



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:07 AM GMT

PDB ID : 2JJM
Title : CRYSTAL STRUCTURE OF A FAMILY GT4 GLYCOSYLTRANSFERASE
FROM BACILLUS ANTHRACIS ORF BA1558.
Authors : Ruane, K.M.; Davies, G.J.; Martinez-Fleites, C.
Deposited on : 2008-04-15
Resolution : 3.10 Å(reported)

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

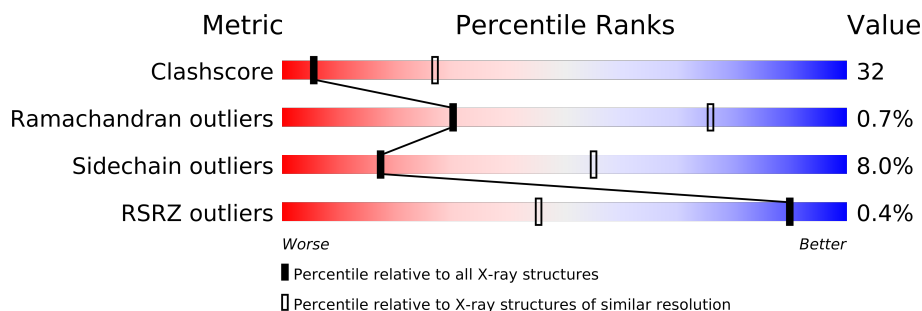
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.10 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 79885 | 1078 (3.16-3.04) |
| Ramachandran outliers | 78287 | 1044 (3.16-3.04) |
| Sidechain outliers | 78261 | 1044 (3.16-3.04) |
| RSRZ outliers | 66119 | 1008 (3.18-3.02) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 394 | |
| 1 | B | 394 | |
| 1 | C | 394 | |
| 1 | D | 394 | |
| 1 | E | 394 | |
| 1 | F | 394 | |
| 1 | G | 394 | |
| 1 | H | 394 | |
| 1 | I | 394 | |
| 1 | J | 394 | |
| 1 | K | 394 | |
| 1 | L | 394 | |

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 33924 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN.

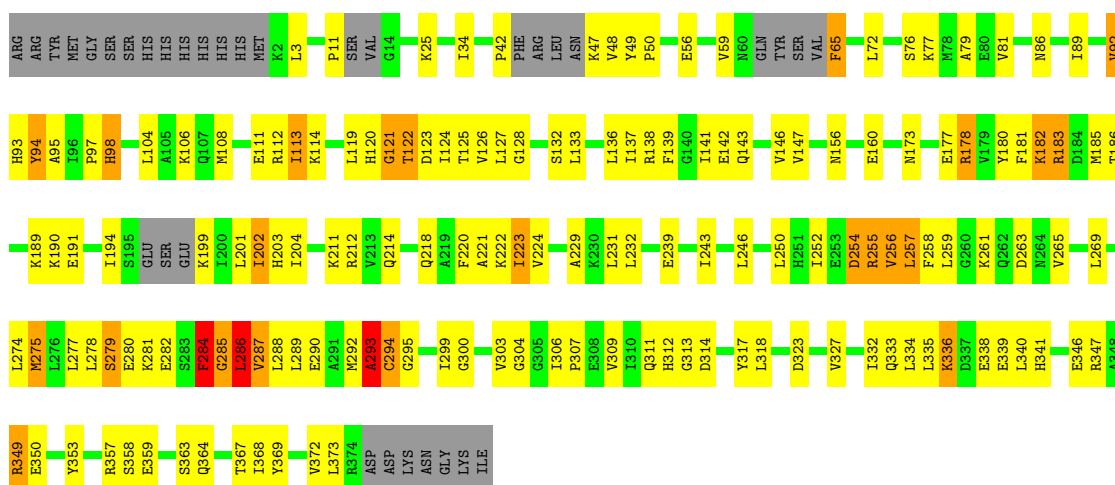
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 360 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 2827 | 1806 | 477 | 531 | 13 | | | |
| 1 | B | 360 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 2827 | 1806 | 477 | 531 | 13 | | | |
| 1 | C | 360 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 2827 | 1806 | 477 | 531 | 13 | | | |
| 1 | D | 360 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 2827 | 1806 | 477 | 531 | 13 | | | |
| 1 | E | 360 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 2827 | 1806 | 477 | 531 | 13 | | | |
| 1 | F | 360 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 2827 | 1806 | 477 | 531 | 13 | | | |
| 1 | G | 360 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 2827 | 1806 | 477 | 531 | 13 | | | |
| 1 | H | 360 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 2827 | 1806 | 477 | 531 | 13 | | | |
| 1 | I | 360 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 2827 | 1806 | 477 | 531 | 13 | | | |
| 1 | J | 360 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 2827 | 1806 | 477 | 531 | 13 | | | |
| 1 | K | 360 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 2827 | 1806 | 477 | 531 | 13 | | | |
| 1 | L | 360 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 2827 | 1806 | 477 | 531 | 13 | | | |

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.

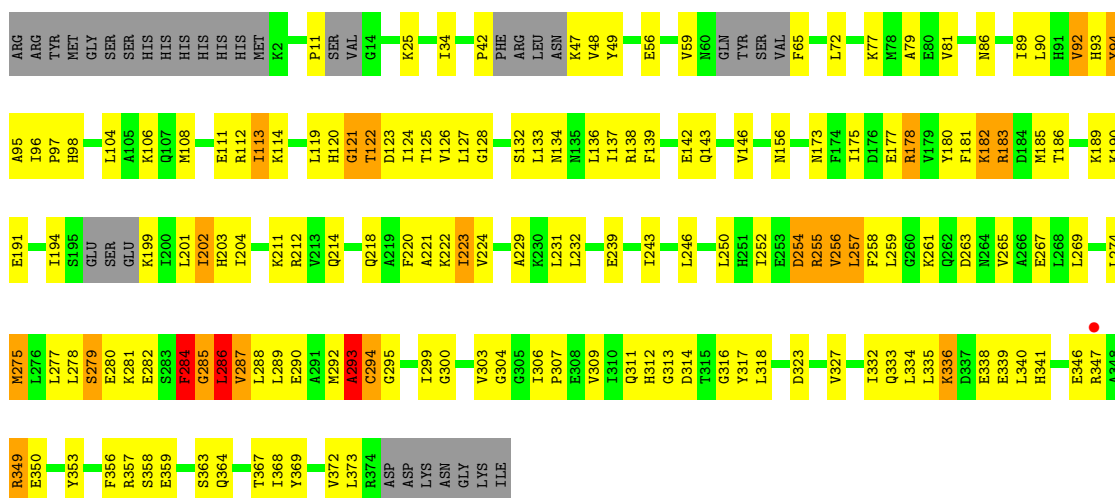
• Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

Chain A:



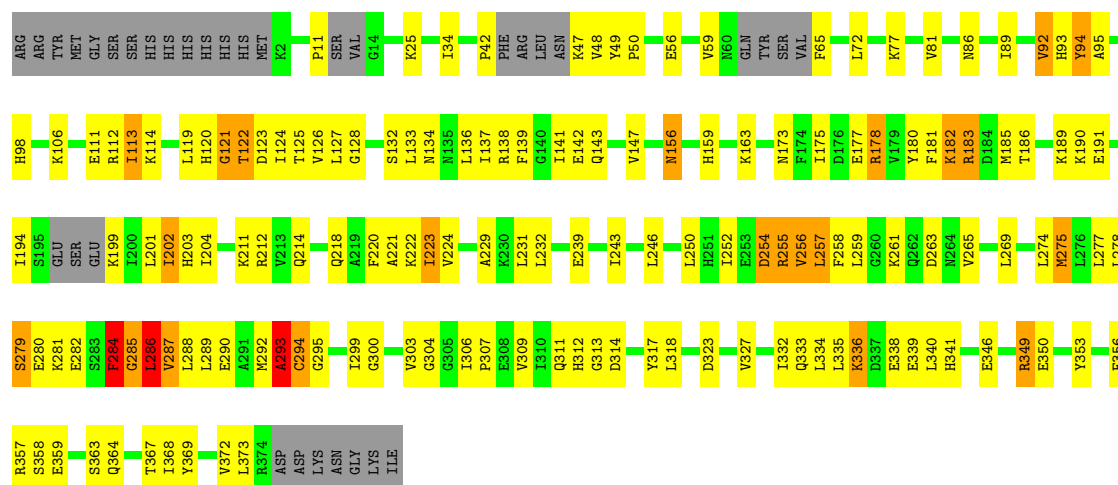
• Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

Chain B:



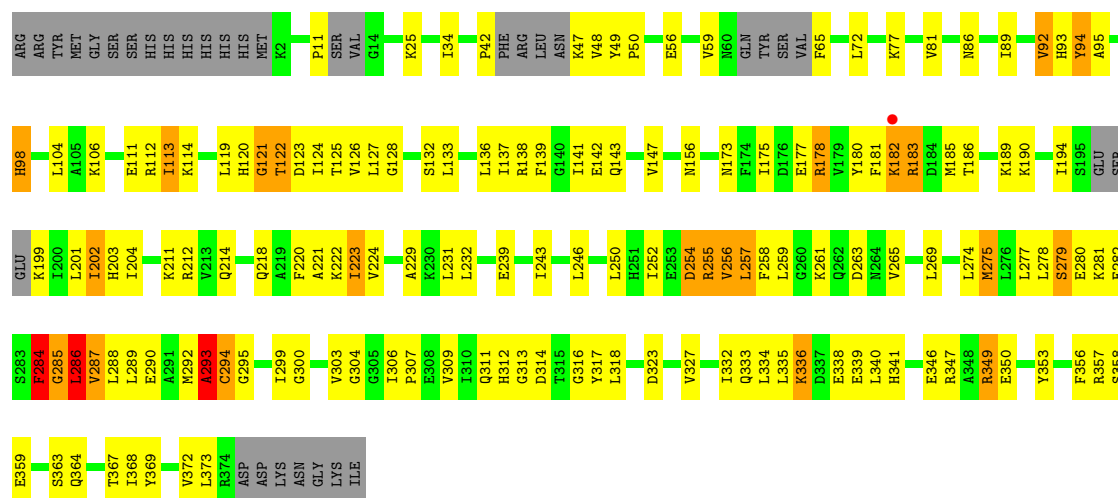
• Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

Chain C:



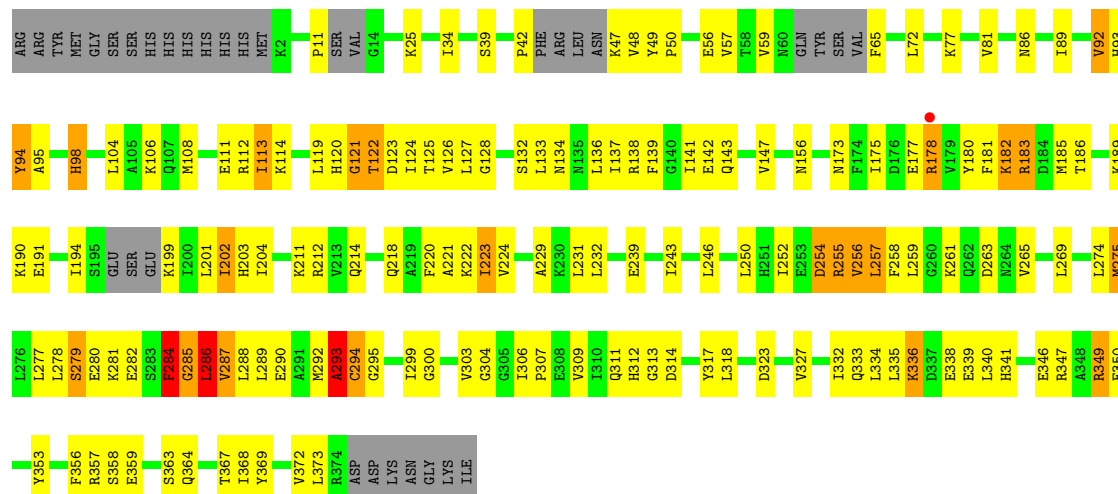
• Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

Chain D:



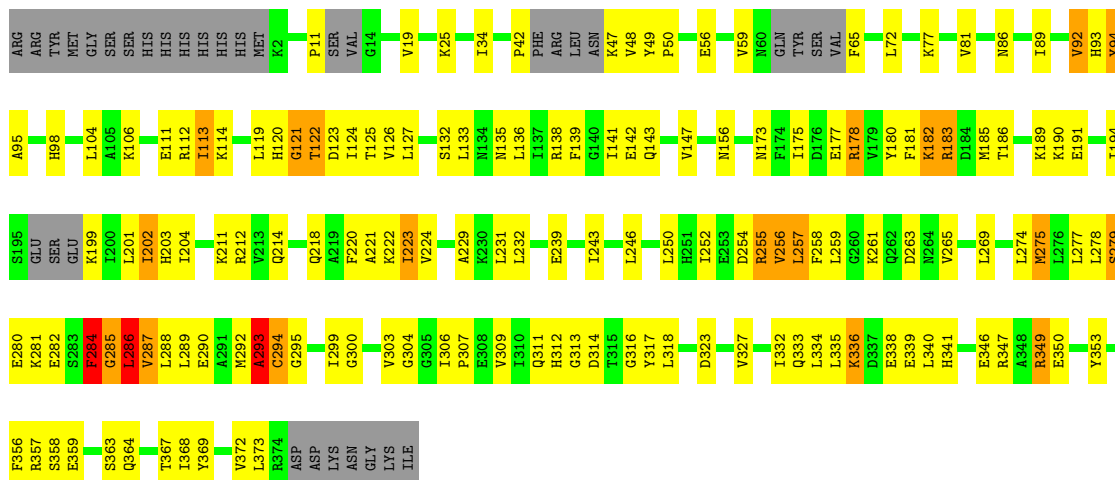
• Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

Chain E:



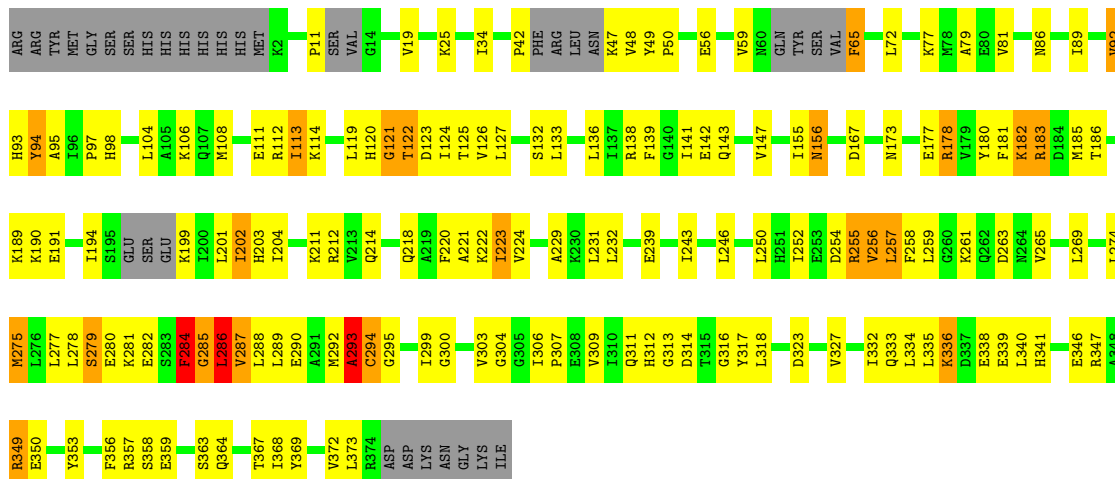
● Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

Chain F:



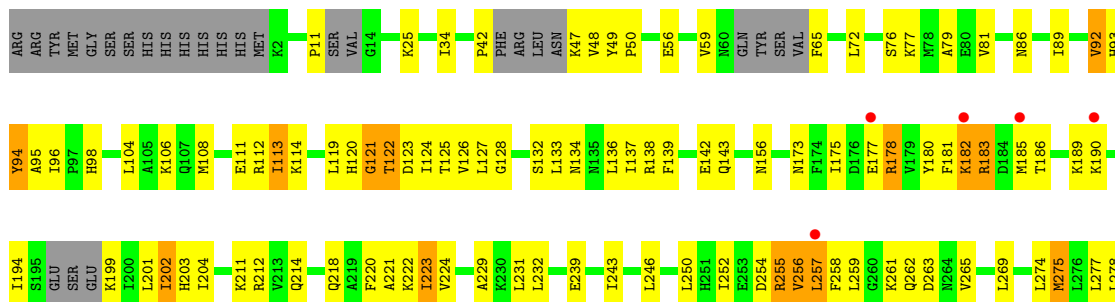
● Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

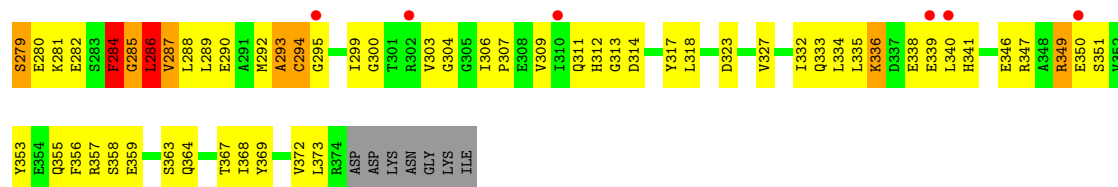
Chain G:



● Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

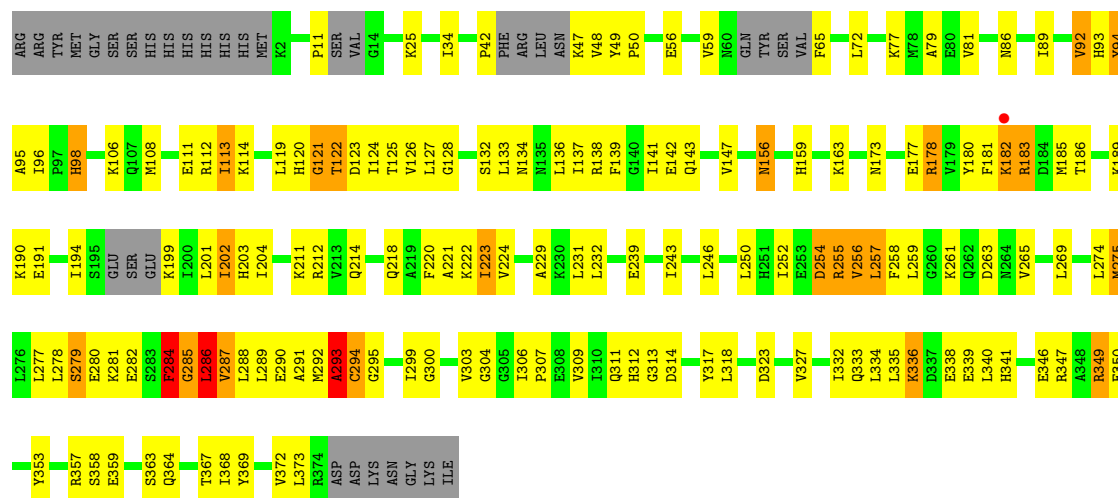
Chain H:





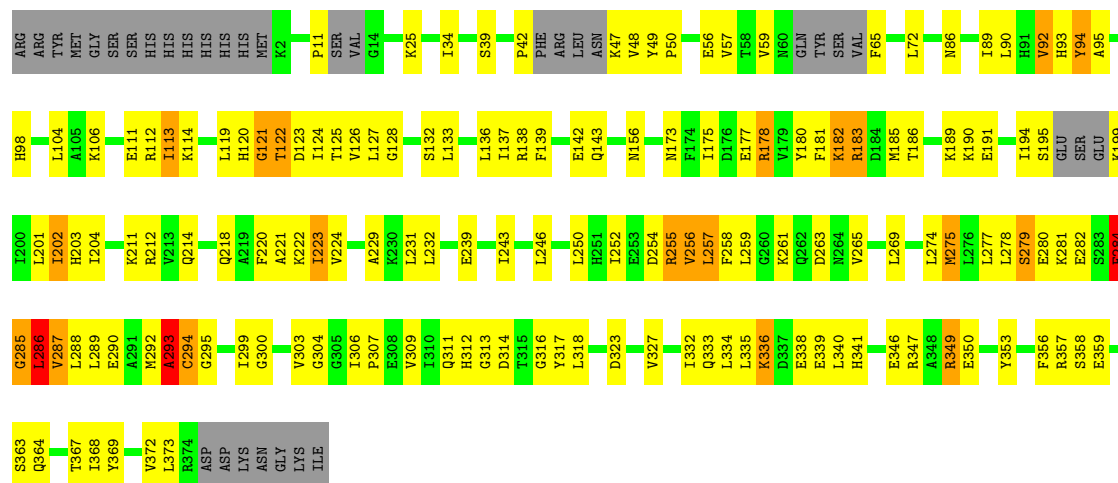
• Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

Chain I:



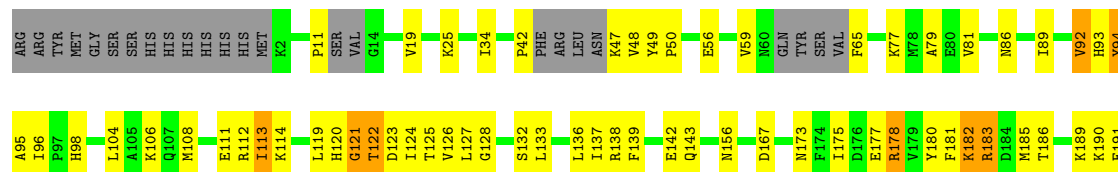
• Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

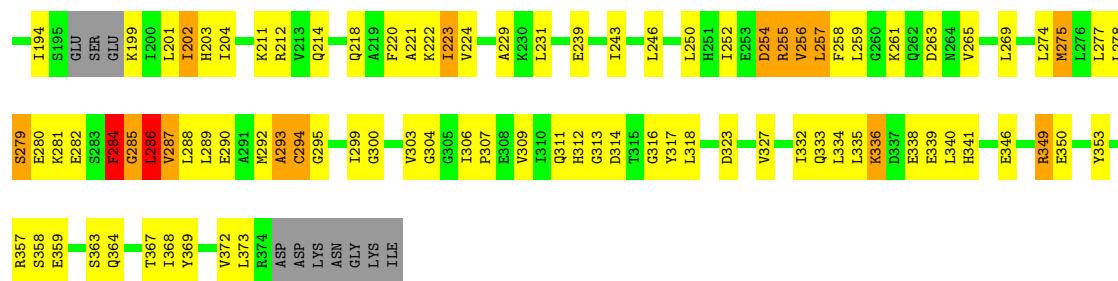
Chain J:



• Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

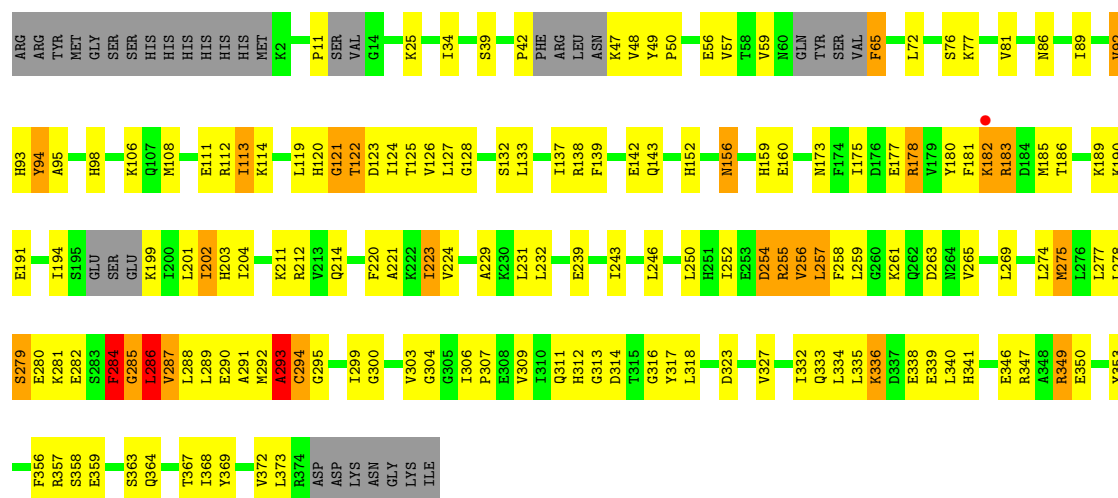
Chain K:





• Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

Chain L:



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 134.60Å 204.67Å 135.33Å 90.00° 115.49° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 3.10 78.27 – 2.70 | Depositor EDS |
| % Data completeness (in resolution range) | 98.3 (20.00-3.10) 89.5 (78.27-2.70) | Depositor EDS |
| R_{merge} | 0.11 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.39 (at 2.69Å) | Xtriage |
| Refinement program | CNS 1.2 | Depositor |
| R, R_{free} | 0.254 , 0.262 0.266 , (Not available) | Depositor DCC |
| R_{free} test set | No test flags present. | DCC |
| Wilson B-factor (Å ²) | 88.0 | Xtriage |
| Anisotropy | 0.099 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.35 , 59.6 | EDS |
| Estimated twinning fraction | 0.022 for l,-k,h | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Outliers | 0 of 161831 reflections | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 33924 | wwPDB-VP |
| Average B, all atoms (Å ²) | 91.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.86 | 8/2873 (0.3%) | 0.89 | 10/3884 (0.3%) |
| 1 | B | 0.86 | 7/2873 (0.2%) | 0.90 | 10/3884 (0.3%) |
| 1 | C | 0.87 | 8/2873 (0.3%) | 0.89 | 10/3884 (0.3%) |
| 1 | D | 0.86 | 8/2873 (0.3%) | 0.89 | 10/3884 (0.3%) |
| 1 | E | 0.87 | 8/2873 (0.3%) | 0.89 | 10/3884 (0.3%) |
| 1 | F | 0.86 | 8/2873 (0.3%) | 0.89 | 9/3884 (0.2%) |
| 1 | G | 0.87 | 8/2873 (0.3%) | 0.90 | 9/3884 (0.2%) |
| 1 | H | 0.86 | 6/2873 (0.2%) | 0.90 | 9/3884 (0.2%) |
| 1 | I | 0.87 | 8/2873 (0.3%) | 0.90 | 10/3884 (0.3%) |
| 1 | J | 0.89 | 8/2873 (0.3%) | 0.89 | 8/3884 (0.2%) |
| 1 | K | 0.87 | 7/2873 (0.2%) | 0.89 | 10/3884 (0.3%) |
| 1 | L | 0.87 | 7/2873 (0.2%) | 0.89 | 10/3884 (0.3%) |
| All | All | 0.87 | 91/34476 (0.3%) | 0.89 | 115/46608 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 2 |
| 1 | B | 0 | 2 |
| 1 | C | 0 | 2 |
| 1 | D | 0 | 2 |
| 1 | E | 0 | 2 |
| 1 | F | 0 | 2 |
| 1 | G | 0 | 2 |
| 1 | H | 0 | 2 |
| 1 | I | 0 | 3 |
| 1 | J | 0 | 2 |
| 1 | K | 0 | 2 |
| 1 | L | 0 | 2 |
| All | All | 0 | 25 |

All (91) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | J | 287 | VAL | CA-CB | -7.51 | 1.39 | 1.54 |
| 1 | F | 287 | VAL | CA-CB | -7.43 | 1.39 | 1.54 |
| 1 | D | 287 | VAL | CA-CB | -7.41 | 1.39 | 1.54 |
| 1 | I | 287 | VAL | CA-CB | -7.41 | 1.39 | 1.54 |
| 1 | G | 287 | VAL | CA-CB | -7.39 | 1.39 | 1.54 |
| 1 | A | 287 | VAL | CA-CB | -7.34 | 1.39 | 1.54 |
| 1 | B | 287 | VAL | CA-CB | -7.32 | 1.39 | 1.54 |
| 1 | E | 287 | VAL | CA-CB | -7.32 | 1.39 | 1.54 |
| 1 | L | 287 | VAL | CA-CB | -7.30 | 1.39 | 1.54 |
| 1 | C | 287 | VAL | CA-CB | -7.30 | 1.39 | 1.54 |
| 1 | K | 287 | VAL | CA-CB | -7.26 | 1.39 | 1.54 |
| 1 | H | 287 | VAL | CA-CB | -7.17 | 1.39 | 1.54 |
| 1 | F | 92 | VAL | CA-CB | -7.15 | 1.39 | 1.54 |
| 1 | K | 92 | VAL | CA-CB | -7.12 | 1.39 | 1.54 |
| 1 | G | 92 | VAL | CA-CB | -7.09 | 1.39 | 1.54 |
| 1 | L | 92 | VAL | CA-CB | -7.06 | 1.40 | 1.54 |
| 1 | A | 92 | VAL | CA-CB | -7.01 | 1.40 | 1.54 |
| 1 | B | 92 | VAL | CA-CB | -7.01 | 1.40 | 1.54 |
| 1 | G | 256 | VAL | CA-CB | -7.00 | 1.40 | 1.54 |
| 1 | E | 256 | VAL | CA-CB | -6.97 | 1.40 | 1.54 |
| 1 | H | 256 | VAL | CA-CB | -6.96 | 1.40 | 1.54 |
| 1 | L | 256 | VAL | CA-CB | -6.95 | 1.40 | 1.54 |
| 1 | E | 92 | VAL | CA-CB | -6.94 | 1.40 | 1.54 |
| 1 | A | 256 | VAL | CA-CB | -6.92 | 1.40 | 1.54 |
| 1 | D | 92 | VAL | CA-CB | -6.91 | 1.40 | 1.54 |
| 1 | B | 256 | VAL | CA-CB | -6.90 | 1.40 | 1.54 |
| 1 | I | 92 | VAL | CA-CB | -6.89 | 1.40 | 1.54 |
| 1 | D | 256 | VAL | CA-CB | -6.89 | 1.40 | 1.54 |
| 1 | H | 92 | VAL | CA-CB | -6.89 | 1.40 | 1.54 |
| 1 | J | 256 | VAL | CA-CB | -6.87 | 1.40 | 1.54 |
| 1 | C | 256 | VAL | CA-CB | -6.86 | 1.40 | 1.54 |
| 1 | C | 92 | VAL | CA-CB | -6.84 | 1.40 | 1.54 |
| 1 | F | 256 | VAL | CA-CB | -6.83 | 1.40 | 1.54 |
| 1 | K | 256 | VAL | CA-CB | -6.80 | 1.40 | 1.54 |
| 1 | I | 256 | VAL | CA-CB | -6.79 | 1.40 | 1.54 |
| 1 | J | 92 | VAL | CA-CB | -6.62 | 1.40 | 1.54 |
| 1 | K | 92 | VAL | CB-CG2 | -6.36 | 1.39 | 1.52 |
| 1 | F | 92 | VAL | CB-CG2 | -6.36 | 1.39 | 1.52 |
| 1 | L | 92 | VAL | CB-CG2 | -6.28 | 1.39 | 1.52 |
| 1 | G | 92 | VAL | CB-CG2 | -6.28 | 1.39 | 1.52 |
| 1 | B | 92 | VAL | CB-CG2 | -6.25 | 1.39 | 1.52 |
| 1 | C | 92 | VAL | CB-CG2 | -6.21 | 1.39 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | I | 92 | VAL | CB-CG2 | -6.20 | 1.39 | 1.52 |
| 1 | D | 92 | VAL | CB-CG2 | -6.17 | 1.39 | 1.52 |
| 1 | A | 92 | VAL | CB-CG2 | -6.16 | 1.40 | 1.52 |
| 1 | F | 294 | CYS | CB-SG | -6.13 | 1.71 | 1.82 |
| 1 | J | 294 | CYS | CB-SG | -6.12 | 1.71 | 1.82 |
| 1 | J | 92 | VAL | CB-CG2 | -6.12 | 1.40 | 1.52 |
| 1 | K | 294 | CYS | CB-SG | -6.11 | 1.71 | 1.82 |
| 1 | G | 294 | CYS | CB-SG | -6.11 | 1.71 | 1.82 |
| 1 | E | 92 | VAL | CB-CG2 | -6.10 | 1.40 | 1.52 |
| 1 | A | 294 | CYS | CB-SG | -6.10 | 1.71 | 1.82 |
| 1 | E | 294 | CYS | CB-SG | -6.07 | 1.72 | 1.82 |
| 1 | H | 92 | VAL | CB-CG2 | -6.06 | 1.40 | 1.52 |
| 1 | H | 294 | CYS | CB-SG | -5.96 | 1.72 | 1.81 |
| 1 | L | 294 | CYS | CB-SG | -5.92 | 1.72 | 1.81 |
| 1 | B | 294 | CYS | CB-SG | -5.84 | 1.72 | 1.81 |
| 1 | D | 294 | CYS | CB-SG | -5.79 | 1.72 | 1.81 |
| 1 | K | 95 | ALA | CA-CB | -5.74 | 1.40 | 1.52 |
| 1 | C | 294 | CYS | CB-SG | -5.71 | 1.72 | 1.81 |
| 1 | I | 294 | CYS | CB-SG | -5.62 | 1.72 | 1.81 |
| 1 | L | 95 | ALA | CA-CB | -5.52 | 1.40 | 1.52 |
| 1 | J | 95 | ALA | CA-CB | -5.45 | 1.41 | 1.52 |
| 1 | G | 95 | ALA | CA-CB | -5.44 | 1.41 | 1.52 |
| 1 | K | 92 | VAL | CB-CG1 | -5.44 | 1.41 | 1.52 |
| 1 | J | 92 | VAL | CB-CG1 | -5.37 | 1.41 | 1.52 |
| 1 | I | 95 | ALA | CA-CB | -5.37 | 1.41 | 1.52 |
| 1 | B | 95 | ALA | CA-CB | -5.35 | 1.41 | 1.52 |
| 1 | C | 92 | VAL | CB-CG1 | -5.32 | 1.41 | 1.52 |
| 1 | E | 95 | ALA | CA-CB | -5.30 | 1.41 | 1.52 |
| 1 | C | 95 | ALA | CA-CB | -5.29 | 1.41 | 1.52 |
| 1 | D | 95 | ALA | CA-CB | -5.28 | 1.41 | 1.52 |
| 1 | E | 92 | VAL | CB-CG1 | -5.23 | 1.41 | 1.52 |
| 1 | H | 95 | ALA | CA-CB | -5.21 | 1.41 | 1.52 |
| 1 | F | 95 | ALA | CA-CB | -5.21 | 1.41 | 1.52 |
| 1 | L | 293 | ALA | CA-CB | -5.21 | 1.41 | 1.52 |
| 1 | F | 92 | VAL | CB-CG1 | -5.20 | 1.42 | 1.52 |
| 1 | A | 95 | ALA | CA-CB | -5.15 | 1.41 | 1.52 |
| 1 | I | 92 | VAL | CB-CG1 | -5.15 | 1.42 | 1.52 |
| 1 | J | 293 | ALA | CA-CB | -5.14 | 1.41 | 1.52 |
| 1 | G | 293 | ALA | CA-CB | -5.12 | 1.41 | 1.52 |
| 1 | D | 293 | ALA | CA-CB | -5.12 | 1.41 | 1.52 |
| 1 | C | 293 | ALA | CA-CB | -5.10 | 1.41 | 1.52 |
| 1 | A | 293 | ALA | CA-CB | -5.07 | 1.41 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | G | 92 | VAL | CB-CG1 | -5.07 | 1.42 | 1.52 |
| 1 | F | 293 | ALA | CA-CB | -5.06 | 1.41 | 1.52 |
| 1 | A | 92 | VAL | CB-CG1 | -5.05 | 1.42 | 1.52 |
| 1 | E | 293 | ALA | CA-CB | -5.04 | 1.41 | 1.52 |
| 1 | I | 293 | ALA | CA-CB | -5.04 | 1.41 | 1.52 |
| 1 | D | 92 | VAL | CB-CG1 | -5.03 | 1.42 | 1.52 |
| 1 | B | 293 | ALA | CA-CB | -5.02 | 1.42 | 1.52 |

All (115) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | L | 121 | GLY | N-CA-C | 9.49 | 136.84 | 113.10 |
| 1 | J | 121 | GLY | N-CA-C | 9.48 | 136.80 | 113.10 |
| 1 | H | 121 | GLY | N-CA-C | 9.46 | 136.74 | 113.10 |
| 1 | B | 121 | GLY | N-CA-C | 9.45 | 136.72 | 113.10 |
| 1 | D | 121 | GLY | N-CA-C | 9.44 | 136.70 | 113.10 |
| 1 | I | 121 | GLY | N-CA-C | 9.44 | 136.69 | 113.10 |
| 1 | K | 121 | GLY | N-CA-C | 9.43 | 136.66 | 113.10 |
| 1 | E | 121 | GLY | N-CA-C | 9.42 | 136.66 | 113.10 |
| 1 | A | 121 | GLY | N-CA-C | 9.41 | 136.62 | 113.10 |
| 1 | C | 121 | GLY | N-CA-C | 9.39 | 136.59 | 113.10 |
| 1 | G | 121 | GLY | N-CA-C | 9.39 | 136.58 | 113.10 |
| 1 | F | 121 | GLY | N-CA-C | 9.35 | 136.48 | 113.10 |
| 1 | G | 284 | PHE | N-CA-C | 9.18 | 135.78 | 111.00 |
| 1 | E | 284 | PHE | N-CA-C | 9.14 | 135.69 | 111.00 |
| 1 | E | 285 | GLY | N-CA-C | -9.13 | 90.27 | 113.10 |
| 1 | K | 284 | PHE | N-CA-C | 9.10 | 135.57 | 111.00 |
| 1 | K | 285 | GLY | N-CA-C | -9.10 | 90.35 | 113.10 |
| 1 | C | 285 | GLY | N-CA-C | -9.05 | 90.47 | 113.10 |
| 1 | F | 284 | PHE | N-CA-C | 9.05 | 135.44 | 111.00 |
| 1 | B | 284 | PHE | N-CA-C | 9.02 | 135.36 | 111.00 |
| 1 | J | 284 | PHE | N-CA-C | 9.02 | 135.35 | 111.00 |
| 1 | C | 284 | PHE | N-CA-C | 9.01 | 135.33 | 111.00 |
| 1 | F | 285 | GLY | N-CA-C | -9.01 | 90.58 | 113.10 |
| 1 | A | 285 | GLY | N-CA-C | -9.00 | 90.59 | 113.10 |
| 1 | I | 284 | PHE | N-CA-C | 9.00 | 135.30 | 111.00 |
| 1 | L | 284 | PHE | N-CA-C | 9.00 | 135.30 | 111.00 |
| 1 | D | 284 | PHE | N-CA-C | 8.99 | 135.28 | 111.00 |
| 1 | I | 285 | GLY | N-CA-C | -8.96 | 90.71 | 113.10 |
| 1 | D | 285 | GLY | N-CA-C | -8.95 | 90.73 | 113.10 |
| 1 | G | 285 | GLY | N-CA-C | -8.95 | 90.72 | 113.10 |
| 1 | A | 284 | PHE | N-CA-C | 8.93 | 135.11 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | L | 285 | GLY | N-CA-C | -8.92 | 90.81 | 113.10 |
| 1 | H | 284 | PHE | N-CA-C | 8.89 | 135.01 | 111.00 |
| 1 | B | 285 | GLY | N-CA-C | -8.89 | 90.87 | 113.10 |
| 1 | H | 285 | GLY | N-CA-C | -8.89 | 90.87 | 113.10 |
| 1 | J | 285 | GLY | N-CA-C | -8.45 | 91.97 | 113.10 |
| 1 | H | 286 | LEU | C-N-CA | -7.71 | 102.41 | 121.70 |
| 1 | B | 286 | LEU | C-N-CA | -7.69 | 102.47 | 121.70 |
| 1 | D | 286 | LEU | C-N-CA | -7.64 | 102.59 | 121.70 |
| 1 | J | 286 | LEU | C-N-CA | -7.63 | 102.61 | 121.70 |
| 1 | E | 286 | LEU | C-N-CA | -7.63 | 102.64 | 121.70 |
| 1 | I | 286 | LEU | C-N-CA | -7.61 | 102.67 | 121.70 |
| 1 | G | 286 | LEU | C-N-CA | -7.61 | 102.68 | 121.70 |
| 1 | A | 286 | LEU | C-N-CA | -7.60 | 102.69 | 121.70 |
| 1 | L | 286 | LEU | C-N-CA | -7.60 | 102.69 | 121.70 |
| 1 | K | 286 | LEU | C-N-CA | -7.60 | 102.69 | 121.70 |
| 1 | C | 286 | LEU | C-N-CA | -7.58 | 102.76 | 121.70 |
| 1 | F | 286 | LEU | C-N-CA | -7.55 | 102.82 | 121.70 |
| 1 | H | 257 | LEU | CA-CB-CG | -7.13 | 98.90 | 115.30 |
| 1 | B | 257 | LEU | CA-CB-CG | -7.13 | 98.91 | 115.30 |
| 1 | F | 257 | LEU | CA-CB-CG | -7.10 | 98.96 | 115.30 |
| 1 | C | 257 | LEU | CA-CB-CG | -7.08 | 99.00 | 115.30 |
| 1 | I | 257 | LEU | CA-CB-CG | -7.07 | 99.04 | 115.30 |
| 1 | E | 257 | LEU | CA-CB-CG | -7.05 | 99.09 | 115.30 |
| 1 | D | 257 | LEU | CA-CB-CG | -7.04 | 99.11 | 115.30 |
| 1 | A | 257 | LEU | CA-CB-CG | -7.02 | 99.15 | 115.30 |
| 1 | G | 257 | LEU | CA-CB-CG | -7.01 | 99.17 | 115.30 |
| 1 | J | 257 | LEU | CA-CB-CG | -7.01 | 99.17 | 115.30 |
| 1 | L | 257 | LEU | CA-CB-CG | -7.00 | 99.19 | 115.30 |
| 1 | K | 257 | LEU | CA-CB-CG | -6.98 | 99.25 | 115.30 |
| 1 | L | 93 | HIS | N-CA-C | 6.05 | 127.33 | 111.00 |
| 1 | I | 93 | HIS | N-CA-C | 6.03 | 127.29 | 111.00 |
| 1 | F | 93 | HIS | N-CA-C | 6.03 | 127.28 | 111.00 |
| 1 | G | 93 | HIS | N-CA-C | 6.03 | 127.28 | 111.00 |
| 1 | D | 93 | HIS | N-CA-C | 6.03 | 127.27 | 111.00 |
| 1 | E | 93 | HIS | N-CA-C | 6.02 | 127.25 | 111.00 |
| 1 | B | 93 | HIS | N-CA-C | 6.00 | 127.21 | 111.00 |
| 1 | H | 93 | HIS | N-CA-C | 6.00 | 127.20 | 111.00 |
| 1 | A | 93 | HIS | N-CA-C | 6.00 | 127.19 | 111.00 |
| 1 | C | 93 | HIS | N-CA-C | 5.94 | 127.03 | 111.00 |
| 1 | K | 93 | HIS | N-CA-C | 5.92 | 126.97 | 111.00 |
| 1 | J | 93 | HIS | N-CA-C | 5.81 | 126.69 | 111.00 |
| 1 | C | 284 | PHE | CB-CA-C | -5.54 | 99.32 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | L | 93 | HIS | C-N-CA | -5.53 | 107.87 | 121.70 |
| 1 | A | 93 | HIS | C-N-CA | -5.51 | 107.92 | 121.70 |
| 1 | G | 93 | HIS | C-N-CA | -5.51 | 107.92 | 121.70 |
| 1 | H | 93 | HIS | C-N-CA | -5.46 | 108.05 | 121.70 |
| 1 | D | 93 | HIS | C-N-CA | -5.43 | 108.13 | 121.70 |
| 1 | I | 93 | HIS | C-N-CA | -5.43 | 108.13 | 121.70 |
| 1 | K | 93 | HIS | C-N-CA | -5.42 | 108.14 | 121.70 |
| 1 | B | 93 | HIS | C-N-CA | -5.42 | 108.14 | 121.70 |
| 1 | C | 93 | HIS | C-N-CA | -5.41 | 108.17 | 121.70 |
| 1 | L | 284 | PHE | CB-CA-C | -5.41 | 99.58 | 110.40 |
| 1 | F | 93 | HIS | C-N-CA | -5.41 | 108.19 | 121.70 |
| 1 | E | 93 | HIS | C-N-CA | -5.40 | 108.19 | 121.70 |
| 1 | J | 93 | HIS | C-N-CA | -5.38 | 108.24 | 121.70 |
| 1 | I | 284 | PHE | CB-CA-C | -5.37 | 99.67 | 110.40 |
| 1 | K | 284 | PHE | CB-CA-C | -5.30 | 99.79 | 110.40 |
| 1 | B | 284 | PHE | CB-CA-C | -5.29 | 99.83 | 110.40 |
| 1 | J | 94 | TYR | N-CA-C | -5.25 | 96.84 | 111.00 |
| 1 | A | 284 | PHE | CB-CA-C | -5.24 | 99.92 | 110.40 |
| 1 | G | 284 | PHE | CB-CA-C | -5.24 | 99.93 | 110.40 |
| 1 | K | 254 | ASP | CB-CG-OD1 | -5.23 | 113.59 | 118.30 |
| 1 | B | 94 | TYR | N-CA-C | -5.23 | 96.88 | 111.00 |
| 1 | G | 94 | TYR | N-CA-C | -5.21 | 96.93 | 111.00 |
| 1 | C | 254 | ASP | CB-CG-OD1 | -5.20 | 113.62 | 118.30 |
| 1 | K | 94 | TYR | N-CA-C | -5.19 | 97.00 | 111.00 |
| 1 | H | 284 | PHE | CB-CA-C | -5.18 | 100.03 | 110.40 |
| 1 | E | 284 | PHE | CB-CA-C | -5.17 | 100.06 | 110.40 |
| 1 | A | 94 | TYR | N-CA-C | -5.17 | 97.04 | 111.00 |
| 1 | D | 284 | PHE | CB-CA-C | -5.17 | 100.06 | 110.40 |
| 1 | D | 94 | TYR | N-CA-C | -5.15 | 97.10 | 111.00 |
| 1 | F | 284 | PHE | CB-CA-C | -5.14 | 100.12 | 110.40 |
| 1 | H | 94 | TYR | N-CA-C | -5.14 | 97.11 | 111.00 |
| 1 | C | 94 | TYR | N-CA-C | -5.13 | 97.14 | 111.00 |
| 1 | E | 94 | TYR | N-CA-C | -5.13 | 97.16 | 111.00 |
| 1 | F | 94 | TYR | N-CA-C | -5.12 | 97.19 | 111.00 |
| 1 | I | 94 | TYR | N-CA-C | -5.12 | 97.19 | 111.00 |
| 1 | L | 94 | TYR | N-CA-C | -5.10 | 97.22 | 111.00 |
| 1 | D | 254 | ASP | CB-CG-OD1 | -5.07 | 113.73 | 118.30 |
| 1 | B | 254 | ASP | CB-CG-OD1 | -5.06 | 113.74 | 118.30 |
| 1 | E | 254 | ASP | CB-CG-OD1 | -5.02 | 113.78 | 118.30 |
| 1 | L | 254 | ASP | CB-CG-OD1 | -5.01 | 113.79 | 118.30 |
| 1 | A | 254 | ASP | CB-CG-OD1 | -5.00 | 113.80 | 118.30 |
| 1 | I | 254 | ASP | CB-CG-OD1 | -5.00 | 113.80 | 118.30 |

There are no chirality outliers.

All (25) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 1 | A | 284 | PHE | Mainchain,Peptide |
| 1 | B | 284 | PHE | Mainchain,Peptide |
| 1 | C | 284 | PHE | Mainchain,Peptide |
| 1 | D | 284 | PHE | Mainchain,Peptide |
| 1 | E | 284 | PHE | Mainchain,Peptide |
| 1 | F | 284 | PHE | Mainchain,Peptide |
| 1 | G | 284 | PHE | Mainchain,Peptide |
| 1 | H | 284 | PHE | Mainchain,Peptide |
| 1 | I | 284 | PHE | Mainchain,Peptide |
| 1 | I | 96 | ILE | Mainchain |
| 1 | J | 284 | PHE | Mainchain,Peptide |
| 1 | K | 284 | PHE | Mainchain,Peptide |
| 1 | L | 284 | PHE | Mainchain,Peptide |

5.2 Close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 2827 | 0 | 2856 | 182 | 1 |
| 1 | B | 2827 | 0 | 2856 | 191 | 0 |
| 1 | C | 2827 | 0 | 2856 | 188 | 0 |
| 1 | D | 2827 | 0 | 2856 | 182 | 0 |
| 1 | E | 2827 | 0 | 2856 | 182 | 0 |
| 1 | F | 2827 | 0 | 2856 | 185 | 0 |
| 1 | G | 2827 | 0 | 2856 | 195 | 0 |
| 1 | H | 2827 | 0 | 2856 | 187 | 0 |
| 1 | I | 2827 | 0 | 2856 | 189 | 0 |
| 1 | J | 2827 | 0 | 2856 | 183 | 0 |
| 1 | K | 2827 | 0 | 2856 | 186 | 1 |
| 1 | L | 2827 | 0 | 2856 | 190 | 0 |
| All | All | 33924 | 0 | 34272 | 2180 | 1 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 32.

All (2180) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:G:167:ASP:OD2 | 1:L:160:GLU:HA | 1.15 | 1.27 |
| 1:A:286:LEU:HD12 | 1:A:286:LEU:N | 1.55 | 1.17 |
| 1:B:286:LEU:CD1 | 1:B:286:LEU:H | 1.54 | 1.16 |
| 1:K:280:GLU:O | 1:K:281:LYS:HG2 | 1.46 | 1.16 |
| 1:G:280:GLU:O | 1:G:281:LYS:HG2 | 1.47 | 1.15 |
| 1:A:280:GLU:O | 1:A:281:LYS:HG2 | 1.46 | 1.15 |
| 1:E:280:GLU:O | 1:E:281:LYS:HG2 | 1.46 | 1.15 |
| 1:I:280:GLU:O | 1:I:281:LYS:HG2 | 1.47 | 1.15 |
| 1:C:280:GLU:O | 1:C:281:LYS:HG2 | 1.47 | 1.14 |
| 1:L:280:GLU:O | 1:L:281:LYS:HG2 | 1.47 | 1.14 |
| 1:I:286:LEU:N | 1:I:286:LEU:HD12 | 1.54 | 1.14 |
| 1:B:280:GLU:O | 1:B:281:LYS:HG2 | 1.46 | 1.13 |
| 1:F:286:LEU:CD1 | 1:F:286:LEU:H | 1.54 | 1.13 |
| 1:D:286:LEU:N | 1:D:286:LEU:HD12 | 1.55 | 1.13 |
| 1:H:280:GLU:O | 1:H:281:LYS:HG2 | 1.46 | 1.12 |
| 1:J:280:GLU:O | 1:J:281:LYS:HG2 | 1.47 | 1.12 |
| 1:F:280:GLU:O | 1:F:281:LYS:HG2 | 1.47 | 1.10 |
| 1:C:286:LEU:HD12 | 1:C:286:LEU:N | 1.55 | 1.10 |
| 1:D:280:GLU:O | 1:D:281:LYS:HG2 | 1.47 | 1.10 |
| 1:C:286:LEU:CD1 | 1:C:286:LEU:H | 1.54 | 1.09 |
| 1:I:286:LEU:CD1 | 1:I:286:LEU:H | 1.53 | 1.09 |
| 1:K:286:LEU:HD12 | 1:K:286:LEU:N | 1.54 | 1.08 |
| 1:J:286:LEU:N | 1:J:286:LEU:HD12 | 1.56 | 1.08 |
| 1:D:286:LEU:H | 1:D:286:LEU:CD1 | 1.55 | 1.08 |
| 1:E:286:LEU:H | 1:E:286:LEU:CD1 | 1.54 | 1.08 |
| 1:E:286:LEU:N | 1:E:286:LEU:HD12 | 1.55 | 1.08 |
| 1:L:286:LEU:CD1 | 1:L:286:LEU:H | 1.54 | 1.08 |
| 1:J:286:LEU:H | 1:J:286:LEU:CD1 | 1.56 | 1.07 |
| 1:B:286:LEU:HD12 | 1:B:286:LEU:N | 1.55 | 1.07 |
| 1:H:286:LEU:HD12 | 1:H:286:LEU:N | 1.55 | 1.07 |
| 1:H:286:LEU:CD1 | 1:H:286:LEU:H | 1.55 | 1.06 |
| 1:L:286:LEU:HD12 | 1:L:286:LEU:N | 1.55 | 1.06 |
| 1:G:286:LEU:H | 1:G:286:LEU:CD1 | 1.54 | 1.06 |
| 1:A:286:LEU:O | 1:A:287:VAL:C | 1.91 | 1.05 |
| 1:G:286:LEU:N | 1:G:286:LEU:HD12 | 1.55 | 1.05 |
| 1:F:286:LEU:N | 1:F:286:LEU:HD12 | 1.55 | 1.04 |
| 1:K:286:LEU:CD1 | 1:K:286:LEU:H | 1.54 | 1.04 |
| 1:F:256:VAL:C | 1:F:257:LEU:HD12 | 1.78 | 1.04 |
| 1:K:256:VAL:C | 1:K:257:LEU:HD12 | 1.78 | 1.04 |
| 1:L:256:VAL:C | 1:L:257:LEU:HD12 | 1.78 | 1.03 |
| 1:G:256:VAL:C | 1:G:257:LEU:HD12 | 1.78 | 1.03 |
| 1:L:286:LEU:O | 1:L:287:VAL:C | 1.90 | 1.03 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:256:VAL:C | 1:A:257:LEU:HD12 | 1.78 | 1.03 |
| 1:F:286:LEU:O | 1:F:287:VAL:C | 1.90 | 1.03 |
| 1:H:256:VAL:C | 1:H:257:LEU:HD12 | 1.78 | 1.03 |
| 1:C:256:VAL:C | 1:C:257:LEU:HD12 | 1.78 | 1.03 |
| 1:A:286:LEU:H | 1:A:286:LEU:CD1 | 1.54 | 1.03 |
| 1:I:256:VAL:C | 1:I:257:LEU:HD12 | 1.78 | 1.03 |
| 1:B:256:VAL:C | 1:B:257:LEU:HD12 | 1.78 | 1.03 |
| 1:E:256:VAL:C | 1:E:257:LEU:HD12 | 1.78 | 1.03 |
| 1:G:286:LEU:O | 1:G:287:VAL:C | 1.91 | 1.03 |
| 1:J:256:VAL:C | 1:J:257:LEU:HD12 | 1.78 | 1.02 |
| 1:D:256:VAL:C | 1:D:257:LEU:HD12 | 1.78 | 1.02 |
| 1:K:220:PHE:HA | 1:K:223:ILE:HG22 | 1.42 | 1.02 |
| 1:E:286:LEU:O | 1:E:287:VAL:C | 1.91 | 1.02 |
| 1:I:220:PHE:HA | 1:I:223:ILE:HG22 | 1.42 | 1.01 |
| 1:A:220:PHE:HA | 1:A:223:ILE:HG22 | 1.42 | 1.01 |
| 1:H:220:PHE:HA | 1:H:223:ILE:HG22 | 1.41 | 1.01 |
| 1:L:220:PHE:HA | 1:L:223:ILE:HG22 | 1.42 | 1.01 |
| 1:B:220:PHE:HA | 1:B:223:ILE:HG22 | 1.42 | 1.01 |
| 1:G:167:ASP:OD2 | 1:L:160:GLU:CA | 2.07 | 1.01 |
| 1:C:220:PHE:HA | 1:C:223:ILE:HG22 | 1.41 | 1.01 |
| 1:F:220:PHE:HA | 1:F:223:ILE:HG22 | 1.41 | 1.00 |
| 1:E:220:PHE:HA | 1:E:223:ILE:HG22 | 1.42 | 1.00 |
| 1:B:281:LYS:HA | 1:B:303:VAL:HG11 | 1.44 | 0.99 |
| 1:E:281:LYS:HA | 1:E:303:VAL:HG11 | 1.44 | 0.99 |
| 1:I:281:LYS:HA | 1:I:303:VAL:HG11 | 1.44 | 0.99 |
| 1:C:281:LYS:HA | 1:C:303:VAL:HG11 | 1.44 | 0.99 |
| 1:G:281:LYS:HA | 1:G:303:VAL:HG11 | 1.44 | 0.99 |
| 1:I:286:LEU:O | 1:I:287:VAL:C | 1.91 | 0.99 |
| 1:H:281:LYS:HA | 1:H:303:VAL:HG11 | 1.44 | 0.99 |
| 1:D:220:PHE:HA | 1:D:223:ILE:HG22 | 1.41 | 0.99 |
| 1:J:281:LYS:HA | 1:J:303:VAL:HG11 | 1.44 | 0.98 |
| 1:G:220:PHE:HA | 1:G:223:ILE:HG22 | 1.42 | 0.98 |
| 1:E:284:PHE:HB3 | 1:E:285:GLY:HA2 | 1.46 | 0.98 |
| 1:F:281:LYS:HA | 1:F:303:VAL:HG11 | 1.44 | 0.98 |
| 1:J:286:LEU:O | 1:J:287:VAL:C | 1.90 | 0.98 |
| 1:H:257:LEU:HD12 | 1:H:257:LEU:N | 1.79 | 0.98 |
| 1:A:257:LEU:N | 1:A:257:LEU:HD12 | 1.79 | 0.98 |
| 1:J:220:PHE:HA | 1:J:223:ILE:HG22 | 1.42 | 0.98 |
| 1:H:284:PHE:HB3 | 1:H:285:GLY:HA2 | 1.46 | 0.97 |
| 1:H:286:LEU:O | 1:H:287:VAL:C | 1.91 | 0.97 |
| 1:D:281:LYS:HA | 1:D:303:VAL:HG11 | 1.44 | 0.97 |
| 1:I:284:PHE:HB3 | 1:I:285:GLY:HA2 | 1.46 | 0.97 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:K:257:LEU:HD12 | 1:K:257:LEU:N | 1.79 | 0.97 |
| 1:G:284:PHE:HB3 | 1:G:285:GLY:HA2 | 1.45 | 0.97 |
| 1:L:281:LYS:HA | 1:L:303:VAL:HG11 | 1.44 | 0.97 |
| 1:I:257:LEU:N | 1:I:257:LEU:HD12 | 1.79 | 0.97 |
| 1:B:284:PHE:HB3 | 1:B:285:GLY:HA2 | 1.46 | 0.97 |
| 1:J:257:LEU:HD12 | 1:J:257:LEU:N | 1.78 | 0.97 |
| 1:K:281:LYS:HA | 1:K:303:VAL:HG11 | 1.45 | 0.97 |
| 1:G:257:LEU:HD12 | 1:G:257:LEU:N | 1.79 | 0.97 |
| 1:A:284:PHE:HB3 | 1:A:285:GLY:HA2 | 1.46 | 0.96 |
| 1:C:284:PHE:HB3 | 1:C:285:GLY:HA2 | 1.45 | 0.96 |
| 1:D:286:LEU:O | 1:D:287:VAL:C | 1.91 | 0.96 |
| 1:D:257:LEU:N | 1:D:257:LEU:HD12 | 1.79 | 0.96 |
| 1:C:286:LEU:O | 1:C:287:VAL:C | 1.91 | 0.96 |
| 1:A:281:LYS:HA | 1:A:303:VAL:HG11 | 1.44 | 0.96 |
| 1:J:284:PHE:HB3 | 1:J:285:GLY:HA2 | 1.44 | 0.96 |
| 1:K:284:PHE:HB3 | 1:K:285:GLY:HA2 | 1.47 | 0.96 |
| 1:B:286:LEU:O | 1:B:287:VAL:C | 1.91 | 0.96 |
| 1:F:284:PHE:HB3 | 1:F:285:GLY:HA2 | 1.46 | 0.95 |
| 1:D:284:PHE:HB3 | 1:D:285:GLY:HA2 | 1.46 | 0.95 |
| 1:E:191:GLU:HG2 | 1:H:50:PRO:HG2 | 1.47 | 0.95 |
| 1:F:11:PRO:HG3 | 1:F:42:PRO:HG3 | 1.49 | 0.95 |
| 1:K:286:LEU:O | 1:K:287:VAL:C | 1.90 | 0.95 |
| 1:L:284:PHE:HB3 | 1:L:285:GLY:HA2 | 1.46 | 0.95 |
| 1:C:11:PRO:HG3 | 1:C:42:PRO:HG3 | 1.49 | 0.95 |
| 1:I:50:PRO:HG2 | 1:K:191:GLU:HG2 | 1.48 | 0.94 |
| 1:I:11:PRO:HG3 | 1:I:42:PRO:HG3 | 1.49 | 0.94 |
| 1:B:11:PRO:HG3 | 1:B:42:PRO:HG3 | 1.49 | 0.94 |
| 1:L:11:PRO:HG3 | 1:L:42:PRO:HG3 | 1.48 | 0.94 |
| 1:H:11:PRO:HG3 | 1:H:42:PRO:HG3 | 1.49 | 0.94 |
| 1:E:11:PRO:HG3 | 1:E:42:PRO:HG3 | 1.49 | 0.94 |
| 1:K:11:PRO:HG3 | 1:K:42:PRO:HG3 | 1.48 | 0.94 |
| 1:G:11:PRO:HG3 | 1:G:42:PRO:HG3 | 1.49 | 0.94 |
| 1:D:286:LEU:O | 1:D:288:LEU:N | 2.01 | 0.93 |
| 1:G:286:LEU:O | 1:G:288:LEU:N | 2.01 | 0.93 |
| 1:J:11:PRO:HG3 | 1:J:42:PRO:HG3 | 1.49 | 0.93 |
| 1:F:286:LEU:O | 1:F:288:LEU:N | 2.01 | 0.93 |
| 1:L:286:LEU:O | 1:L:288:LEU:N | 2.01 | 0.93 |
| 1:E:257:LEU:HD12 | 1:E:257:LEU:N | 1.79 | 0.93 |
| 1:K:286:LEU:O | 1:K:288:LEU:N | 2.00 | 0.93 |
| 1:E:286:LEU:O | 1:E:288:LEU:N | 2.01 | 0.93 |
| 1:A:286:LEU:O | 1:A:288:LEU:N | 2.01 | 0.92 |
| 1:J:286:LEU:O | 1:J:288:LEU:N | 2.02 | 0.92 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:C:286:LEU:O | 1:C:288:LEU:N | 2.02 | 0.92 |
| 1:D:11:PRO:HG3 | 1:D:42:PRO:HG3 | 1.49 | 0.92 |
| 1:B:286:LEU:O | 1:B:288:LEU:N | 2.02 | 0.92 |
| 1:K:199:LYS:HB2 | 1:K:229:ALA:HB2 | 1.52 | 0.92 |
| 1:A:11:PRO:HG3 | 1:A:42:PRO:HG3 | 1.49 | 0.92 |
| 1:I:286:LEU:O | 1:I:288:LEU:N | 2.02 | 0.92 |
| 1:F:199:LYS:HB2 | 1:F:229:ALA:HB2 | 1.52 | 0.92 |
| 1:J:199:LYS:HB2 | 1:J:229:ALA:HB2 | 1.51 | 0.92 |
| 1:A:199:LYS:HB2 | 1:A:229:ALA:HB2 | 1.52 | 0.92 |
| 1:G:199:LYS:HB2 | 1:G:229:ALA:HB2 | 1.52 | 0.91 |
| 1:H:286:LEU:O | 1:H:288:LEU:N | 2.02 | 0.91 |
| 1:E:199:LYS:HB2 | 1:E:229:ALA:HB2 | 1.52 | 0.90 |
| 1:I:199:LYS:HB2 | 1:I:229:ALA:HB2 | 1.52 | 0.90 |
| 1:K:280:GLU:C | 1:K:281:LYS:HG2 | 1.92 | 0.90 |
| 1:D:199:LYS:HB2 | 1:D:229:ALA:HB2 | 1.52 | 0.90 |
| 1:I:257:LEU:CD1 | 1:I:257:LEU:N | 2.35 | 0.89 |
| 1:J:257:LEU:CD1 | 1:J:257:LEU:N | 2.35 | 0.89 |
| 1:H:199:LYS:HB2 | 1:H:229:ALA:HB2 | 1.52 | 0.89 |
| 1:C:47:LYS:HG2 | 1:C:48:VAL:H | 1.37 | 0.89 |
| 1:I:47:LYS:HG2 | 1:I:48:VAL:H | 1.37 | 0.89 |
| 1:B:199:LYS:HB2 | 1:B:229:ALA:HB2 | 1.52 | 0.89 |
| 1:H:257:LEU:CD1 | 1:H:257:LEU:N | 2.36 | 0.89 |
| 1:C:199:LYS:HB2 | 1:C:229:ALA:HB2 | 1.52 | 0.89 |
| 1:I:280:GLU:C | 1:I:281:LYS:HG2 | 1.93 | 0.89 |
| 1:D:280:GLU:C | 1:D:281:LYS:HG2 | 1.93 | 0.89 |
| 1:A:257:LEU:N | 1:A:257:LEU:CD1 | 2.36 | 0.89 |
| 1:G:156:ASN:OD1 | 1:L:152:HIS:CG | 2.26 | 0.89 |
| 1:C:257:LEU:CD1 | 1:C:257:LEU:N | 2.36 | 0.89 |
| 1:E:257:LEU:CD1 | 1:E:257:LEU:N | 2.36 | 0.89 |
| 1:F:280:GLU:C | 1:F:281:LYS:HG2 | 1.93 | 0.89 |
| 1:K:257:LEU:CD1 | 1:K:257:LEU:N | 2.35 | 0.89 |
| 1:J:286:LEU:H | 1:J:286:LEU:HD12 | 0.72 | 0.88 |
| 1:E:47:LYS:HG2 | 1:E:48:VAL:H | 1.37 | 0.88 |
| 1:H:280:GLU:C | 1:H:281:LYS:HG2 | 1.93 | 0.88 |
| 1:D:257:LEU:N | 1:D:257:LEU:CD1 | 2.36 | 0.88 |
| 1:L:199:LYS:HB2 | 1:L:229:ALA:HB2 | 1.52 | 0.88 |
| 1:G:257:LEU:N | 1:G:257:LEU:CD1 | 2.35 | 0.88 |
| 1:D:47:LYS:HG2 | 1:D:48:VAL:H | 1.37 | 0.88 |
| 1:H:47:LYS:HG2 | 1:H:48:VAL:H | 1.38 | 0.88 |
| 1:B:257:LEU:N | 1:B:257:LEU:CD1 | 2.35 | 0.88 |
| 1:A:280:GLU:C | 1:A:281:LYS:HG2 | 1.93 | 0.88 |
| 1:J:47:LYS:HG2 | 1:J:48:VAL:H | 1.36 | 0.88 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:G:47:LYS:HG2 | 1:G:48:VAL:H | 1.37 | 0.88 |
| 1:F:47:LYS:HG2 | 1:F:48:VAL:H | 1.37 | 0.88 |
| 1:B:280:GLU:C | 1:B:281:LYS:HG2 | 1.93 | 0.87 |
| 1:L:257:LEU:CD1 | 1:L:257:LEU:N | 2.35 | 0.87 |
| 1:L:280:GLU:C | 1:L:281:LYS:HG2 | 1.93 | 0.87 |
| 1:E:286:LEU:H | 1:E:286:LEU:HD12 | 0.70 | 0.87 |
| 1:F:257:LEU:N | 1:F:257:LEU:HD12 | 1.79 | 0.87 |
| 1:F:257:LEU:N | 1:F:257:LEU:CD1 | 2.36 | 0.87 |
| 1:B:286:LEU:HD12 | 1:B:286:LEU:H | 0.71 | 0.86 |
| 1:A:47:LYS:HG2 | 1:A:48:VAL:H | 1.37 | 0.86 |
| 1:L:286:LEU:HD12 | 1:L:286:LEU:H | 0.71 | 0.86 |
| 1:L:47:LYS:HG2 | 1:L:48:VAL:H | 1.38 | 0.86 |
| 1:B:47:LYS:HG2 | 1:B:48:VAL:H | 1.37 | 0.86 |
| 1:E:280:GLU:C | 1:E:281:LYS:HG2 | 1.93 | 0.86 |
| 1:G:286:LEU:H | 1:G:286:LEU:HD12 | 0.71 | 0.86 |
| 1:H:286:LEU:HD12 | 1:H:286:LEU:H | 0.71 | 0.86 |
| 1:K:47:LYS:HG2 | 1:K:48:VAL:H | 1.39 | 0.85 |
| 1:L:257:LEU:HD12 | 1:L:257:LEU:N | 1.79 | 0.85 |
| 1:A:286:LEU:HD12 | 1:A:286:LEU:H | 0.71 | 0.85 |
| 1:C:286:LEU:HD12 | 1:C:286:LEU:H | 0.70 | 0.85 |
| 1:C:257:LEU:HD12 | 1:C:257:LEU:N | 1.79 | 0.85 |
| 1:I:286:LEU:H | 1:I:286:LEU:HD12 | 0.70 | 0.85 |
| 1:K:286:LEU:HD12 | 1:K:286:LEU:H | 0.70 | 0.84 |
| 1:J:280:GLU:C | 1:J:281:LYS:HG2 | 1.94 | 0.84 |
| 1:G:280:GLU:C | 1:G:281:LYS:HG2 | 1.93 | 0.84 |
| 1:D:286:LEU:H | 1:D:286:LEU:HD12 | 0.71 | 0.83 |
| 1:H:211:LYS:HA | 1:H:279:SER:HB3 | 1.61 | 0.83 |
| 1:B:257:LEU:HD12 | 1:B:257:LEU:N | 1.79 | 0.83 |
| 1:G:167:ASP:CG | 1:L:160:GLU:HA | 1.98 | 0.82 |
| 1:D:220:PHE:HA | 1:D:223:ILE:CG2 | 2.09 | 0.82 |
| 1:F:211:LYS:HA | 1:F:279:SER:HB3 | 1.62 | 0.82 |
| 1:A:220:PHE:HA | 1:A:223:ILE:CG2 | 2.10 | 0.82 |
| 1:B:211:LYS:HA | 1:B:279:SER:HB3 | 1.61 | 0.82 |
| 1:G:72:LEU:HB3 | 1:H:136:LEU:HD21 | 1.61 | 0.82 |
| 1:G:167:ASP:OD1 | 1:L:159:HIS:C | 2.18 | 0.82 |
| 1:C:280:GLU:C | 1:C:281:LYS:HG2 | 1.93 | 0.82 |
| 1:L:211:LYS:HA | 1:L:279:SER:HB3 | 1.62 | 0.82 |
| 1:J:220:PHE:HA | 1:J:223:ILE:CG2 | 2.10 | 0.82 |
| 1:K:220:PHE:HA | 1:K:223:ILE:CG2 | 2.10 | 0.82 |
| 1:B:220:PHE:HA | 1:B:223:ILE:CG2 | 2.10 | 0.82 |
| 1:C:220:PHE:HA | 1:C:223:ILE:CG2 | 2.10 | 0.82 |
| 1:C:211:LYS:HA | 1:C:279:SER:HB3 | 1.62 | 0.82 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:L:220:PHE:HA | 1:L:223:ILE:CG2 | 2.10 | 0.81 |
| 1:F:286:LEU:HD12 | 1:F:286:LEU:H | 0.71 | 0.81 |
| 1:I:211:LYS:HA | 1:I:279:SER:HB3 | 1.61 | 0.81 |
| 1:I:220:PHE:HA | 1:I:223:ILE:CG2 | 2.10 | 0.81 |
| 1:E:220:PHE:HA | 1:E:223:ILE:CG2 | 2.10 | 0.81 |
| 1:H:256:VAL:HG11 | 1:H:258:PHE:CE2 | 2.16 | 0.81 |
| 1:E:256:VAL:HG11 | 1:E:258:PHE:CE2 | 2.16 | 0.81 |
| 1:H:220:PHE:HA | 1:H:223:ILE:CG2 | 2.10 | 0.81 |
| 1:F:220:PHE:HA | 1:F:223:ILE:CG2 | 2.09 | 0.81 |
| 1:G:349:ARG:HH11 | 1:G:349:ARG:HB2 | 1.46 | 0.81 |
| 1:D:211:LYS:HA | 1:D:279:SER:HB3 | 1.61 | 0.80 |
| 1:J:211:LYS:HA | 1:J:279:SER:HB3 | 1.61 | 0.80 |
| 1:F:256:VAL:HG11 | 1:F:258:PHE:CE2 | 2.16 | 0.80 |
| 1:C:256:VAL:HG11 | 1:C:258:PHE:CE2 | 2.17 | 0.80 |
| 1:G:220:PHE:HA | 1:G:223:ILE:CG2 | 2.10 | 0.80 |
| 1:A:211:LYS:HA | 1:A:279:SER:HB3 | 1.62 | 0.80 |
| 1:G:211:LYS:HA | 1:G:279:SER:HB3 | 1.62 | 0.80 |
| 1:E:211:LYS:HA | 1:E:279:SER:HB3 | 1.62 | 0.80 |
| 1:H:94:TYR:CE2 | 1:H:123:ASP:HB3 | 2.17 | 0.80 |
| 1:H:349:ARG:HH11 | 1:H:349:ARG:HB2 | 1.47 | 0.80 |
| 1:G:256:VAL:HG11 | 1:G:258:PHE:CE2 | 2.17 | 0.80 |
| 1:B:256:VAL:HG11 | 1:B:258:PHE:CE2 | 2.17 | 0.80 |
| 1:C:94:TYR:CE2 | 1:C:123:ASP:HB3 | 2.17 | 0.80 |
| 1:D:256:VAL:HG11 | 1:D:258:PHE:CE2 | 2.17 | 0.80 |
| 1:L:94:TYR:CE2 | 1:L:123:ASP:HB3 | 2.17 | 0.80 |
| 1:J:306:ILE:HB | 1:J:307:PRO:HD3 | 1.64 | 0.80 |
| 1:D:94:TYR:CE2 | 1:D:123:ASP:HB3 | 2.17 | 0.79 |
| 1:I:349:ARG:HB2 | 1:I:349:ARG:HH11 | 1.47 | 0.79 |
| 1:J:349:ARG:HB2 | 1:J:349:ARG:HH11 | 1.47 | 0.79 |
| 1:C:349:ARG:HB2 | 1:C:349:ARG:HH11 | 1.47 | 0.79 |
| 1:L:256:VAL:HG11 | 1:L:258:PHE:CE2 | 2.17 | 0.79 |
| 1:K:211:LYS:HA | 1:K:279:SER:HB3 | 1.62 | 0.79 |
| 1:F:349:ARG:HH11 | 1:F:349:ARG:HB2 | 1.47 | 0.79 |
| 1:I:256:VAL:HG11 | 1:I:258:PHE:CE2 | 2.17 | 0.79 |
| 1:E:94:TYR:CE2 | 1:E:123:ASP:HB3 | 2.18 | 0.79 |
| 1:A:306:ILE:HB | 1:A:307:PRO:HD3 | 1.65 | 0.79 |
| 1:H:306:ILE:HB | 1:H:307:PRO:HD3 | 1.65 | 0.79 |
| 1:I:94:TYR:CE2 | 1:I:123:ASP:HB3 | 2.18 | 0.79 |
| 1:A:94:TYR:CE2 | 1:A:123:ASP:HB3 | 2.18 | 0.79 |
| 1:J:94:TYR:CE2 | 1:J:123:ASP:HB3 | 2.17 | 0.79 |
| 1:A:256:VAL:HG11 | 1:A:258:PHE:CE2 | 2.17 | 0.79 |
| 1:G:94:TYR:CE2 | 1:G:123:ASP:HB3 | 2.17 | 0.79 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 1:F:306:ILE:HB | 1:F:307:PRO:HD3 | 1.64 | 0.79 |
| 1:K:256:VAL:HG11 | 1:K:258:PHE:CE2 | 2.17 | 0.78 |
| 1:B:306:ILE:HB | 1:B:307:PRO:HD3 | 1.65 | 0.78 |
| 1:B:349:ARG:HH11 | 1:B:349:ARG:HB2 | 1.47 | 0.78 |
| 1:K:94:TYR:CE2 | 1:K:123:ASP:HB3 | 2.18 | 0.78 |
| 1:J:256:VAL:HG11 | 1:J:258:PHE:CE2 | 2.17 | 0.78 |
| 1:C:306:ILE:HB | 1:C:307:PRO:HD3 | 1.65 | 0.78 |
| 1:K:306:ILE:HB | 1:K:307:PRO:HD3 | 1.65 | 0.78 |
| 1:L:306:ILE:HB | 1:L:307:PRO:HD3 | 1.65 | 0.78 |
| 1:D:349:ARG:HH11 | 1:D:349:ARG:HB2 | 1.47 | 0.78 |
| 1:B:94:TYR:CE2 | 1:B:123:ASP:HB3 | 2.17 | 0.78 |
| 1:E:349:ARG:HH11 | 1:E:349:ARG:HB2 | 1.47 | 0.78 |
| 1:I:306:ILE:HB | 1:I:307:PRO:HD3 | 1.65 | 0.78 |
| 1:F:94:TYR:CE2 | 1:F:123:ASP:HB3 | 2.17 | 0.78 |
| 1:K:349:ARG:HH11 | 1:K:349:ARG:HB2 | 1.47 | 0.78 |
| 1:A:191:GLU:HG2 | 1:C:50:PRO:HG2 | 1.66 | 0.78 |
| 1:K:136:LEU:HD21 | 1:L:72:LEU:HB3 | 1.66 | 0.78 |
| 1:G:306:ILE:HB | 1:G:307:PRO:HD3 | 1.65 | 0.77 |
| 1:F:50:PRO:HG2 | 1:G:191:GLU:HG2 | 1.65 | 0.77 |
| 1:H:286:LEU:O | 1:H:289:LEU:N | 2.18 | 0.77 |
| 1:L:349:ARG:HH11 | 1:L:349:ARG:HB2 | 1.47 | 0.77 |
| 1:D:306:ILE:HB | 1:D:307:PRO:HD3 | 1.65 | 0.77 |
| 1:A:286:LEU:O | 1:A:289:LEU:N | 2.18 | 0.77 |
| 1:D:286:LEU:O | 1:D:289:LEU:N | 2.18 | 0.77 |
| 1:E:306:ILE:HB | 1:E:307:PRO:HD3 | 1.65 | 0.77 |
| 1:K:94:TYR:OH | 1:K:123:ASP:N | 2.18 | 0.77 |
| 1:A:349:ARG:HH11 | 1:A:349:ARG:HB2 | 1.47 | 0.76 |
| 1:I:286:LEU:O | 1:I:289:LEU:N | 2.18 | 0.76 |
| 1:C:286:LEU:O | 1:C:289:LEU:N | 2.19 | 0.76 |
| 1:F:286:LEU:O | 1:F:289:LEU:N | 2.18 | 0.76 |
| 1:J:94:TYR:OH | 1:J:123:ASP:N | 2.19 | 0.76 |
| 1:B:286:LEU:O | 1:B:289:LEU:N | 2.18 | 0.76 |
| 1:G:286:LEU:O | 1:G:289:LEU:N | 2.18 | 0.76 |
| 1:L:94:TYR:OH | 1:L:123:ASP:N | 2.19 | 0.76 |
| 1:C:136:LEU:HD21 | 1:D:72:LEU:HB3 | 1.65 | 0.76 |
| 1:B:94:TYR:OH | 1:B:123:ASP:N | 2.19 | 0.76 |
| 1:F:94:TYR:OH | 1:F:123:ASP:N | 2.19 | 0.76 |
| 1:K:286:LEU:O | 1:K:289:LEU:N | 2.19 | 0.75 |
| 1:C:94:TYR:OH | 1:C:123:ASP:N | 2.19 | 0.75 |
| 1:H:94:TYR:OH | 1:H:123:ASP:N | 2.19 | 0.75 |
| 1:J:286:LEU:O | 1:J:289:LEU:N | 2.20 | 0.75 |
| 1:J:47:LYS:HG2 | 1:J:48:VAL:N | 2.02 | 0.75 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:G:94:TYR:OH | 1:G:123:ASP:N | 2.19 | 0.75 |
| 1:B:191:GLU:HG2 | 1:D:50:PRO:HG2 | 1.69 | 0.75 |
| 1:D:94:TYR:OH | 1:D:123:ASP:N | 2.19 | 0.75 |
| 1:A:94:TYR:OH | 1:A:123:ASP:N | 2.20 | 0.75 |
| 1:E:186:THR:HA | 1:E:189:LYS:HD2 | 1.69 | 0.75 |
| 1:H:369:TYR:O | 1:H:372:VAL:HG12 | 1.87 | 0.75 |
| 1:I:94:TYR:OH | 1:I:123:ASP:N | 2.20 | 0.75 |
| 1:H:186:THR:HA | 1:H:189:LYS:HD2 | 1.69 | 0.75 |
| 1:L:286:LEU:O | 1:L:289:LEU:N | 2.18 | 0.75 |
| 1:E:286:LEU:O | 1:E:289:LEU:N | 2.19 | 0.75 |
| 1:K:186:THR:HA | 1:K:189:LYS:HD2 | 1.68 | 0.75 |
| 1:E:136:LEU:HD21 | 1:F:72:LEU:HB3 | 1.69 | 0.75 |
| 1:D:47:LYS:HG2 | 1:D:48:VAL:N | 2.02 | 0.74 |
| 1:E:94:TYR:OH | 1:E:123:ASP:N | 2.19 | 0.74 |
| 1:E:369:TYR:O | 1:E:372:VAL:HG12 | 1.87 | 0.74 |
| 1:D:369:TYR:O | 1:D:372:VAL:HG12 | 1.87 | 0.74 |
| 1:G:186:THR:HA | 1:G:189:LYS:HD2 | 1.69 | 0.74 |
| 1:A:186:THR:HA | 1:A:189:LYS:HD2 | 1.69 | 0.74 |
| 1:D:186:THR:HA | 1:D:189:LYS:HD2 | 1.69 | 0.74 |
| 1:L:186:THR:HA | 1:L:189:LYS:HD2 | 1.69 | 0.74 |
| 1:L:369:TYR:O | 1:L:372:VAL:HG12 | 1.87 | 0.74 |
| 1:G:369:TYR:O | 1:G:372:VAL:HG12 | 1.88 | 0.74 |
| 1:B:186:THR:HA | 1:B:189:LYS:HD2 | 1.69 | 0.74 |
| 1:I:186:THR:HA | 1:I:189:LYS:HD2 | 1.69 | 0.74 |
| 1:C:186:THR:HA | 1:C:189:LYS:HD2 | 1.69 | 0.74 |
| 1:J:186:THR:HA | 1:J:189:LYS:HD2 | 1.70 | 0.74 |
| 1:F:369:TYR:O | 1:F:372:VAL:HG12 | 1.88 | 0.74 |
| 1:B:369:TYR:O | 1:B:372:VAL:HG12 | 1.88 | 0.74 |
| 1:B:47:LYS:HG2 | 1:B:48:VAL:N | 2.03 | 0.74 |
| 1:E:47:LYS:HG2 | 1:E:48:VAL:N | 2.03 | 0.74 |
| 1:F:186:THR:HA | 1:F:189:LYS:HD2 | 1.69 | 0.74 |
| 1:F:47:LYS:HG2 | 1:F:48:VAL:N | 2.03 | 0.74 |
| 1:I:369:TYR:O | 1:I:372:VAL:HG12 | 1.88 | 0.73 |
| 1:H:47:LYS:HG2 | 1:H:48:VAL:N | 2.03 | 0.73 |
| 1:A:369:TYR:O | 1:A:372:VAL:HG12 | 1.87 | 0.73 |
| 1:G:47:LYS:HG2 | 1:G:48:VAL:N | 2.03 | 0.73 |
| 1:J:191:GLU:HG2 | 1:L:50:PRO:HG2 | 1.71 | 0.73 |
| 1:C:47:LYS:HG2 | 1:C:48:VAL:N | 2.03 | 0.73 |
| 1:K:47:LYS:HG2 | 1:K:48:VAL:N | 2.04 | 0.73 |
| 1:A:47:LYS:HG2 | 1:A:48:VAL:N | 2.03 | 0.73 |
| 1:L:47:LYS:HG2 | 1:L:48:VAL:N | 2.03 | 0.73 |
| 1:C:369:TYR:O | 1:C:372:VAL:HG12 | 1.88 | 0.73 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|----------------|------------------|-------------|----------|
| 1:K:280:GLU:C | 1:K:281:LYS:CG | 2.57 | 0.72 |
| 1:I:47:LYS:HG2 | 1:I:48:VAL:N | 2.03 | 0.72 |
| 1:K:369:TYR:O | 1:K:372:VAL:HG12 | 1.88 | 0.72 |
| 1:K:11:PRO:CG | 1:K:42:PRO:HG3 | 2.20 | 0.72 |
| 1:F:280:GLU:C | 1:F:281:LYS:CG | 2.58 | 0.72 |
| 1:A:11:PRO:CG | 1:A:42:PRO:HG3 | 2.20 | 0.72 |
| 1:A:257:LEU:O | 1:A:258:PHE:C | 2.27 | 0.72 |
| 1:A:280:GLU:C | 1:A:281:LYS:CG | 2.58 | 0.72 |
| 1:D:280:GLU:C | 1:D:281:LYS:CG | 2.58 | 0.72 |
| 1:G:257:LEU:O | 1:G:258:PHE:C | 2.27 | 0.72 |
| 1:I:257:LEU:O | 1:I:258:PHE:C | 2.27 | 0.72 |
| 1:K:256:VAL:C | 1:K:257:LEU:CD1 | 2.58 | 0.71 |
| 1:G:280:GLU:C | 1:G:281:LYS:CG | 2.58 | 0.71 |
| 1:J:280:GLU:C | 1:J:281:LYS:CG | 2.58 | 0.71 |
| 1:L:11:PRO:CG | 1:L:42:PRO:HG3 | 2.20 | 0.71 |
| 1:J:369:TYR:O | 1:J:372:VAL:HG12 | 1.89 | 0.71 |
| 1:H:280:GLU:C | 1:H:281:LYS:CG | 2.58 | 0.71 |
| 1:E:11:PRO:CG | 1:E:42:PRO:HG3 | 2.20 | 0.71 |
| 1:B:212:ARG:HA | 1:B:214:GLN:HE22 | 1.56 | 0.71 |
| 1:B:280:GLU:C | 1:B:281:LYS:CG | 2.58 | 0.71 |
| 1:J:212:ARG:HA | 1:J:214:GLN:HE22 | 1.56 | 0.71 |
| 1:D:11:PRO:CG | 1:D:42:PRO:HG3 | 2.20 | 0.71 |
| 1:I:280:GLU:C | 1:I:281:LYS:CG | 2.58 | 0.71 |
| 1:L:280:GLU:C | 1:L:281:LYS:CG | 2.58 | 0.71 |
| 1:D:212:ARG:HA | 1:D:214:GLN:HE22 | 1.56 | 0.71 |
| 1:B:11:PRO:CG | 1:B:42:PRO:HG3 | 2.20 | 0.71 |
| 1:H:11:PRO:CG | 1:H:42:PRO:HG3 | 2.20 | 0.71 |
| 1:K:212:ARG:HA | 1:K:214:GLN:HE22 | 1.56 | 0.71 |
| 1:E:280:GLU:C | 1:E:281:LYS:CG | 2.58 | 0.71 |
| 1:C:286:LEU:C | 1:C:288:LEU:N | 2.43 | 0.71 |
| 1:H:212:ARG:HA | 1:H:214:GLN:HE22 | 1.56 | 0.70 |
| 1:B:257:LEU:O | 1:B:258:PHE:C | 2.27 | 0.70 |
| 1:J:257:LEU:O | 1:J:258:PHE:C | 2.28 | 0.70 |
| 1:D:257:LEU:O | 1:D:258:PHE:C | 2.28 | 0.70 |
| 1:C:280:GLU:C | 1:C:281:LYS:CG | 2.58 | 0.70 |
| 1:L:212:ARG:HA | 1:L:214:GLN:HE22 | 1.56 | 0.70 |
| 1:F:212:ARG:HA | 1:F:214:GLN:HE22 | 1.56 | 0.70 |
| 1:G:256:VAL:C | 1:G:257:LEU:CD1 | 2.59 | 0.70 |
| 1:C:11:PRO:CG | 1:C:42:PRO:HG3 | 2.20 | 0.70 |
| 1:A:212:ARG:HA | 1:A:214:GLN:HE22 | 1.56 | 0.70 |
| 1:H:256:VAL:C | 1:H:257:LEU:CD1 | 2.59 | 0.70 |
| 1:F:11:PRO:CG | 1:F:42:PRO:HG3 | 2.20 | 0.70 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:I:212:ARG:HA | 1:I:214:GLN:HE22 | 1.56 | 0.70 |
| 1:G:11:PRO:CG | 1:G:42:PRO:HG3 | 2.20 | 0.70 |
| 1:A:50:PRO:HG2 | 1:C:191:GLU:HG2 | 1.72 | 0.70 |
| 1:C:212:ARG:HA | 1:C:214:GLN:HE22 | 1.56 | 0.70 |
| 1:I:11:PRO:CG | 1:I:42:PRO:HG3 | 2.20 | 0.70 |
| 1:G:220:PHE:CA | 1:G:223:ILE:HG22 | 2.21 | 0.69 |
| 1:I:72:LEU:HB3 | 1:J:136:LEU:HD21 | 1.73 | 0.69 |
| 1:C:220:PHE:CA | 1:C:223:ILE:HG22 | 2.21 | 0.69 |
| 1:K:180:TYR:CE2 | 1:K:290:GLU:HB3 | 2.27 | 0.69 |
| 1:H:180:TYR:CE2 | 1:H:290:GLU:HB3 | 2.28 | 0.69 |
| 1:I:256:VAL:C | 1:I:257:LEU:CD1 | 2.59 | 0.69 |
| 1:G:212:ARG:HA | 1:G:214:GLN:HE22 | 1.56 | 0.69 |
| 1:H:286:LEU:C | 1:H:288:LEU:N | 2.43 | 0.69 |
| 1:D:220:PHE:CA | 1:D:223:ILE:HG22 | 2.20 | 0.69 |
| 1:B:180:TYR:CE2 | 1:B:290:GLU:HB3 | 2.28 | 0.69 |
| 1:I:286:LEU:C | 1:I:288:LEU:N | 2.43 | 0.69 |
| 1:K:220:PHE:CA | 1:K:223:ILE:HG22 | 2.21 | 0.69 |
| 1:J:11:PRO:CG | 1:J:42:PRO:HG3 | 2.20 | 0.69 |
| 1:L:357:ARG:HG3 | 1:L:359:GLU:HG3 | 1.75 | 0.69 |
| 1:E:357:ARG:HG3 | 1:E:359:GLU:HG3 | 1.75 | 0.69 |
| 1:A:180:TYR:CE2 | 1:A:290:GLU:HB3 | 2.28 | 0.69 |
| 1:D:180:TYR:CE2 | 1:D:290:GLU:HB3 | 2.28 | 0.69 |
| 1:J:180:TYR:CE2 | 1:J:290:GLU:HB3 | 2.28 | 0.69 |
| 1:F:257:LEU:O | 1:F:258:PHE:C | 2.27 | 0.69 |
| 1:I:220:PHE:CA | 1:I:223:ILE:HG22 | 2.21 | 0.69 |
| 1:A:220:PHE:CA | 1:A:223:ILE:HG22 | 2.21 | 0.69 |
| 1:H:220:PHE:CA | 1:H:223:ILE:HG22 | 2.21 | 0.69 |
| 1:C:357:ARG:HG3 | 1:C:359:GLU:HG3 | 1.75 | 0.69 |
| 1:B:357:ARG:HG3 | 1:B:359:GLU:HG3 | 1.75 | 0.69 |
| 1:F:180:TYR:CE2 | 1:F:290:GLU:HB3 | 2.28 | 0.69 |
| 1:A:256:VAL:C | 1:A:257:LEU:CD1 | 2.59 | 0.69 |
| 1:E:212:ARG:HA | 1:E:214:GLN:HE22 | 1.56 | 0.68 |
| 1:L:180:TYR:CE2 | 1:L:290:GLU:HB3 | 2.28 | 0.68 |
| 1:J:286:LEU:C | 1:J:288:LEU:N | 2.43 | 0.68 |
| 1:G:357:ARG:HG3 | 1:G:359:GLU:HG3 | 1.75 | 0.68 |
| 1:I:180:TYR:CE2 | 1:I:290:GLU:HB3 | 2.28 | 0.68 |
| 1:I:136:LEU:HD21 | 1:J:72:LEU:HB3 | 1.75 | 0.68 |
| 1:C:180:TYR:CE2 | 1:C:290:GLU:HB3 | 2.28 | 0.68 |
| 1:J:220:PHE:CA | 1:J:223:ILE:HG22 | 2.21 | 0.68 |
| 1:A:94:TYR:H | 1:A:98:HIS:HD2 | 1.41 | 0.68 |
| 1:A:357:ARG:HG3 | 1:A:359:GLU:HG3 | 1.75 | 0.68 |
| 1:H:357:ARG:HG3 | 1:H:359:GLU:HG3 | 1.75 | 0.68 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:K:357:ARG:HG3 | 1:K:359:GLU:HG3 | 1.75 | 0.68 |
| 1:D:286:LEU:C | 1:D:288:LEU:N | 2.43 | 0.68 |
| 1:B:220:PHE:CA | 1:B:223:ILE:HG22 | 2.21 | 0.68 |
| 1:K:286:LEU:C | 1:K:288:LEU:N | 2.42 | 0.68 |
| 1:C:257:LEU:O | 1:C:258:PHE:C | 2.28 | 0.68 |
| 1:E:94:TYR:H | 1:E:98:HIS:HD2 | 1.42 | 0.68 |
| 1:J:94:TYR:H | 1:J:98:HIS:HD2 | 1.42 | 0.68 |
| 1:G:180:TYR:CE2 | 1:G:290:GLU:HB3 | 2.28 | 0.68 |
| 1:D:357:ARG:HG3 | 1:D:359:GLU:HG3 | 1.75 | 0.68 |
| 1:F:357:ARG:HG3 | 1:F:359:GLU:HG3 | 1.75 | 0.68 |
| 1:J:357:ARG:HG3 | 1:J:359:GLU:HG3 | 1.75 | 0.68 |
| 1:J:256:VAL:C | 1:J:257:LEU:CD1 | 2.59 | 0.68 |
| 1:D:94:TYR:H | 1:D:98:HIS:HD2 | 1.42 | 0.68 |
| 1:I:357:ARG:HG3 | 1:I:359:GLU:HG3 | 1.75 | 0.67 |
| 1:E:180:TYR:CE2 | 1:E:290:GLU:HB3 | 2.28 | 0.67 |
| 1:G:94:TYR:H | 1:G:98:HIS:HD2 | 1.42 | 0.67 |
| 1:F:286:LEU:C | 1:F:288:LEU:N | 2.43 | 0.67 |
| 1:C:256:VAL:C | 1:C:257:LEU:CD1 | 2.59 | 0.67 |
| 1:E:220:PHE:CA | 1:E:223:ILE:HG22 | 2.21 | 0.67 |
| 1:I:94:TYR:H | 1:I:98:HIS:HD2 | 1.43 | 0.67 |
| 1:D:256:VAL:C | 1:D:257:LEU:CD1 | 2.59 | 0.67 |
| 1:D:257:LEU:HB3 | 1:D:259:LEU:CD1 | 2.25 | 0.67 |
| 1:F:220:PHE:CA | 1:F:223:ILE:HG22 | 2.20 | 0.67 |
| 1:C:94:TYR:H | 1:C:98:HIS:HD2 | 1.42 | 0.67 |
| 1:H:257:LEU:HB3 | 1:H:259:LEU:CD1 | 2.25 | 0.67 |
| 1:B:286:LEU:C | 1:B:288:LEU:N | 2.43 | 0.66 |
| 1:B:256:VAL:C | 1:B:257:LEU:CD1 | 2.59 | 0.66 |
| 1:E:257:LEU:HB3 | 1:E:259:LEU:CD1 | 2.25 | 0.66 |
| 1:E:257:LEU:O | 1:E:258:PHE:C | 2.28 | 0.66 |
| 1:K:94:TYR:H | 1:K:98:HIS:HD2 | 1.42 | 0.66 |
| 1:A:286:LEU:C | 1:A:288:LEU:N | 2.42 | 0.66 |
| 1:E:286:LEU:C | 1:E:288:LEU:N | 2.43 | 0.66 |
| 1:K:257:LEU:O | 1:K:258:PHE:C | 2.27 | 0.66 |
| 1:C:257:LEU:HB3 | 1:C:259:LEU:CD1 | 2.25 | 0.66 |
| 1:B:257:LEU:HB3 | 1:B:259:LEU:CD1 | 2.25 | 0.66 |
| 1:J:257:LEU:HB3 | 1:J:259:LEU:CD1 | 2.25 | 0.66 |
| 1:L:94:TYR:H | 1:L:98:HIS:HD2 | 1.42 | 0.66 |
| 1:F:256:VAL:C | 1:F:257:LEU:CD1 | 2.59 | 0.66 |
| 1:K:257:LEU:HB3 | 1:K:259:LEU:CD1 | 2.26 | 0.66 |
| 1:A:257:LEU:HB3 | 1:A:259:LEU:CD1 | 2.25 | 0.66 |
| 1:L:220:PHE:CA | 1:L:223:ILE:HG22 | 2.21 | 0.66 |
| 1:F:333:GLN:HE22 | 1:F:340:LEU:HD23 | 1.61 | 0.66 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:I:257:LEU:HB3 | 1:I:259:LEU:CD1 | 2.25 | 0.66 |
| 1:F:223:ILE:HD11 | 1:F:335:LEU:HD12 | 1.78 | 0.66 |
| 1:F:94:TYR:H | 1:F:98:HIS:HD2 | 1.42 | 0.66 |
| 1:L:257:LEU:HB3 | 1:L:259:LEU:CD1 | 2.25 | 0.66 |
| 1:L:257:LEU:O | 1:L:258:PHE:C | 2.28 | 0.66 |
| 1:C:333:GLN:HE22 | 1:C:340:LEU:HD23 | 1.61 | 0.66 |
| 1:E:223:ILE:HD11 | 1:E:335:LEU:HD12 | 1.78 | 0.66 |
| 1:G:333:GLN:HE22 | 1:G:340:LEU:HD23 | 1.61 | 0.66 |
| 1:H:94:TYR:H | 1:H:98:HIS:HD2 | 1.43 | 0.66 |
| 1:I:223:ILE:HD11 | 1:I:335:LEU:HD12 | 1.78 | 0.66 |
| 1:H:223:ILE:HD11 | 1:H:335:LEU:HD12 | 1.78 | 0.66 |
| 1:B:94:TYR:H | 1:B:98:HIS:HD2 | 1.42 | 0.66 |
| 1:F:257:LEU:HB3 | 1:F:259:LEU:CD1 | 2.25 | 0.66 |
| 1:G:223:ILE:HD11 | 1:G:335:LEU:HD12 | 1.78 | 0.66 |
| 1:G:257:LEU:HB3 | 1:G:259:LEU:CD1 | 2.26 | 0.65 |
| 1:C:223:ILE:HD11 | 1:C:335:LEU:HD12 | 1.78 | 0.65 |
| 1:A:333:GLN:HE22 | 1:A:340:LEU:HD23 | 1.61 | 0.65 |
| 1:B:223:ILE:HD11 | 1:B:335:LEU:HD12 | 1.78 | 0.65 |
| 1:K:333:GLN:HE22 | 1:K:340:LEU:HD23 | 1.61 | 0.65 |
| 1:I:333:GLN:HE22 | 1:I:340:LEU:HD23 | 1.61 | 0.65 |
| 1:L:333:GLN:HE22 | 1:L:340:LEU:HD23 | 1.61 | 0.65 |
| 1:L:223:ILE:HD11 | 1:L:335:LEU:HD12 | 1.78 | 0.65 |
| 1:K:353:TYR:O | 1:K:357:ARG:HB2 | 1.97 | 0.65 |
| 1:D:223:ILE:HD11 | 1:D:335:LEU:HD12 | 1.78 | 0.65 |
| 1:D:333:GLN:HE22 | 1:D:340:LEU:HD23 | 1.61 | 0.65 |
| 1:B:221:ALA:O | 1:B:224:VAL:HG12 | 1.97 | 0.65 |
| 1:E:256:VAL:C | 1:E:257:LEU:CD1 | 2.59 | 0.65 |
| 1:K:223:ILE:HD11 | 1:K:335:LEU:HD12 | 1.78 | 0.65 |
| 1:J:333:GLN:HE22 | 1:J:340:LEU:HD23 | 1.61 | 0.65 |
| 1:J:353:TYR:O | 1:J:357:ARG:HB2 | 1.97 | 0.65 |
| 1:E:333:GLN:HE22 | 1:E:340:LEU:HD23 | 1.61 | 0.65 |
| 1:G:353:TYR:O | 1:G:357:ARG:HB2 | 1.97 | 0.65 |
| 1:I:221:ALA:O | 1:I:224:VAL:HG12 | 1.97 | 0.65 |
| 1:C:353:TYR:O | 1:C:357:ARG:HB2 | 1.97 | 0.64 |
| 1:B:353:TYR:O | 1:B:357:ARG:HB2 | 1.97 | 0.64 |
| 1:I:353:TYR:O | 1:I:357:ARG:HB2 | 1.97 | 0.64 |
| 1:B:323:ASP:O | 1:B:327:VAL:HG23 | 1.98 | 0.64 |
| 1:K:221:ALA:O | 1:K:224:VAL:HG12 | 1.98 | 0.64 |
| 1:A:223:ILE:HD11 | 1:A:335:LEU:HD12 | 1.78 | 0.64 |
| 1:I:284:PHE:HB3 | 1:I:285:GLY:CA | 2.26 | 0.64 |
| 1:F:353:TYR:O | 1:F:357:ARG:HB2 | 1.97 | 0.64 |
| 1:K:256:VAL:O | 1:K:257:LEU:HD12 | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:H:257:LEU:O | 1:H:258:PHE:C | 2.28 | 0.64 |
| 1:H:333:GLN:HE22 | 1:H:340:LEU:HD23 | 1.61 | 0.64 |
| 1:B:333:GLN:HE22 | 1:B:340:LEU:HD23 | 1.61 | 0.64 |
| 1:L:221:ALA:O | 1:L:224:VAL:HG12 | 1.97 | 0.64 |
| 1:H:349:ARG:HB2 | 1:H:349:ARG:NH1 | 2.13 | 0.64 |
| 1:A:306:ILE:N | 1:A:307:PRO:CD | 2.61 | 0.64 |
| 1:H:353:TYR:O | 1:H:357:ARG:HB2 | 1.97 | 0.64 |
| 1:K:257:LEU:O | 1:K:259:LEU:CD1 | 2.46 | 0.64 |
| 1:E:349:ARG:HB2 | 1:E:349:ARG:NH1 | 2.13 | 0.64 |
| 1:I:323:ASP:O | 1:I:327:VAL:HG23 | 1.98 | 0.64 |
| 1:B:306:ILE:N | 1:B:307:PRO:CD | 2.61 | 0.64 |
| 1:D:353:TYR:O | 1:D:357:ARG:HB2 | 1.97 | 0.64 |
| 1:C:221:ALA:O | 1:C:224:VAL:HG12 | 1.98 | 0.64 |
| 1:D:221:ALA:O | 1:D:224:VAL:HG12 | 1.97 | 0.64 |
| 1:E:221:ALA:O | 1:E:224:VAL:HG12 | 1.98 | 0.64 |
| 1:E:323:ASP:O | 1:E:327:VAL:HG23 | 1.98 | 0.64 |
| 1:A:353:TYR:O | 1:A:357:ARG:HB2 | 1.97 | 0.64 |
| 1:F:323:ASP:O | 1:F:327:VAL:HG23 | 1.98 | 0.64 |
| 1:C:323:ASP:O | 1:C:327:VAL:HG23 | 1.98 | 0.64 |
| 1:L:256:VAL:C | 1:L:257:LEU:CD1 | 2.59 | 0.64 |
| 1:G:306:ILE:N | 1:G:307:PRO:CD | 2.61 | 0.64 |
| 1:J:221:ALA:O | 1:J:224:VAL:HG12 | 1.98 | 0.64 |
| 1:G:221:ALA:O | 1:G:224:VAL:HG12 | 1.98 | 0.64 |
| 1:J:223:ILE:HD11 | 1:J:335:LEU:HD12 | 1.79 | 0.63 |
| 1:E:353:TYR:O | 1:E:357:ARG:HB2 | 1.97 | 0.63 |
| 1:H:323:ASP:O | 1:H:327:VAL:HG23 | 1.98 | 0.63 |
| 1:L:289:LEU:O | 1:L:290:GLU:C | 2.36 | 0.63 |
| 1:C:257:LEU:O | 1:C:259:LEU:CD1 | 2.46 | 0.63 |
| 1:B:256:VAL:O | 1:B:257:LEU:HD12 | 1.97 | 0.63 |
| 1:L:306:ILE:N | 1:L:307:PRO:CD | 2.62 | 0.63 |
| 1:L:353:TYR:O | 1:L:357:ARG:HB2 | 1.97 | 0.63 |
| 1:F:254:ASP:C | 1:F:254:ASP:OD1 | 2.34 | 0.63 |
| 1:A:323:ASP:O | 1:A:327:VAL:HG23 | 1.98 | 0.63 |
| 1:E:72:LEU:HB3 | 1:F:136:LEU:HD21 | 1.79 | 0.63 |
| 1:A:349:ARG:NH1 | 1:A:349:ARG:HB2 | 2.13 | 0.63 |
| 1:A:221:ALA:O | 1:A:224:VAL:HG12 | 1.98 | 0.63 |
| 1:A:257:LEU:O | 1:A:259:LEU:CD1 | 2.46 | 0.63 |
| 1:E:256:VAL:O | 1:E:257:LEU:HD12 | 1.98 | 0.63 |
| 1:L:323:ASP:O | 1:L:327:VAL:HG23 | 1.98 | 0.63 |
| 1:E:257:LEU:O | 1:E:259:LEU:CD1 | 2.47 | 0.63 |
| 1:C:349:ARG:NH1 | 1:C:349:ARG:HB2 | 2.13 | 0.63 |
| 1:K:306:ILE:N | 1:K:307:PRO:CD | 2.62 | 0.63 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:E:306:ILE:N | 1:E:307:PRO:CD | 2.62 | 0.63 |
| 1:K:254:ASP:C | 1:K:254:ASP:OD1 | 2.33 | 0.63 |
| 1:F:221:ALA:O | 1:F:224:VAL:HG12 | 1.97 | 0.63 |
| 1:L:257:LEU:O | 1:L:259:LEU:CD1 | 2.47 | 0.63 |
| 1:J:257:LEU:O | 1:J:259:LEU:CD1 | 2.46 | 0.63 |
| 1:D:256:VAL:O | 1:D:257:LEU:HD12 | 1.98 | 0.63 |
| 1:B:349:ARG:NH1 | 1:B:349:ARG:HB2 | 2.13 | 0.63 |
| 1:C:306:ILE:N | 1:C:307:PRO:CD | 2.62 | 0.63 |
| 1:G:132:SER:O | 1:G:133:LEU:HD23 | 1.99 | 0.63 |
| 1:C:256:VAL:O | 1:C:257:LEU:HD12 | 1.98 | 0.63 |
| 1:D:306:ILE:N | 1:D:307:PRO:CD | 2.62 | 0.63 |
| 1:H:221:ALA:O | 1:H:224:VAL:HG12 | 1.98 | 0.63 |
| 1:G:254:ASP:C | 1:G:254:ASP:OD1 | 2.34 | 0.63 |
| 1:L:256:VAL:O | 1:L:257:LEU:HD12 | 1.98 | 0.63 |
| 1:A:256:VAL:O | 1:A:257:LEU:HD12 | 1.98 | 0.63 |
| 1:H:306:ILE:N | 1:H:307:PRO:CD | 2.61 | 0.63 |
| 1:I:306:ILE:N | 1:I:307:PRO:CD | 2.62 | 0.63 |
| 1:K:323:ASP:O | 1:K:327:VAL:HG23 | 1.98 | 0.63 |
| 1:F:257:LEU:O | 1:F:259:LEU:CD1 | 2.46 | 0.62 |
| 1:G:257:LEU:O | 1:G:259:LEU:CD1 | 2.47 | 0.62 |
| 1:H:256:VAL:O | 1:H:257:LEU:HD12 | 1.98 | 0.62 |
| 1:B:257:LEU:O | 1:B:259:LEU:CD1 | 2.46 | 0.62 |
| 1:E:256:VAL:HG12 | 1:E:256:VAL:O | 1.97 | 0.62 |
| 1:J:323:ASP:O | 1:J:327:VAL:HG23 | 1.98 | 0.62 |
| 1:C:284:PHE:HB3 | 1:C:285:GLY:CA | 2.26 | 0.62 |
| 1:I:256:VAL:O | 1:I:257:LEU:HD12 | 1.98 | 0.62 |
| 1:J:132:SER:O | 1:J:133:LEU:HD23 | 1.98 | 0.62 |
| 1:G:286:LEU:C | 1:G:288:LEU:N | 2.43 | 0.62 |
| 1:F:256:VAL:O | 1:F:257:LEU:HD12 | 1.98 | 0.62 |
| 1:I:349:ARG:HB2 | 1:I:349:ARG:NH1 | 2.13 | 0.62 |
| 1:G:323:ASP:O | 1:G:327:VAL:HG23 | 1.98 | 0.62 |
| 1:L:286:LEU:C | 1:L:288:LEU:N | 2.42 | 0.62 |
| 1:H:257:LEU:O | 1:H:259:LEU:CD1 | 2.47 | 0.62 |
| 1:I:257:LEU:O | 1:I:259:LEU:CD1 | 2.47 | 0.62 |
| 1:J:306:ILE:N | 1:J:307:PRO:CD | 2.62 | 0.62 |
| 1:D:323:ASP:O | 1:D:327:VAL:HG23 | 1.98 | 0.62 |
| 1:E:132:SER:O | 1:E:133:LEU:HD23 | 1.99 | 0.62 |
| 1:B:204:ILE:HD13 | 1:B:265:VAL:HG21 | 1.82 | 0.62 |
| 1:J:256:VAL:O | 1:J:256:VAL:HG12 | 1.97 | 0.62 |
| 1:J:256:VAL:O | 1:J:257:LEU:HD12 | 1.99 | 0.62 |
| 1:D:257:LEU:O | 1:D:259:LEU:CD1 | 2.47 | 0.62 |
| 1:C:204:ILE:HD13 | 1:C:265:VAL:HG21 | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:G:349:ARG:HB2 | 1:G:349:ARG:NH1 | 2.13 | 0.62 |
| 1:A:132:SER:O | 1:A:133:LEU:HD23 | 2.00 | 0.62 |
| 1:K:204:ILE:HD13 | 1:K:265:VAL:HG21 | 1.82 | 0.62 |
| 1:I:204:ILE:HD13 | 1:I:265:VAL:HG21 | 1.82 | 0.62 |
| 1:B:132:SER:O | 1:B:133:LEU:HD23 | 1.99 | 0.62 |
| 1:E:204:ILE:HD13 | 1:E:265:VAL:HG21 | 1.82 | 0.62 |
| 1:L:204:ILE:HD13 | 1:L:265:VAL:HG21 | 1.82 | 0.62 |
| 1:L:132:SER:O | 1:L:133:LEU:HD23 | 2.00 | 0.62 |
| 1:B:284:PHE:HB3 | 1:B:285:GLY:CA | 2.27 | 0.62 |
| 1:D:204:ILE:HD13 | 1:D:265:VAL:HG21 | 1.82 | 0.62 |
| 1:G:204:ILE:HD13 | 1:G:265:VAL:HG21 | 1.82 | 0.62 |
| 1:F:132:SER:O | 1:F:133:LEU:HD23 | 1.99 | 0.62 |
| 1:G:289:LEU:O | 1:G:290:GLU:C | 2.36 | 0.62 |
| 1:L:256:VAL:HG12 | 1:L:256:VAL:O | 1.97 | 0.62 |
| 1:J:349:ARG:HB2 | 1:J:349:ARG:NH1 | 2.13 | 0.62 |
| 1:I:132:SER:O | 1:I:133:LEU:HD23 | 1.99 | 0.62 |
| 1:L:349:ARG:HB2 | 1:L:349:ARG:NH1 | 2.13 | 0.62 |
| 1:C:132:SER:O | 1:C:133:LEU:HD23 | 1.99 | 0.62 |
| 1:F:306:ILE:N | 1:F:307:PRO:CD | 2.61 | 0.61 |
| 1:D:349:ARG:HB2 | 1:D:349:ARG:NH1 | 2.13 | 0.61 |
| 1:F:123:ASP:HA | 1:F:127:LEU:HD12 | 1.82 | 0.61 |
| 1:J:50:PRO:HG2 | 1:L:191:GLU:HG2 | 1.81 | 0.61 |
| 1:C:72:LEU:HB3 | 1:D:136:LEU:HD21 | 1.80 | 0.61 |
| 1:K:289:LEU:O | 1:K:290:GLU:C | 2.36 | 0.61 |
| 1:J:289:LEU:O | 1:J:290:GLU:C | 2.35 | 0.61 |
| 1:G:256:VAL:O | 1:G:257:LEU:HD12 | 1.98 | 0.61 |
| 1:D:256:VAL:HG12 | 1:D:256:VAL:O | 1.97 | 0.61 |
| 1:A:72:LEU:HB3 | 1:B:136:LEU:HD21 | 1.82 | 0.61 |
| 1:H:281:LYS:CB | 1:H:281:LYS:NZ | 2.63 | 0.61 |
| 1:H:289:LEU:O | 1:H:290:GLU:C | 2.36 | 0.61 |
| 1:K:123:ASP:HA | 1:K:127:LEU:HD12 | 1.82 | 0.61 |
| 1:B:122:THR:HG22 | 1:B:126:VAL:CG1 | 2.31 | 0.61 |
| 1:L:281:LYS:CB | 1:L:281:LYS:NZ | 2.64 | 0.61 |
| 1:E:123:ASP:HA | 1:E:127:LEU:HD12 | 1.82 | 0.61 |
| 1:G:123:ASP:HA | 1:G:127:LEU:HD12 | 1.82 | 0.61 |
| 1:H:204:ILE:HD13 | 1:H:265:VAL:HG21 | 1.82 | 0.61 |
| 1:G:256:VAL:HG12 | 1:G:256:VAL:O | 1.97 | 0.61 |
| 1:H:122:THR:HG22 | 1:H:126:VAL:CG1 | 2.31 | 0.61 |
| 1:H:132:SER:O | 1:H:133:LEU:HD23 | 2.00 | 0.61 |
| 1:A:254:ASP:C | 1:A:254:ASP:OD1 | 2.33 | 0.61 |
| 1:J:122:THR:HG22 | 1:J:126:VAL:CG1 | 2.31 | 0.61 |
| 1:K:132:SER:O | 1:K:133:LEU:HD23 | 1.99 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:J:204:ILE:HD13 | 1:J:265:VAL:HG21 | 1.82 | 0.61 |
| 1:H:123:ASP:HA | 1:H:127:LEU:HD12 | 1.82 | 0.61 |
| 1:D:122:THR:HG22 | 1:D:126:VAL:CG1 | 2.31 | 0.61 |
| 1:D:132:SER:O | 1:D:133:LEU:HD23 | 2.00 | 0.61 |
| 1:A:204:ILE:HD13 | 1:A:265:VAL:HG21 | 1.82 | 0.61 |
| 1:G:281:LYS:CB | 1:G:281:LYS:NZ | 2.64 | 0.61 |
| 1:E:281:LYS:NZ | 1:E:281:LYS:CB | 2.64 | 0.61 |
| 1:J:284:PHE:HB3 | 1:J:285:GLY:CA | 2.26 | 0.61 |
| 1:K:292:MET:O | 1:K:294:CYS:N | 2.34 | 0.61 |
| 1:J:123:ASP:HA | 1:J:127:LEU:HD12 | 1.81 | 0.61 |
| 1:F:122:THR:HG22 | 1:F:126:VAL:CG1 | 2.31 | 0.61 |
| 1:J:254:ASP:OD1 | 1:J:254:ASP:C | 2.33 | 0.61 |
| 1:B:292:MET:O | 1:B:294:CYS:N | 2.34 | 0.61 |
| 1:C:281:LYS:NZ | 1:C:281:LYS:CB | 2.64 | 0.61 |
| 1:L:123:ASP:HA | 1:L:127:LEU:HD12 | 1.82 | 0.61 |
| 1:G:167:ASP:OD1 | 1:L:160:GLU:N | 2.34 | 0.61 |
| 1:L:292:MET:O | 1:L:294:CYS:N | 2.34 | 0.61 |
| 1:B:256:VAL:HG12 | 1:B:256:VAL:O | 1.97 | 0.61 |
| 1:C:122:THR:HG22 | 1:C:126:VAL:CG1 | 2.30 | 0.61 |
| 1:L:122:THR:HG22 | 1:L:126:VAL:CG1 | 2.31 | 0.61 |
| 1:D:254:ASP:C | 1:D:254:ASP:OD1 | 2.34 | 0.61 |
| 1:F:281:LYS:CB | 1:F:281:LYS:NZ | 2.64 | 0.61 |
| 1:C:123:ASP:HA | 1:C:127:LEU:HD12 | 1.82 | 0.61 |
| 1:F:349:ARG:NH1 | 1:F:349:ARG:HB2 | 2.13 | 0.61 |
| 1:A:123:ASP:HA | 1:A:127:LEU:HD12 | 1.83 | 0.61 |
| 1:I:281:LYS:O | 1:I:282:GLU:HB2 | 2.01 | 0.60 |
| 1:D:292:MET:O | 1:D:294:CYS:N | 2.34 | 0.60 |
| 1:C:292:MET:O | 1:C:294:CYS:N | 2.34 | 0.60 |
| 1:D:284:PHE:HB3 | 1:D:285:GLY:CA | 2.27 | 0.60 |
| 1:H:254:ASP:OD1 | 1:H:254:ASP:C | 2.34 | 0.60 |
| 1:C:254:ASP:C | 1:C:254:ASP:OD1 | 2.33 | 0.60 |
| 1:D:281:LYS:NZ | 1:D:281:LYS:CB | 2.64 | 0.60 |
| 1:E:292:MET:O | 1:E:294:CYS:N | 2.34 | 0.60 |
| 1:I:123:ASP:HA | 1:I:127:LEU:HD12 | 1.82 | 0.60 |
| 1:K:349:ARG:HB2 | 1:K:349:ARG:NH1 | 2.13 | 0.60 |
| 1:E:122:THR:HG22 | 1:E:126:VAL:CG1 | 2.31 | 0.60 |
| 1:D:281:LYS:O | 1:D:282:GLU:HB2 | 2.01 | 0.60 |
| 1:H:182:LYS:HZ1 | 1:H:349:ARG:HD3 | 1.66 | 0.60 |
| 1:I:122:THR:HG22 | 1:I:126:VAL:CG1 | 2.31 | 0.60 |
| 1:I:254:ASP:C | 1:I:254:ASP:OD1 | 2.34 | 0.60 |
| 1:A:122:THR:HG22 | 1:A:126:VAL:CG1 | 2.31 | 0.60 |
| 1:K:212:ARG:HA | 1:K:214:GLN:NE2 | 2.17 | 0.60 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:281:LYS:NZ | 1:A:281:LYS:CB | 2.64 | 0.60 |
| 1:G:292:MET:O | 1:G:294:CYS:N | 2.34 | 0.60 |
| 1:D:123:ASP:HA | 1:D:127:LEU:HD12 | 1.83 | 0.60 |
| 1:F:204:ILE:HD13 | 1:F:265:VAL:HG21 | 1.82 | 0.60 |
| 1:K:281:LYS:CB | 1:K:281:LYS:NZ | 2.64 | 0.60 |
| 1:I:281:LYS:NZ | 1:I:281:LYS:CB | 2.64 | 0.60 |
| 1:H:284:PHE:HB3 | 1:H:285:GLY:CA | 2.27 | 0.60 |
| 1:B:123:ASP:HA | 1:B:127:LEU:HD12 | 1.82 | 0.60 |
| 1:A:281:LYS:O | 1:A:282:GLU:HB2 | 2.01 | 0.60 |
| 1:I:292:MET:O | 1:I:294:CYS:N | 2.34 | 0.60 |
| 1:J:281:LYS:O | 1:J:282:GLU:HB2 | 2.01 | 0.60 |
| 1:E:289:LEU:O | 1:E:290:GLU:C | 2.36 | 0.60 |
| 1:A:292:MET:O | 1:A:294:CYS:N | 2.34 | 0.60 |
| 1:K:281:LYS:O | 1:K:282:GLU:HB2 | 2.01 | 0.60 |
| 1:F:292:MET:O | 1:F:294:CYS:N | 2.34 | 0.60 |
| 1:A:289:LEU:O | 1:A:290:GLU:C | 2.36 | 0.60 |
| 1:G:281:LYS:O | 1:G:282:GLU:HB2 | 2.01 | 0.60 |
| 1:D:289:LEU:O | 1:D:290:GLU:C | 2.36 | 0.60 |
| 1:K:256:VAL:HG12 | 1:K:256:VAL:O | 1.98 | 0.60 |
| 1:F:191:GLU:HG2 | 1:G:50:PRO:HG2 | 1.83 | 0.60 |
| 1:F:289:LEU:O | 1:F:290:GLU:C | 2.36 | 0.60 |
| 1:D:113:ILE:HD13 | 1:D:114:LYS:H | 1.67 | 0.60 |
| 1:K:122:THR:HG22 | 1:K:126:VAL:CG1 | 2.32 | 0.60 |
| 1:L:281:LYS:O | 1:L:282:GLU:HB2 | 2.01 | 0.60 |
| 1:J:292:MET:O | 1:J:294:CYS:N | 2.35 | 0.60 |
| 1:C:256:VAL:O | 1:C:256:VAL:HG12 | 1.97 | 0.60 |
| 1:I:113:ILE:HD13 | 1:I:114:LYS:H | 1.67 | 0.60 |
| 1:A:212:ARG:HA | 1:A:214:GLN:NE2 | 2.17 | 0.59 |
| 1:H:212:ARG:HA | 1:H:214:GLN:NE2 | 2.17 | 0.59 |
| 1:J:287:VAL:O | 1:J:287:VAL:HG23 | 2.02 | 0.59 |
| 1:B:281:LYS:NZ | 1:B:281:LYS:CB | 2.64 | 0.59 |
| 1:J:173:ASN:OD1 | 1:J:284:PHE:CD1 | 2.55 | 0.59 |
| 1:E:94:TYR:CD2 | 1:E:123:ASP:HB3 | 2.37 | 0.59 |
| 1:J:94:TYR:CD2 | 1:J:123:ASP:HB3 | 2.37 | 0.59 |
| 1:L:106:LYS:HG2 | 1:L:111:GLU:HA | 1.84 | 0.59 |
| 1:G:173:ASN:OD1 | 1:G:284:PHE:CD1 | 2.56 | 0.59 |
| 1:A:173:ASN:OD1 | 1:A:284:PHE:CD1 | 2.55 | 0.59 |
| 1:E:212:ARG:HA | 1:E:214:GLN:NE2 | 2.17 | 0.59 |
| 1:C:281:LYS:O | 1:C:282:GLU:HB2 | 2.01 | 0.59 |
| 1:H:292:MET:O | 1:H:294:CYS:N | 2.35 | 0.59 |
| 1:L:254:ASP:C | 1:L:254:ASP:OD1 | 2.33 | 0.59 |
| 1:G:122:THR:HG22 | 1:G:126:VAL:CG1 | 2.31 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:173:ASN:OD1 | 1:B:284:PHE:CD1 | 2.56 | 0.59 |
| 1:B:212:ARG:HA | 1:B:214:GLN:NE2 | 2.17 | 0.59 |
| 1:H:281:LYS:O | 1:H:282:GLU:HB2 | 2.01 | 0.59 |
| 1:F:281:LYS:O | 1:F:282:GLU:HB2 | 2.01 | 0.59 |
| 1:D:173:ASN:OD1 | 1:D:284:PHE:CD1 | 2.56 | 0.59 |
| 1:A:256:VAL:O | 1:A:256:VAL:HG12 | 1.97 | 0.59 |
| 1:E:254:ASP:OD1 | 1:E:254:ASP:C | 2.33 | 0.59 |
| 1:B:106:LYS:HG2 | 1:B:111:GLU:HA | 1.84 | 0.59 |
| 1:J:281:LYS:CB | 1:J:281:LYS:NZ | 2.64 | 0.59 |
| 1:B:113:ILE:HD13 | 1:B:114:LYS:H | 1.67 | 0.59 |
| 1:H:106:LYS:HG2 | 1:H:111:GLU:HA | 1.84 | 0.59 |
| 1:L:173:ASN:OD1 | 1:L:284:PHE:CD1 | 2.55 | 0.59 |
| 1:J:212:ARG:HA | 1:J:214:GLN:NE2 | 2.17 | 0.59 |
| 1:H:94:TYR:CD2 | 1:H:123:ASP:HB3 | 2.37 | 0.59 |
| 1:C:182:LYS:HZ1 | 1:C:349:ARG:HD3 | 1.66 | 0.59 |
| 1:G:250:LEU:HD23 | 1:G:252:ILE:HD11 | 1.85 | 0.59 |
| 1:B:204:ILE:CD1 | 1:B:265:VAL:HG21 | 2.33 | 0.59 |
| 1:G:284:PHE:HB3 | 1:G:285:GLY:CA | 2.26 | 0.59 |
| 1:L:284:PHE:HB3 | 1:L:285:GLY:CA | 2.27 | 0.59 |
| 1:L:333:GLN:HE22 | 1:L:340:LEU:CD2 | 2.16 | 0.59 |
| 1:C:204:ILE:CD1 | 1:C:265:VAL:HG21 | 2.33 | 0.59 |
| 1:I:250:LEU:HD23 | 1:I:252:ILE:HD11 | 1.85 | 0.59 |
| 1:L:113:ILE:HD13 | 1:L:114:LYS:H | 1.68 | 0.59 |
| 1:E:281:LYS:O | 1:E:282:GLU:HB2 | 2.01 | 0.59 |
| 1:B:281:LYS:O | 1:B:282:GLU:HB2 | 2.01 | 0.59 |
| 1:H:173:ASN:OD1 | 1:H:284:PHE:CD1 | 2.56 | 0.59 |
| 1:G:204:ILE:CD1 | 1:G:265:VAL:HG21 | 2.33 | 0.59 |
| 1:A:204:ILE:CD1 | 1:A:265:VAL:HG21 | 2.33 | 0.59 |
| 1:C:250:LEU:HD23 | 1:C:252:ILE:HD11 | 1.85 | 0.59 |
| 1:F:204:ILE:CD1 | 1:F:265:VAL:HG21 | 2.33 | 0.59 |
| 1:J:106:LYS:HG2 | 1:J:111:GLU:HA | 1.84 | 0.59 |
| 1:C:113:ILE:HD13 | 1:C:114:LYS:H | 1.68 | 0.59 |
| 1:F:113:ILE:HD13 | 1:F:114:LYS:H | 1.67 | 0.59 |
| 1:L:121:GLY:O | 1:L:125:THR:OG1 | 2.20 | 0.59 |
| 1:F:212:ARG:HA | 1:F:214:GLN:NE2 | 2.17 | 0.59 |
| 1:F:284:PHE:HB3 | 1:F:285:GLY:CA | 2.27 | 0.59 |
| 1:A:94:TYR:CD2 | 1:A:123:ASP:HB3 | 2.38 | 0.59 |
| 1:I:204:ILE:CD1 | 1:I:265:VAL:HG21 | 2.33 | 0.59 |
| 1:D:106:LYS:HG2 | 1:D:111:GLU:HA | 1.84 | 0.59 |
| 1:G:281:LYS:CB | 1:G:281:LYS:HZ3 | 2.15 | 0.59 |
| 1:I:281:LYS:HZ3 | 1:I:281:LYS:CB | 2.15 | 0.59 |
| 1:C:212:ARG:HA | 1:C:214:GLN:NE2 | 2.17 | 0.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:I:289:LEU:O | 1:I:290:GLU:C | 2.36 | 0.59 |
| 1:C:289:LEU:O | 1:C:290:GLU:C | 2.36 | 0.59 |
| 1:F:333:GLN:HE22 | 1:F:340:LEU:CD2 | 2.16 | 0.59 |
| 1:F:94:TYR:CD2 | 1:F:123:ASP:HB3 | 2.38 | 0.59 |
| 1:K:250:LEU:HD23 | 1:K:252:ILE:HD11 | 1.85 | 0.59 |
| 1:K:204:ILE:CD1 | 1:K:265:VAL:HG21 | 2.33 | 0.59 |
| 1:A:250:LEU:HD23 | 1:A:252:ILE:HD11 | 1.85 | 0.59 |
| 1:E:113:ILE:HD13 | 1:E:114:LYS:H | 1.67 | 0.59 |
| 1:B:254:ASP:OD1 | 1:B:254:ASP:C | 2.34 | 0.59 |
| 1:G:113:ILE:HD13 | 1:G:114:LYS:H | 1.67 | 0.59 |
| 1:L:212:ARG:HA | 1:L:214:GLN:NE2 | 2.17 | 0.58 |
| 1:F:173:ASN:OD1 | 1:F:284:PHE:CD1 | 2.55 | 0.58 |
| 1:B:333:GLN:HE22 | 1:B:340:LEU:CD2 | 2.16 | 0.58 |
| 1:G:333:GLN:HE22 | 1:G:340:LEU:CD2 | 2.16 | 0.58 |
| 1:D:94:TYR:CD2 | 1:D:123:ASP:HB3 | 2.38 | 0.58 |
| 1:G:106:LYS:HG2 | 1:G:111:GLU:HA | 1.84 | 0.58 |
| 1:G:212:ARG:HA | 1:G:214:GLN:NE2 | 2.17 | 0.58 |
| 1:D:287:VAL:O | 1:D:287:VAL:HG23 | 2.03 | 0.58 |
| 1:K:257:LEU:O | 1:K:259:LEU:HD13 | 2.04 | 0.58 |
| 1:E:256:VAL:CG1 | 1:E:258:PHE:CE2 | 2.86 | 0.58 |
| 1:D:333:GLN:HE22 | 1:D:340:LEU:CD2 | 2.16 | 0.58 |
| 1:I:94:TYR:CD2 | 1:I:123:ASP:HB3 | 2.38 | 0.58 |
| 1:G:94:TYR:CD2 | 1:G:123:ASP:HB3 | 2.38 | 0.58 |
| 1:F:250:LEU:HD23 | 1:F:252:ILE:HD11 | 1.85 | 0.58 |
| 1:J:250:LEU:HD23 | 1:J:252:ILE:HD11 | 1.85 | 0.58 |
| 1:L:250:LEU:HD23 | 1:L:252:ILE:HD11 | 1.85 | 0.58 |
| 1:K:113:ILE:HD13 | 1:K:114:LYS:H | 1.68 | 0.58 |
| 1:I:212:ARG:HA | 1:I:214:GLN:NE2 | 2.17 | 0.58 |
| 1:B:94:TYR:CD2 | 1:B:123:ASP:HB3 | 2.38 | 0.58 |
| 1:D:204:ILE:CD1 | 1:D:265:VAL:HG21 | 2.33 | 0.58 |
| 1:E:173:ASN:OD1 | 1:E:284:PHE:CD1 | 2.56 | 0.58 |
| 1:F:290:GLU:O | 1:F:293:ALA:HB3 | 2.04 | 0.58 |
| 1:J:257:LEU:O | 1:J:259:LEU:HD13 | 2.04 | 0.58 |
| 1:L:94:TYR:CD2 | 1:L:123:ASP:HB3 | 2.38 | 0.58 |
| 1:F:182:LYS:HZ1 | 1:F:349:ARG:HD3 | 1.67 | 0.58 |
| 1:K:96:ILE:CG2 | 1:L:65:PHE:HZ | 2.17 | 0.58 |
| 1:A:290:GLU:O | 1:A:293:ALA:HB3 | 2.04 | 0.58 |
| 1:I:173:ASN:OD1 | 1:I:284:PHE:CD1 | 2.56 | 0.58 |
| 1:D:212:ARG:HA | 1:D:214:GLN:NE2 | 2.17 | 0.58 |
| 1:E:333:GLN:HE22 | 1:E:340:LEU:CD2 | 2.16 | 0.58 |
| 1:J:204:ILE:CD1 | 1:J:265:VAL:HG21 | 2.34 | 0.58 |
| 1:F:106:LYS:HG2 | 1:F:111:GLU:HA | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:C:106:LYS:HG2 | 1:C:111:GLU:HA | 1.84 | 0.58 |
| 1:H:113:ILE:HD13 | 1:H:114:LYS:H | 1.67 | 0.58 |
| 1:A:257:LEU:O | 1:A:259:LEU:HD13 | 2.04 | 0.58 |
| 1:D:250:LEU:HD23 | 1:D:252:ILE:HD11 | 1.85 | 0.58 |
| 1:C:290:GLU:O | 1:C:293:ALA:HB3 | 2.04 | 0.58 |
| 1:H:333:GLN:HE22 | 1:H:340:LEU:CD2 | 2.16 | 0.58 |
| 1:E:106:LYS:HG2 | 1:E:111:GLU:HA | 1.84 | 0.58 |
| 1:C:287:VAL:HG23 | 1:C:287:VAL:O | 2.04 | 0.58 |
| 1:I:333:GLN:HE22 | 1:I:340:LEU:CD2 | 2.16 | 0.58 |
| 1:A:113:ILE:HD13 | 1:A:114:LYS:H | 1.67 | 0.58 |
| 1:G:257:LEU:O | 1:G:259:LEU:HD13 | 2.04 | 0.58 |
| 1:A:256:VAL:CG1 | 1:A:258:PHE:CE2 | 2.87 | 0.58 |
| 1:B:257:LEU:O | 1:B:259:LEU:HD13 | 2.04 | 0.58 |
| 1:K:333:GLN:HE22 | 1:K:340:LEU:CD2 | 2.17 | 0.58 |
| 1:C:333:GLN:HE22 | 1:C:340:LEU:CD2 | 2.16 | 0.58 |
| 1:E:204:ILE:CD1 | 1:E:265:VAL:HG21 | 2.33 | 0.58 |
| 1:L:204:ILE:CD1 | 1:L:265:VAL:HG21 | 2.33 | 0.58 |
| 1:H:204:ILE:CD1 | 1:H:265:VAL:HG21 | 2.33 | 0.58 |
| 1:H:250:LEU:HD23 | 1:H:252:ILE:HD11 | 1.85 | 0.58 |
| 1:I:287:VAL:O | 1:I:287:VAL:HG23 | 2.03 | 0.58 |
| 1:C:257:LEU:O | 1:C:259:LEU:HD13 | 2.04 | 0.58 |
| 1:A:333:GLN:HE22 | 1:A:340:LEU:CD2 | 2.16 | 0.58 |
| 1:B:250:LEU:HD23 | 1:B:252:ILE:HD11 | 1.85 | 0.58 |
| 1:K:106:LYS:HG2 | 1:K:111:GLU:HA | 1.84 | 0.58 |
| 1:K:290:GLU:O | 1:K:293:ALA:HB3 | 2.04 | 0.57 |
| 1:C:317:TYR:HE1 | 1:C:334:LEU:HD22 | 1.69 | 0.57 |
| 1:J:290:GLU:O | 1:J:293:ALA:HB3 | 2.04 | 0.57 |
| 1:G:287:VAL:HG23 | 1:G:287:VAL:O | 2.03 | 0.57 |
| 1:D:257:LEU:O | 1:D:259:LEU:HD13 | 2.05 | 0.57 |
| 1:C:94:TYR:CD2 | 1:C:123:ASP:HB3 | 2.38 | 0.57 |
| 1:A:106:LYS:HG2 | 1:A:111:GLU:HA | 1.84 | 0.57 |
| 1:C:256:VAL:CG1 | 1:C:258:PHE:CE2 | 2.87 | 0.57 |
| 1:I:256:VAL:O | 1:I:256:VAL:HG12 | 1.97 | 0.57 |
| 1:B:289:LEU:O | 1:B:290:GLU:C | 2.36 | 0.57 |
| 1:D:292:MET:O | 1:D:293:ALA:C | 2.42 | 0.57 |
| 1:K:256:VAL:CG1 | 1:K:258:PHE:CE2 | 2.87 | 0.57 |
| 1:E:257:LEU:O | 1:E:259:LEU:HD13 | 2.04 | 0.57 |
| 1:J:182:LYS:NZ | 1:J:349:ARG:HD3 | 2.19 | 0.57 |
| 1:B:306:ILE:H | 1:B:307:PRO:CD | 2.18 | 0.57 |
| 1:J:113:ILE:HD13 | 1:J:114:LYS:H | 1.68 | 0.57 |
| 1:I:290:GLU:O | 1:I:293:ALA:HB3 | 2.04 | 0.57 |
| 1:H:290:GLU:O | 1:H:293:ALA:HB3 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:F:256:VAL:CG1 | 1:F:258:PHE:CE2 | 2.87 | 0.57 |
| 1:L:256:VAL:CG1 | 1:L:258:PHE:CE2 | 2.88 | 0.57 |
| 1:K:332:ILE:HD12 | 1:K:333:GLN:N | 2.20 | 0.57 |
| 1:H:317:TYR:HE1 | 1:H:334:LEU:HD22 | 1.69 | 0.57 |
| 1:G:182:LYS:NZ | 1:G:349:ARG:HD3 | 2.20 | 0.57 |
| 1:H:94:TYR:CZ | 1:H:123:ASP:HB3 | 2.40 | 0.57 |
| 1:K:94:TYR:CD2 | 1:K:123:ASP:HB3 | 2.39 | 0.57 |
| 1:E:250:LEU:HD23 | 1:E:252:ILE:HD11 | 1.85 | 0.57 |
| 1:K:173:ASN:OD1 | 1:K:284:PHE:CD1 | 2.58 | 0.57 |
| 1:B:256:VAL:CG1 | 1:B:258:PHE:CE2 | 2.87 | 0.57 |
| 1:D:256:VAL:CG1 | 1:D:258:PHE:CE2 | 2.87 | 0.57 |
| 1:A:317:TYR:HE1 | 1:A:334:LEU:HD22 | 1.69 | 0.57 |
| 1:G:332:ILE:HD12 | 1:G:333:GLN:N | 2.20 | 0.57 |
| 1:J:332:ILE:HD12 | 1:J:333:GLN:N | 2.20 | 0.57 |
| 1:J:317:TYR:HE1 | 1:J:334:LEU:HD22 | 1.69 | 0.57 |
| 1:A:306:ILE:H | 1:A:307:PRO:CD | 2.17 | 0.57 |
| 1:H:306:ILE:H | 1:H:307:PRO:CD | 2.18 | 0.57 |
| 1:G:167:ASP:CG | 1:L:160:GLU:CA | 2.67 | 0.57 |
| 1:A:275:MET:SD | 1:A:287:VAL:CG2 | 2.93 | 0.57 |
| 1:L:275:MET:SD | 1:L:287:VAL:CG2 | 2.93 | 0.57 |
| 1:H:275:MET:SD | 1:H:287:VAL:CG2 | 2.93 | 0.57 |
| 1:L:257:LEU:O | 1:L:259:LEU:HD13 | 2.05 | 0.57 |
| 1:F:317:TYR:HE1 | 1:F:334:LEU:HD22 | 1.69 | 0.57 |
| 1:H:284:PHE:C | 1:H:284:PHE:CD2 | 2.75 | 0.57 |
| 1:L:290:GLU:O | 1:L:293:ALA:HB3 | 2.04 | 0.57 |
| 1:G:256:VAL:CG1 | 1:G:258:PHE:CE2 | 2.87 | 0.57 |
| 1:J:333:GLN:HE22 | 1:J:340:LEU:CD2 | 2.17 | 0.57 |
| 1:B:182:LYS:NZ | 1:B:349:ARG:HD3 | 2.20 | 0.57 |
| 1:K:284:PHE:HB3 | 1:K:285:GLY:CA | 2.28 | 0.57 |
| 1:E:290:GLU:O | 1:E:293:ALA:HB3 | 2.04 | 0.57 |
| 1:H:257:LEU:O | 1:H:259:LEU:HD13 | 2.04 | 0.57 |
| 1:C:182:LYS:NZ | 1:C:349:ARG:HD3 | 2.20 | 0.57 |
| 1:L:182:LYS:NZ | 1:L:349:ARG:HD3 | 2.20 | 0.57 |
| 1:B:290:GLU:O | 1:B:293:ALA:HB3 | 2.04 | 0.57 |
| 1:A:284:PHE:HB3 | 1:A:285:GLY:CA | 2.27 | 0.57 |
| 1:I:332:ILE:HD12 | 1:I:333:GLN:N | 2.20 | 0.57 |
| 1:A:332:ILE:HD12 | 1:A:333:GLN:N | 2.20 | 0.57 |
| 1:L:332:ILE:HD12 | 1:L:333:GLN:N | 2.20 | 0.57 |
| 1:B:317:TYR:HE1 | 1:B:334:LEU:HD22 | 1.69 | 0.57 |
| 1:D:332:ILE:HD12 | 1:D:333:GLN:N | 2.20 | 0.57 |
| 1:K:182:LYS:NZ | 1:K:349:ARG:HD3 | 2.19 | 0.57 |
| 1:I:106:LYS:HG2 | 1:I:111:GLU:HA | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:J:292:MET:O | 1:J:293:ALA:C | 2.43 | 0.56 |
| 1:G:290:GLU:O | 1:G:293:ALA:HB3 | 2.04 | 0.56 |
| 1:H:256:VAL:CG1 | 1:H:258:PHE:CE2 | 2.87 | 0.56 |
| 1:H:332:ILE:HD12 | 1:H:333:GLN:N | 2.20 | 0.56 |
| 1:F:332:ILE:HD12 | 1:F:333:GLN:N | 2.20 | 0.56 |
| 1:F:182:LYS:NZ | 1:F:349:ARG:HD3 | 2.20 | 0.56 |
| 1:I:306:ILE:H | 1:I:307:PRO:CD | 2.18 | 0.56 |
| 1:G:306:ILE:H | 1:G:307:PRO:CD | 2.17 | 0.56 |
| 1:E:173:ASN:HB2 | 1:E:284:PHE:HE1 | 1.71 | 0.56 |
| 1:I:292:MET:O | 1:I:293:ALA:C | 2.42 | 0.56 |
| 1:E:292:MET:O | 1:E:293:ALA:C | 2.42 | 0.56 |
| 1:I:312:HIS:NE2 | 1:I:317:TYR:HD2 | 2.03 | 0.56 |
| 1:B:332:ILE:HD12 | 1:B:333:GLN:N | 2.20 | 0.56 |
| 1:D:317:TYR:HE1 | 1:D:334:LEU:HD22 | 1.69 | 0.56 |
| 1:F:287:VAL:O | 1:F:287:VAL:HG23 | 2.03 | 0.56 |
| 1:I:317:TYR:HE1 | 1:I:334:LEU:HD22 | 1.69 | 0.56 |
| 1:C:312:HIS:NE2 | 1:C:317:TYR:HD2 | 2.04 | 0.56 |
| 1:E:317:TYR:HE1 | 1:E:334:LEU:HD22 | 1.69 | 0.56 |
| 1:G:317:TYR:HE1 | 1:G:334:LEU:HD22 | 1.69 | 0.56 |
| 1:F:306:ILE:H | 1:F:307:PRO:CD | 2.18 | 0.56 |
| 1:L:306:ILE:H | 1:L:307:PRO:CD | 2.18 | 0.56 |
| 1:D:182:LYS:NZ | 1:D:349:ARG:HD3 | 2.20 | 0.56 |
| 1:A:182:LYS:NZ | 1:A:349:ARG:HD3 | 2.20 | 0.56 |
| 1:K:177:GLU:HG3 | 1:K:357:ARG:NH1 | 2.20 | 0.56 |
| 1:H:119:LEU:HD22 | 1:H:124:ILE:HD11 | 1.88 | 0.56 |
| 1:C:292:MET:O | 1:C:293:ALA:C | 2.42 | 0.56 |
| 1:E:275:MET:SD | 1:E:287:VAL:CG2 | 2.94 | 0.56 |
| 1:E:292:MET:O | 1:E:295:GLY:N | 2.37 | 0.56 |
| 1:G:275:MET:SD | 1:G:287:VAL:CG2 | 2.93 | 0.56 |
| 1:H:312:HIS:NE2 | 1:H:317:TYR:HD2 | 2.03 | 0.56 |
| 1:L:317:TYR:HE1 | 1:L:334:LEU:HD22 | 1.69 | 0.56 |
| 1:I:182:LYS:NZ | 1:I:349:ARG:HD3 | 2.20 | 0.56 |
| 1:E:182:LYS:NZ | 1:E:349:ARG:HD3 | 2.20 | 0.56 |
| 1:D:254:ASP:N | 1:D:254:ASP:OD1 | 2.36 | 0.56 |
| 1:I:257:LEU:O | 1:I:259:LEU:HD13 | 2.04 | 0.56 |
| 1:I:317:TYR:OH | 1:I:340:LEU:HD21 | 2.06 | 0.56 |
| 1:B:254:ASP:OD1 | 1:B:254:ASP:N | 2.36 | 0.56 |
| 1:G:119:LEU:HD22 | 1:G:124:ILE:HD11 | 1.88 | 0.56 |
| 1:D:290:GLU:O | 1:D:293:ALA:HB3 | 2.04 | 0.56 |
| 1:H:173:ASN:HB2 | 1:H:284:PHE:HE1 | 1.71 | 0.56 |
| 1:F:257:LEU:O | 1:F:259:LEU:HD13 | 2.04 | 0.56 |
| 1:A:317:TYR:OH | 1:A:340:LEU:HD21 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:L:317:TYR:OH | 1:L:340:LEU:HD21 | 2.06 | 0.56 |
| 1:E:332:ILE:HD12 | 1:E:333:GLN:N | 2.20 | 0.56 |
| 1:C:173:ASN:OD1 | 1:C:284:PHE:CD1 | 2.58 | 0.56 |
| 1:F:275:MET:SD | 1:F:287:VAL:CG2 | 2.93 | 0.56 |
| 1:D:275:MET:SD | 1:D:287:VAL:CG2 | 2.93 | 0.56 |
| 1:K:286:LEU:CD1 | 1:K:286:LEU:N | 2.31 | 0.56 |
| 1:C:332:ILE:HD12 | 1:C:333:GLN:N | 2.20 | 0.56 |
| 1:H:182:LYS:NZ | 1:H:349:ARG:HD3 | 2.20 | 0.56 |
| 1:E:119:LEU:HD22 | 1:E:124:ILE:HD11 | 1.87 | 0.56 |
| 1:J:256:VAL:CG1 | 1:J:258:PHE:CE2 | 2.87 | 0.56 |
| 1:B:317:TYR:OH | 1:B:340:LEU:HD21 | 2.06 | 0.56 |
| 1:C:317:TYR:OH | 1:C:340:LEU:HD21 | 2.06 | 0.56 |
| 1:J:306:ILE:H | 1:J:307:PRO:CD | 2.18 | 0.56 |
| 1:G:94:TYR:CZ | 1:G:123:ASP:HB3 | 2.41 | 0.56 |
| 1:D:119:LEU:HD22 | 1:D:124:ILE:HD11 | 1.88 | 0.56 |
| 1:B:275:MET:SD | 1:B:287:VAL:CG2 | 2.93 | 0.56 |
| 1:C:286:LEU:CD1 | 1:C:286:LEU:N | 2.31 | 0.56 |
| 1:J:312:HIS:NE2 | 1:J:317:TYR:HD2 | 2.04 | 0.56 |
| 1:E:306:ILE:H | 1:E:307:PRO:CD | 2.18 | 0.56 |
| 1:I:121:GLY:O | 1:I:125:THR:OG1 | 2.20 | 0.56 |
| 1:J:202:ILE:HD13 | 1:J:203:HIS:N | 2.21 | 0.56 |
| 1:C:284:PHE:C | 1:C:284:PHE:CD2 | 2.74 | 0.56 |
| 1:E:287:VAL:HG23 | 1:E:287:VAL:O | 2.03 | 0.56 |
| 1:H:292:MET:O | 1:H:293:ALA:C | 2.43 | 0.56 |
| 1:F:312:HIS:NE2 | 1:F:317:TYR:HD2 | 2.04 | 0.56 |
| 1:F:317:TYR:OH | 1:F:340:LEU:HD21 | 2.06 | 0.56 |
| 1:I:94:TYR:CZ | 1:I:123:ASP:HB3 | 2.41 | 0.56 |
| 1:B:202:ILE:HD13 | 1:B:203:HIS:N | 2.21 | 0.56 |
| 1:A:292:MET:O | 1:A:293:ALA:C | 2.42 | 0.55 |
| 1:L:312:HIS:NE2 | 1:L:317:TYR:HD2 | 2.04 | 0.55 |
| 1:B:312:HIS:NE2 | 1:B:317:TYR:HD2 | 2.04 | 0.55 |
| 1:B:177:GLU:HG3 | 1:B:357:ARG:NH1 | 2.22 | 0.55 |
| 1:E:121:GLY:O | 1:E:125:THR:OG1 | 2.20 | 0.55 |
| 1:G:173:ASN:HB2 | 1:G:284:PHE:HE1 | 1.71 | 0.55 |
| 1:I:173:ASN:HB2 | 1:I:284:PHE:HE1 | 1.71 | 0.55 |
| 1:F:94:TYR:CZ | 1:F:123:ASP:HB3 | 2.41 | 0.55 |
| 1:A:177:GLU:HG3 | 1:A:357:ARG:NH1 | 2.22 | 0.55 |
| 1:K:317:TYR:HE1 | 1:K:334:LEU:HD22 | 1.70 | 0.55 |
| 1:L:94:TYR:CZ | 1:L:123:ASP:HB3 | 2.41 | 0.55 |
| 1:E:94:TYR:CZ | 1:E:123:ASP:HB3 | 2.40 | 0.55 |
| 1:D:202:ILE:HD13 | 1:D:203:HIS:N | 2.22 | 0.55 |
| 1:L:202:ILE:HD13 | 1:L:203:HIS:N | 2.22 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:292:MET:O | 1:B:293:ALA:C | 2.42 | 0.55 |
| 1:C:275:MET:SD | 1:C:287:VAL:CG2 | 2.94 | 0.55 |
| 1:K:275:MET:SD | 1:K:287:VAL:CG2 | 2.94 | 0.55 |
| 1:K:287:VAL:HG23 | 1:K:287:VAL:O | 2.04 | 0.55 |
| 1:G:317:TYR:OH | 1:G:340:LEU:HD21 | 2.06 | 0.55 |
| 1:C:94:TYR:CZ | 1:C:123:ASP:HB3 | 2.41 | 0.55 |
| 1:C:177:GLU:HG3 | 1:C:357:ARG:NH1 | 2.22 | 0.55 |
| 1:F:177:GLU:HG3 | 1:F:357:ARG:NH1 | 2.22 | 0.55 |
| 1:I:177:GLU:HG3 | 1:I:357:ARG:NH1 | 2.22 | 0.55 |
| 1:J:122:THR:HG22 | 1:J:126:VAL:HG11 | 1.89 | 0.55 |
| 1:F:119:LEU:HD22 | 1:F:124:ILE:HD11 | 1.88 | 0.55 |
| 1:H:202:ILE:HD13 | 1:H:203:HIS:N | 2.22 | 0.55 |
| 1:A:173:ASN:HB2 | 1:A:284:PHE:HE1 | 1.72 | 0.55 |
| 1:F:292:MET:O | 1:F:293:ALA:C | 2.42 | 0.55 |
| 1:K:292:MET:O | 1:K:293:ALA:C | 2.42 | 0.55 |
| 1:E:317:TYR:OH | 1:E:340:LEU:HD21 | 2.06 | 0.55 |
| 1:G:312:HIS:NE2 | 1:G:317:TYR:HD2 | 2.04 | 0.55 |
| 1:C:306:ILE:H | 1:C:307:PRO:CD | 2.18 | 0.55 |
| 1:D:177:GLU:HG3 | 1:D:357:ARG:NH1 | 2.22 | 0.55 |
| 1:J:177:GLU:HG3 | 1:J:357:ARG:NH1 | 2.22 | 0.55 |
| 1:A:202:ILE:HD13 | 1:A:203:HIS:N | 2.22 | 0.55 |
| 1:I:275:MET:SD | 1:I:287:VAL:CG2 | 2.94 | 0.55 |
| 1:B:173:ASN:HB2 | 1:B:284:PHE:HE1 | 1.71 | 0.55 |
| 1:A:94:TYR:CZ | 1:A:123:ASP:HB3 | 2.41 | 0.55 |
| 1:D:122:THR:HG22 | 1:D:126:VAL:HG11 | 1.89 | 0.55 |
| 1:B:121:GLY:O | 1:B:125:THR:OG1 | 2.20 | 0.55 |
| 1:C:156:ASN:OD1 | 1:I:163:LYS:HA | 2.06 | 0.55 |
| 1:B:178:ARG:NE | 1:B:178:ARG:HA | 2.22 | 0.55 |
| 1:B:292:MET:O | 1:B:295:GLY:N | 2.36 | 0.55 |
| 1:H:287:VAL:HG23 | 1:H:287:VAL:O | 2.04 | 0.55 |
| 1:I:256:VAL:CG1 | 1:I:258:PHE:CE2 | 2.88 | 0.55 |
| 1:L:312:HIS:C | 1:L:312:HIS:CD2 | 2.80 | 0.55 |
| 1:D:317:TYR:OH | 1:D:340:LEU:HD21 | 2.06 | 0.55 |
| 1:K:306:ILE:H | 1:K:307:PRO:CD | 2.19 | 0.55 |
| 1:B:94:TYR:CZ | 1:B:123:ASP:HB3 | 2.41 | 0.55 |
| 1:L:177:GLU:HG3 | 1:L:357:ARG:NH1 | 2.22 | 0.55 |
| 1:H:122:THR:HG22 | 1:H:126:VAL:HG11 | 1.89 | 0.55 |
| 1:E:122:THR:HG22 | 1:E:126:VAL:HG11 | 1.89 | 0.55 |
| 1:G:284:PHE:C | 1:G:284:PHE:CD2 | 2.75 | 0.55 |
| 1:E:284:PHE:HB3 | 1:E:285:GLY:CA | 2.27 | 0.55 |
| 1:E:312:HIS:NE2 | 1:E:317:TYR:HD2 | 2.04 | 0.55 |
| 1:J:317:TYR:OH | 1:J:340:LEU:HD21 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:94:TYR:CZ | 1:D:123:ASP:HB3 | 2.41 | 0.55 |
| 1:G:202:ILE:HD13 | 1:G:203:HIS:N | 2.22 | 0.55 |
| 1:A:119:LEU:HD22 | 1:A:124:ILE:HD11 | 1.88 | 0.55 |
| 1:F:178:ARG:HA | 1:F:178:ARG:NE | 2.22 | 0.55 |
| 1:E:177:GLU:HG3 | 1:E:357:ARG:NH1 | 2.22 | 0.55 |
| 1:L:178:ARG:NE | 1:L:178:ARG:HA | 2.22 | 0.55 |
| 1:H:178:ARG:HA | 1:H:178:ARG:NE | 2.22 | 0.55 |
| 1:C:178:ARG:HA | 1:C:178:ARG:NE | 2.22 | 0.55 |
| 1:B:119:LEU:HD22 | 1:B:124:ILE:HD11 | 1.88 | 0.55 |
| 1:A:173:ASN:OD1 | 1:A:284:PHE:HD1 | 1.91 | 0.54 |
| 1:K:312:HIS:NE2 | 1:K:317:TYR:HD2 | 2.04 | 0.54 |
| 1:D:312:HIS:NE2 | 1:D:317:TYR:HD2 | 2.04 | 0.54 |
| 1:G:254:ASP:OD1 | 1:G:254:ASP:N | 2.36 | 0.54 |
| 1:I:119:LEU:HD22 | 1:I:124:ILE:HD11 | 1.88 | 0.54 |
| 1:I:202:ILE:HD13 | 1:I:203:HIS:N | 2.22 | 0.54 |
| 1:E:202:ILE:HD13 | 1:E:203:HIS:N | 2.22 | 0.54 |
| 1:I:178:ARG:NE | 1:I:178:ARG:HA | 2.23 | 0.54 |
| 1:K:281:LYS:HZ3 | 1:K:281:LYS:CB | 2.19 | 0.54 |
| 1:K:284:PHE:C | 1:K:284:PHE:CD2 | 2.75 | 0.54 |
| 1:F:173:ASN:HB2 | 1:F:284:PHE:HE1 | 1.72 | 0.54 |
| 1:D:173:ASN:HB2 | 1:D:284:PHE:HE1 | 1.72 | 0.54 |
| 1:L:292:MET:O | 1:L:293:ALA:C | 2.42 | 0.54 |
| 1:D:306:ILE:H | 1:D:307:PRO:CD | 2.19 | 0.54 |
| 1:L:119:LEU:HD22 | 1:L:124:ILE:HD11 | 1.88 | 0.54 |
| 1:J:178:ARG:HA | 1:J:178:ARG:NE | 2.22 | 0.54 |
| 1:C:173:ASN:HB2 | 1:C:284:PHE:HE1 | 1.71 | 0.54 |
| 1:L:173:ASN:HB2 | 1:L:284:PHE:HE1 | 1.73 | 0.54 |
| 1:G:292:MET:O | 1:G:293:ALA:C | 2.42 | 0.54 |
| 1:G:177:GLU:HG3 | 1:G:357:ARG:NH1 | 2.22 | 0.54 |
| 1:C:122:THR:HG22 | 1:C:126:VAL:HG11 | 1.89 | 0.54 |
| 1:G:122:THR:HG22 | 1:G:126:VAL:HG11 | 1.89 | 0.54 |
| 1:I:284:PHE:C | 1:I:284:PHE:CD2 | 2.76 | 0.54 |
| 1:H:177:GLU:HG3 | 1:H:357:ARG:NH1 | 2.22 | 0.54 |
| 1:C:119:LEU:HD22 | 1:C:124:ILE:HD11 | 1.88 | 0.54 |
| 1:C:202:ILE:HD13 | 1:C:203:HIS:N | 2.22 | 0.54 |
| 1:G:178:ARG:NE | 1:G:178:ARG:HA | 2.22 | 0.54 |
| 1:A:287:VAL:O | 1:A:287:VAL:HG23 | 2.03 | 0.54 |
| 1:J:284:PHE:C | 1:J:284:PHE:CD2 | 2.77 | 0.54 |
| 1:J:275:MET:SD | 1:J:287:VAL:CG2 | 2.96 | 0.54 |
| 1:H:317:TYR:OH | 1:H:340:LEU:HD21 | 2.06 | 0.54 |
| 1:F:122:THR:HG22 | 1:F:126:VAL:HG11 | 1.89 | 0.54 |
| 1:L:254:ASP:N | 1:L:254:ASP:OD1 | 2.36 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:178:ARG:HA | 1:D:178:ARG:NE | 2.22 | 0.54 |
| 1:E:178:ARG:HA | 1:E:178:ARG:NE | 2.22 | 0.54 |
| 1:B:287:VAL:O | 1:B:287:VAL:HG23 | 2.04 | 0.54 |
| 1:D:286:LEU:N | 1:D:286:LEU:CD1 | 2.31 | 0.54 |
| 1:I:349:ARG:CB | 1:I:349:ARG:HH11 | 2.19 | 0.54 |
| 1:J:94:TYR:CZ | 1:J:123:ASP:HB3 | 2.41 | 0.54 |
| 1:K:306:ILE:O | 1:K:309:VAL:HG22 | 2.08 | 0.54 |
| 1:F:256:VAL:O | 1:F:256:VAL:HG12 | 1.97 | 0.54 |
| 1:A:349:ARG:CB | 1:A:349:ARG:HH11 | 2.19 | 0.54 |
| 1:L:122:THR:HG22 | 1:L:126:VAL:HG11 | 1.89 | 0.54 |
| 1:K:119:LEU:HD22 | 1:K:124:ILE:HD11 | 1.88 | 0.54 |
| 1:J:173:ASN:HB2 | 1:J:284:PHE:HE1 | 1.72 | 0.54 |
| 1:A:312:HIS:NE2 | 1:A:317:TYR:HD2 | 2.05 | 0.54 |
| 1:H:223:ILE:O | 1:H:223:ILE:HD13 | 2.08 | 0.54 |
| 1:G:156:ASN:OD1 | 1:L:152:HIS:ND1 | 2.41 | 0.54 |
| 1:J:254:ASP:N | 1:J:254:ASP:OD1 | 2.37 | 0.54 |
| 1:H:121:GLY:O | 1:H:125:THR:OG1 | 2.19 | 0.54 |
| 1:B:284:PHE:CD2 | 1:B:284:PHE:C | 2.76 | 0.54 |
| 1:G:292:MET:O | 1:G:295:GLY:N | 2.36 | 0.54 |
| 1:F:223:ILE:O | 1:F:223:ILE:HD13 | 2.08 | 0.54 |
| 1:D:223:ILE:O | 1:D:223:ILE:HD13 | 2.08 | 0.54 |
| 1:F:202:ILE:HD13 | 1:F:203:HIS:N | 2.22 | 0.54 |
| 1:K:139:PHE:O | 1:K:143:GLN:HG2 | 2.08 | 0.54 |
| 1:K:178:ARG:HA | 1:K:178:ARG:NE | 2.22 | 0.54 |
| 1:L:284:PHE:CD2 | 1:L:284:PHE:C | 2.76 | 0.54 |
| 1:K:317:TYR:OH | 1:K:340:LEU:HD21 | 2.08 | 0.54 |
| 1:I:223:ILE:O | 1:I:223:ILE:HD13 | 2.08 | 0.54 |
| 1:A:223:ILE:O | 1:A:223:ILE:HD13 | 2.08 | 0.54 |
| 1:D:121:GLY:O | 1:D:125:THR:OG1 | 2.20 | 0.54 |
| 1:L:173:ASN:OD1 | 1:L:284:PHE:HD1 | 1.90 | 0.53 |
| 1:C:292:MET:O | 1:C:295:GLY:N | 2.37 | 0.53 |
| 1:L:223:ILE:O | 1:L:223:ILE:HD13 | 2.08 | 0.53 |
| 1:K:94:TYR:CZ | 1:K:123:ASP:HB3 | 2.42 | 0.53 |
| 1:J:119:LEU:HD22 | 1:J:124:ILE:HD11 | 1.89 | 0.53 |
| 1:A:178:ARG:HA | 1:A:178:ARG:NE | 2.22 | 0.53 |
| 1:K:173:ASN:HB2 | 1:K:284:PHE:HE1 | 1.74 | 0.53 |
| 1:F:292:MET:O | 1:F:295:GLY:N | 2.37 | 0.53 |
| 1:H:312:HIS:CD2 | 1:H:312:HIS:C | 2.81 | 0.53 |
| 1:G:223:ILE:O | 1:G:223:ILE:HD13 | 2.08 | 0.53 |
| 1:K:364:GLN:O | 1:K:368:ILE:HG13 | 2.09 | 0.53 |
| 1:A:312:HIS:C | 1:A:312:HIS:CD2 | 2.80 | 0.53 |
| 1:C:223:ILE:O | 1:C:223:ILE:HD13 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:J:246:LEU:O | 1:J:250:LEU:HB2 | 2.09 | 0.53 |
| 1:K:202:ILE:HD13 | 1:K:203:HIS:N | 2.22 | 0.53 |
| 1:B:223:ILE:HD13 | 1:B:223:ILE:O | 2.08 | 0.53 |
| 1:E:312:HIS:CD2 | 1:E:312:HIS:C | 2.81 | 0.53 |
| 1:J:223:ILE:HD13 | 1:J:223:ILE:O | 2.09 | 0.53 |
| 1:B:122:THR:HG22 | 1:B:126:VAL:HG11 | 1.89 | 0.53 |
| 1:L:292:MET:O | 1:L:295:GLY:N | 2.37 | 0.53 |
| 1:I:312:HIS:C | 1:I:312:HIS:CD2 | 2.81 | 0.53 |
| 1:J:312:HIS:C | 1:J:312:HIS:CD2 | 2.81 | 0.53 |
| 1:F:284:PHE:C | 1:F:284:PHE:CD2 | 2.75 | 0.53 |
| 1:C:312:HIS:CD2 | 1:C:312:HIS:C | 2.81 | 0.53 |
| 1:J:349:ARG:CB | 1:J:349:ARG:HH11 | 2.19 | 0.53 |
| 1:C:349:ARG:CB | 1:C:349:ARG:HH11 | 2.19 | 0.53 |
| 1:F:349:ARG:HH11 | 1:F:349:ARG:CB | 2.19 | 0.53 |
| 1:A:182:LYS:HZ1 | 1:A:349:ARG:HD3 | 1.73 | 0.53 |
| 1:D:292:MET:O | 1:D:295:GLY:N | 2.37 | 0.53 |
| 1:L:287:VAL:O | 1:L:287:VAL:HG23 | 2.04 | 0.53 |
| 1:G:286:LEU:N | 1:G:286:LEU:CD1 | 2.31 | 0.53 |
| 1:K:257:LEU:O | 1:K:259:LEU:HD12 | 2.09 | 0.53 |
| 1:C:257:LEU:O | 1:C:259:LEU:HD12 | 2.09 | 0.53 |
| 1:L:182:LYS:HZ1 | 1:L:349:ARG:HD3 | 1.73 | 0.53 |
| 1:K:122:THR:HG22 | 1:K:126:VAL:HG11 | 1.90 | 0.53 |
| 1:H:257:LEU:O | 1:H:259:LEU:HD12 | 2.09 | 0.53 |
| 1:B:312:HIS:CD2 | 1:B:312:HIS:C | 2.81 | 0.53 |
| 1:B:246:LEU:O | 1:B:250:LEU:HB2 | 2.09 | 0.53 |
| 1:A:139:PHE:O | 1:A:143:GLN:HG2 | 2.09 | 0.53 |
| 1:B:281:LYS:CB | 1:B:281:LYS:HZ3 | 2.22 | 0.53 |
| 1:H:256:VAL:O | 1:H:256:VAL:HG12 | 1.97 | 0.53 |
| 1:D:312:HIS:C | 1:D:312:HIS:CD2 | 2.81 | 0.53 |
| 1:C:306:ILE:O | 1:C:309:VAL:HG22 | 2.09 | 0.53 |
| 1:F:246:LEU:O | 1:F:250:LEU:HB2 | 2.09 | 0.53 |
| 1:H:364:GLN:O | 1:H:368:ILE:HG13 | 2.09 | 0.53 |
| 1:F:173:ASN:OD1 | 1:F:284:PHE:HD1 | 1.91 | 0.53 |
| 1:J:306:ILE:O | 1:J:309:VAL:HG22 | 2.09 | 0.53 |
| 1:E:189:LYS:O | 1:E:194:ILE:HG22 | 2.09 | 0.53 |
| 1:A:189:LYS:O | 1:A:194:ILE:HG22 | 2.09 | 0.53 |
| 1:E:364:GLN:O | 1:E:368:ILE:HG13 | 2.09 | 0.53 |
| 1:E:257:LEU:O | 1:E:259:LEU:HD12 | 2.09 | 0.52 |
| 1:H:139:PHE:O | 1:H:143:GLN:HG2 | 2.10 | 0.52 |
| 1:A:364:GLN:O | 1:A:368:ILE:HG13 | 2.09 | 0.52 |
| 1:A:284:PHE:CD2 | 1:A:284:PHE:C | 2.76 | 0.52 |
| 1:I:281:LYS:HB2 | 1:I:281:LYS:NZ | 2.25 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:257:LEU:O | 1:B:259:LEU:HD12 | 2.09 | 0.52 |
| 1:I:306:ILE:O | 1:I:309:VAL:HG22 | 2.10 | 0.52 |
| 1:D:306:ILE:O | 1:D:309:VAL:HG22 | 2.10 | 0.52 |
| 1:G:189:LYS:O | 1:G:194:ILE:HG22 | 2.09 | 0.52 |
| 1:I:246:LEU:O | 1:I:250:LEU:HB2 | 2.09 | 0.52 |
| 1:E:338:GLU:O | 1:E:338:GLU:HG2 | 2.10 | 0.52 |
| 1:J:257:LEU:O | 1:J:259:LEU:HD12 | 2.09 | 0.52 |
| 1:K:223:ILE:O | 1:K:223:ILE:HD13 | 2.08 | 0.52 |
| 1:G:312:HIS:C | 1:G:312:HIS:CD2 | 2.82 | 0.52 |
| 1:J:199:LYS:HB2 | 1:J:229:ALA:CB | 2.34 | 0.52 |
| 1:C:189:LYS:O | 1:C:194:ILE:HG22 | 2.09 | 0.52 |
| 1:H:254:ASP:OD1 | 1:H:254:ASP:N | 2.36 | 0.52 |
| 1:E:246:LEU:O | 1:E:250:LEU:HB2 | 2.09 | 0.52 |
| 1:J:364:GLN:O | 1:J:368:ILE:HG13 | 2.10 | 0.52 |
| 1:G:338:GLU:HG2 | 1:G:338:GLU:O | 2.09 | 0.52 |
| 1:G:139:PHE:O | 1:G:143:GLN:HG2 | 2.10 | 0.52 |
| 1:D:281:LYS:NZ | 1:D:281:LYS:HB2 | 2.25 | 0.52 |
| 1:H:292:MET:O | 1:H:295:GLY:N | 2.37 | 0.52 |
| 1:I:257:LEU:O | 1:I:259:LEU:HD12 | 2.09 | 0.52 |
| 1:K:189:LYS:O | 1:K:194:ILE:HG22 | 2.10 | 0.52 |
| 1:A:246:LEU:O | 1:A:250:LEU:HB2 | 2.09 | 0.52 |
| 1:A:254:ASP:OD1 | 1:A:254:ASP:N | 2.36 | 0.52 |
| 1:A:122:THR:HG22 | 1:A:126:VAL:HG11 | 1.90 | 0.52 |
| 1:B:139:PHE:O | 1:B:143:GLN:HG2 | 2.09 | 0.52 |
| 1:F:364:GLN:O | 1:F:368:ILE:HG13 | 2.10 | 0.52 |
| 1:G:364:GLN:O | 1:G:368:ILE:HG13 | 2.09 | 0.52 |
| 1:J:338:GLU:O | 1:J:338:GLU:HG2 | 2.09 | 0.52 |
| 1:A:292:MET:O | 1:A:295:GLY:N | 2.37 | 0.52 |
| 1:E:281:LYS:NZ | 1:E:281:LYS:HB2 | 2.25 | 0.52 |
| 1:H:120:HIS:O | 1:H:123:ASP:OD1 | 2.28 | 0.52 |
| 1:H:94:TYR:CZ | 1:H:123:ASP:N | 2.78 | 0.52 |
| 1:G:306:ILE:O | 1:G:309:VAL:HG22 | 2.10 | 0.52 |
| 1:L:349:ARG:HH11 | 1:L:349:ARG:CB | 2.19 | 0.52 |
| 1:F:189:LYS:O | 1:F:194:ILE:HG22 | 2.09 | 0.52 |
| 1:G:246:LEU:O | 1:G:250:LEU:HB2 | 2.09 | 0.52 |
| 1:C:281:LYS:NZ | 1:C:281:LYS:HB2 | 2.25 | 0.52 |
| 1:H:281:LYS:CB | 1:H:281:LYS:HZ3 | 2.22 | 0.52 |
| 1:B:199:LYS:HB2 | 1:B:229:ALA:CB | 2.35 | 0.52 |
| 1:E:349:ARG:HH11 | 1:E:349:ARG:CB | 2.19 | 0.52 |
| 1:H:189:LYS:O | 1:H:194:ILE:HG22 | 2.09 | 0.52 |
| 1:F:254:ASP:N | 1:F:254:ASP:OD1 | 2.36 | 0.52 |
| 1:J:254:ASP:OD1 | 1:J:255:ARG:HG3 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:C:246:LEU:O | 1:C:250:LEU:HB2 | 2.10 | 0.52 |
| 1:I:122:THR:HG22 | 1:I:126:VAL:HG11 | 1.89 | 0.52 |
| 1:E:139:PHE:O | 1:E:143:GLN:HG2 | 2.09 | 0.52 |
| 1:L:139:PHE:O | 1:L:143:GLN:HG2 | 2.10 | 0.52 |
| 1:K:281:LYS:HB2 | 1:K:281:LYS:NZ | 2.25 | 0.52 |
| 1:F:257:LEU:O | 1:F:259:LEU:HD12 | 2.09 | 0.52 |
| 1:K:312:HIS:C | 1:K:312:HIS:CD2 | 2.81 | 0.52 |
| 1:H:25:LYS:HE2 | 1:H:49:TYR:OH | 2.10 | 0.52 |
| 1:H:349:ARG:HH11 | 1:H:349:ARG:CB | 2.19 | 0.52 |
| 1:C:120:HIS:O | 1:C:123:ASP:OD1 | 2.28 | 0.52 |
| 1:G:94:TYR:CZ | 1:G:123:ASP:N | 2.78 | 0.52 |
| 1:D:246:LEU:O | 1:D:250:LEU:HB2 | 2.09 | 0.52 |
| 1:C:254:ASP:N | 1:C:254:ASP:OD1 | 2.36 | 0.52 |
| 1:L:246:LEU:O | 1:L:250:LEU:HB2 | 2.09 | 0.52 |
| 1:L:364:GLN:O | 1:L:368:ILE:HG13 | 2.09 | 0.52 |
| 1:C:338:GLU:HG2 | 1:C:338:GLU:O | 2.09 | 0.52 |
| 1:K:223:ILE:HD11 | 1:K:335:LEU:CD1 | 2.40 | 0.52 |
| 1:C:223:ILE:HD11 | 1:C:335:LEU:CD1 | 2.40 | 0.52 |
| 1:E:94:TYR:CZ | 1:E:123:ASP:N | 2.78 | 0.52 |
| 1:L:189:LYS:O | 1:L:194:ILE:HG22 | 2.09 | 0.52 |
| 1:K:246:LEU:O | 1:K:250:LEU:HB2 | 2.10 | 0.52 |
| 1:A:25:LYS:HE2 | 1:A:49:TYR:OH | 2.10 | 0.52 |
| 1:I:139:PHE:O | 1:I:143:GLN:HG2 | 2.10 | 0.52 |
| 1:D:139:PHE:O | 1:D:143:GLN:HG2 | 2.09 | 0.52 |
| 1:E:223:ILE:HD13 | 1:E:223:ILE:O | 2.09 | 0.52 |
| 1:D:94:TYR:CZ | 1:D:123:ASP:N | 2.78 | 0.52 |
| 1:E:120:HIS:O | 1:E:123:ASP:OD1 | 2.28 | 0.52 |
| 1:A:120:HIS:O | 1:A:123:ASP:OD1 | 2.28 | 0.52 |
| 1:G:120:HIS:O | 1:G:123:ASP:OD1 | 2.28 | 0.52 |
| 1:L:306:ILE:O | 1:L:309:VAL:HG22 | 2.10 | 0.52 |
| 1:F:120:HIS:O | 1:F:123:ASP:OD1 | 2.28 | 0.52 |
| 1:H:246:LEU:O | 1:H:250:LEU:HB2 | 2.09 | 0.52 |
| 1:D:364:GLN:O | 1:D:368:ILE:HG13 | 2.10 | 0.52 |
| 1:K:338:GLU:HG2 | 1:K:338:GLU:O | 2.10 | 0.52 |
| 1:A:212:ARG:HH11 | 1:A:212:ARG:HG3 | 1.75 | 0.52 |
| 1:E:212:ARG:HG3 | 1:E:212:ARG:HH11 | 1.75 | 0.52 |
| 1:E:281:LYS:CB | 1:E:281:LYS:HZ3 | 2.23 | 0.52 |
| 1:C:212:ARG:HG3 | 1:C:212:ARG:HH11 | 1.75 | 0.52 |
| 1:L:281:LYS:NZ | 1:L:281:LYS:HB2 | 2.25 | 0.52 |
| 1:A:257:LEU:O | 1:A:259:LEU:HD12 | 2.09 | 0.52 |
| 1:D:257:LEU:O | 1:D:259:LEU:HD12 | 2.10 | 0.52 |
| 1:D:349:ARG:HH11 | 1:D:349:ARG:CB | 2.19 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:F:139:PHE:O | 1:F:143:GLN:HG2 | 2.10 | 0.52 |
| 1:B:25:LYS:HE2 | 1:B:49:TYR:OH | 2.10 | 0.52 |
| 1:C:364:GLN:O | 1:C:368:ILE:HG13 | 2.10 | 0.52 |
| 1:G:281:LYS:NZ | 1:G:281:LYS:HB2 | 2.25 | 0.51 |
| 1:J:292:MET:O | 1:J:295:GLY:N | 2.37 | 0.51 |
| 1:A:223:ILE:HD11 | 1:A:335:LEU:CD1 | 2.40 | 0.51 |
| 1:J:182:LYS:HZ1 | 1:J:349:ARG:HD3 | 1.75 | 0.51 |
| 1:D:189:LYS:O | 1:D:194:ILE:HG22 | 2.09 | 0.51 |
| 1:F:121:GLY:O | 1:F:125:THR:OG1 | 2.21 | 0.51 |
| 1:F:338:GLU:O | 1:F:338:GLU:HG2 | 2.09 | 0.51 |
| 1:H:338:GLU:HG2 | 1:H:338:GLU:O | 2.09 | 0.51 |
| 1:B:338:GLU:HG2 | 1:B:338:GLU:O | 2.09 | 0.51 |
| 1:A:281:LYS:NZ | 1:A:281:LYS:HB2 | 2.25 | 0.51 |
| 1:D:284:PHE:C | 1:D:284:PHE:CD2 | 2.75 | 0.51 |
| 1:C:94:TYR:CZ | 1:C:123:ASP:N | 2.79 | 0.51 |
| 1:A:306:ILE:O | 1:A:309:VAL:HG22 | 2.10 | 0.51 |
| 1:I:94:TYR:CZ | 1:I:123:ASP:N | 2.79 | 0.51 |
| 1:B:349:ARG:CB | 1:B:349:ARG:HH11 | 2.19 | 0.51 |
| 1:B:94:TYR:CZ | 1:B:123:ASP:N | 2.78 | 0.51 |
| 1:G:25:LYS:HE2 | 1:G:49:TYR:OH | 2.10 | 0.51 |
| 1:H:212:ARG:HG3 | 1:H:212:ARG:HH11 | 1.76 | 0.51 |
| 1:F:281:LYS:NZ | 1:F:281:LYS:HB2 | 2.25 | 0.51 |
| 1:G:257:LEU:O | 1:G:259:LEU:HD12 | 2.10 | 0.51 |
| 1:L:223:ILE:HD11 | 1:L:335:LEU:CD1 | 2.41 | 0.51 |
| 1:L:94:TYR:CZ | 1:L:123:ASP:N | 2.78 | 0.51 |
| 1:I:120:HIS:O | 1:I:123:ASP:OD1 | 2.28 | 0.51 |
| 1:J:94:TYR:CZ | 1:J:123:ASP:N | 2.78 | 0.51 |
| 1:K:94:TYR:CZ | 1:K:123:ASP:N | 2.78 | 0.51 |
| 1:F:25:LYS:HE2 | 1:F:49:TYR:OH | 2.10 | 0.51 |
| 1:L:338:GLU:O | 1:L:338:GLU:HG2 | 2.09 | 0.51 |
| 1:A:338:GLU:O | 1:A:338:GLU:HG2 | 2.10 | 0.51 |
| 1:G:212:ARG:HG3 | 1:G:212:ARG:HH11 | 1.76 | 0.51 |
| 1:A:281:LYS:HZ3 | 1:A:281:LYS:CB | 2.21 | 0.51 |
| 1:J:281:LYS:HB2 | 1:J:281:LYS:NZ | 2.25 | 0.51 |
| 1:B:223:ILE:HD11 | 1:B:335:LEU:CD1 | 2.40 | 0.51 |
| 1:B:306:ILE:O | 1:B:309:VAL:HG22 | 2.09 | 0.51 |
| 1:B:120:HIS:O | 1:B:123:ASP:OD1 | 2.28 | 0.51 |
| 1:L:281:LYS:HZ3 | 1:L:281:LYS:CB | 2.22 | 0.51 |
| 1:B:281:LYS:NZ | 1:B:281:LYS:HB2 | 2.25 | 0.51 |
| 1:I:223:ILE:HD11 | 1:I:335:LEU:CD1 | 2.40 | 0.51 |
| 1:E:223:ILE:HD11 | 1:E:335:LEU:CD1 | 2.40 | 0.51 |
| 1:J:223:ILE:HD11 | 1:J:335:LEU:CD1 | 2.41 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:I:50:PRO:CG | 1:K:191:GLU:HG2 | 2.32 | 0.51 |
| 1:F:94:TYR:CZ | 1:F:123:ASP:N | 2.78 | 0.51 |
| 1:K:349:ARG:CB | 1:K:349:ARG:HH11 | 2.19 | 0.51 |
| 1:J:189:LYS:O | 1:J:194:ILE:HG22 | 2.10 | 0.51 |
| 1:B:364:GLN:O | 1:B:368:ILE:HG13 | 2.09 | 0.51 |
| 1:E:284:PHE:CD2 | 1:E:284:PHE:C | 2.74 | 0.51 |
| 1:K:292:MET:O | 1:K:295:GLY:N | 2.37 | 0.51 |
| 1:H:306:ILE:O | 1:H:309:VAL:HG22 | 2.09 | 0.51 |
| 1:B:189:LYS:O | 1:B:194:ILE:HG22 | 2.09 | 0.51 |
| 1:I:189:LYS:O | 1:I:194:ILE:HG22 | 2.09 | 0.51 |
| 1:L:25:LYS:HE2 | 1:L:49:TYR:OH | 2.10 | 0.51 |
| 1:I:25:LYS:HE2 | 1:I:49:TYR:OH | 2.10 | 0.51 |
| 1:F:312:HIS:CD2 | 1:F:312:HIS:C | 2.81 | 0.51 |
| 1:D:199:LYS:HB2 | 1:D:229:ALA:CB | 2.35 | 0.51 |
| 1:F:306:ILE:O | 1:F:309:VAL:HG22 | 2.10 | 0.51 |
| 1:D:25:LYS:HE2 | 1:D:49:TYR:OH | 2.10 | 0.51 |
| 1:E:25:LYS:HE2 | 1:E:49:TYR:OH | 2.10 | 0.51 |
| 1:J:139:PHE:O | 1:J:143:GLN:HG2 | 2.10 | 0.51 |
| 1:I:364:GLN:O | 1:I:368:ILE:HG13 | 2.10 | 0.51 |
| 1:I:183:ARG:NH1 | 1:I:185:MET:SD | 2.84 | 0.51 |
| 1:I:338:GLU:O | 1:I:338:GLU:HG2 | 2.09 | 0.51 |
| 1:D:338:GLU:HG2 | 1:D:338:GLU:O | 2.09 | 0.51 |
| 1:K:212:ARG:HH11 | 1:K:212:ARG:HG3 | 1.76 | 0.51 |
| 1:I:292:MET:O | 1:I:295:GLY:N | 2.37 | 0.51 |
| 1:L:257:LEU:O | 1:L:259:LEU:HD12 | 2.10 | 0.51 |
| 1:G:121:GLY:O | 1:G:125:THR:OG1 | 2.19 | 0.51 |
| 1:K:121:GLY:O | 1:K:125:THR:OG1 | 2.18 | 0.51 |
| 1:H:281:LYS:HB2 | 1:H:281:LYS:NZ | 2.24 | 0.51 |
| 1:F:281:LYS:CB | 1:F:281:LYS:HZ3 | 2.24 | 0.51 |
| 1:C:254:ASP:OD1 | 1:C:255:ARG:HG3 | 2.11 | 0.51 |
| 1:F:202:ILE:HG21 | 1:F:269:LEU:HD23 | 1.93 | 0.51 |
| 1:K:25:LYS:HE2 | 1:K:49:TYR:OH | 2.11 | 0.51 |
| 1:C:25:LYS:HE2 | 1:C:49:TYR:OH | 2.10 | 0.51 |
| 1:F:223:ILE:HD11 | 1:F:335:LEU:CD1 | 2.40 | 0.51 |
| 1:I:199:LYS:HB2 | 1:I:229:ALA:CB | 2.35 | 0.51 |
| 1:B:267:GLU:OE1 | 1:D:48:VAL:HG12 | 2.11 | 0.51 |
| 1:H:202:ILE:HG21 | 1:H:269:LEU:HD23 | 1.93 | 0.51 |
| 1:H:223:ILE:HD11 | 1:H:335:LEU:CD1 | 2.40 | 0.50 |
| 1:G:182:LYS:HZ1 | 1:G:349:ARG:HD3 | 1.77 | 0.50 |
| 1:K:120:HIS:O | 1:K:123:ASP:OD1 | 2.29 | 0.50 |
| 1:E:306:ILE:O | 1:E:309:VAL:HG22 | 2.10 | 0.50 |
| 1:F:254:ASP:OD1 | 1:F:255:ARG:HG3 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:K:254:ASP:N | 1:K:254:ASP:OD1 | 2.36 | 0.50 |
| 1:G:202:ILE:HG21 | 1:G:269:LEU:HD23 | 1.93 | 0.50 |
| 1:G:183:ARG:NH1 | 1:G:185:MET:SD | 2.85 | 0.50 |
| 1:C:183:ARG:NH1 | 1:C:185:MET:SD | 2.84 | 0.50 |
| 1:J:281:LYS:O | 1:J:282:GLU:CB | 2.58 | 0.50 |
| 1:F:212:ARG:HH11 | 1:F:212:ARG:HG3 | 1.76 | 0.50 |
| 1:J:120:HIS:O | 1:J:123:ASP:OD1 | 2.29 | 0.50 |
| 1:G:254:ASP:OD1 | 1:G:255:ARG:HG3 | 2.11 | 0.50 |
| 1:L:254:ASP:OD1 | 1:L:255:ARG:HG3 | 2.12 | 0.50 |
| 1:H:183:ARG:NH1 | 1:H:185:MET:SD | 2.84 | 0.50 |
| 1:D:212:ARG:HG3 | 1:D:212:ARG:HH11 | 1.76 | 0.50 |
| 1:A:94:TYR:CZ | 1:A:123:ASP:N | 2.78 | 0.50 |
| 1:I:254:ASP:N | 1:I:254:ASP:OD1 | 2.36 | 0.50 |
| 1:E:254:ASP:OD1 | 1:E:255:ARG:HG3 | 2.11 | 0.50 |
| 1:G:136:LEU:HD21 | 1:H:72:LEU:HB3 | 1.93 | 0.50 |
| 1:L:183:ARG:NH1 | 1:L:185:MET:SD | 2.84 | 0.50 |
| 1:L:284:PHE:CB | 1:L:285:GLY:HA2 | 2.32 | 0.50 |
| 1:G:223:ILE:HD11 | 1:G:335:LEU:CD1 | 2.41 | 0.50 |
| 1:I:50:PRO:HG2 | 1:K:191:GLU:CG | 2.30 | 0.50 |
| 1:B:254:ASP:OD1 | 1:B:255:ARG:HG3 | 2.11 | 0.50 |
| 1:K:254:ASP:OD1 | 1:K:255:ARG:HG3 | 2.11 | 0.50 |
| 1:D:254:ASP:OD1 | 1:D:255:ARG:HG3 | 2.11 | 0.50 |
| 1:I:202:ILE:HG21 | 1:I:269:LEU:HD23 | 1.93 | 0.50 |
| 1:C:202:ILE:HG21 | 1:C:269:LEU:HD23 | 1.93 | 0.50 |
| 1:C:139:PHE:O | 1:C:143:GLN:HG2 | 2.10 | 0.50 |
| 1:D:183:ARG:NH1 | 1:D:185:MET:SD | 2.85 | 0.50 |
| 1:B:212:ARG:HG3 | 1:B:212:ARG:HH11 | 1.75 | 0.50 |
| 1:D:173:ASN:OD1 | 1:D:284:PHE:HD1 | 1.93 | 0.50 |
| 1:A:254:ASP:OD1 | 1:A:255:ARG:HG3 | 2.11 | 0.50 |
| 1:B:202:ILE:HG21 | 1:B:269:LEU:HD23 | 1.93 | 0.50 |
| 1:H:254:ASP:OD1 | 1:H:255:ARG:HG3 | 2.11 | 0.50 |
| 1:I:191:GLU:HG2 | 1:K:50:PRO:HG2 | 1.94 | 0.50 |
| 1:K:183:ARG:NH1 | 1:K:185:MET:SD | 2.84 | 0.50 |
| 1:L:120:HIS:O | 1:L:123:ASP:OD1 | 2.29 | 0.50 |
| 1:K:202:ILE:HG21 | 1:K:269:LEU:HD23 | 1.93 | 0.50 |
| 1:E:183:ARG:NH1 | 1:E:185:MET:SD | 2.85 | 0.50 |
| 1:A:183:ARG:NH1 | 1:A:185:MET:SD | 2.85 | 0.50 |
| 1:K:284:PHE:CB | 1:K:285:GLY:HA2 | 2.33 | 0.50 |
| 1:G:97:PRO:HB3 | 1:H:72:LEU:CD2 | 2.42 | 0.50 |
| 1:E:254:ASP:OD1 | 1:E:254:ASP:N | 2.36 | 0.49 |
| 1:D:202:ILE:HG21 | 1:D:269:LEU:HD23 | 1.93 | 0.49 |
| 1:A:202:ILE:HG21 | 1:A:269:LEU:HD23 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:120:HIS:O | 1:D:123:ASP:OD1 | 2.29 | 0.49 |
| 1:K:182:LYS:HZ2 | 1:K:349:ARG:CD | 2.25 | 0.49 |
| 1:I:212:ARG:HG3 | 1:I:212:ARG:HH11 | 1.76 | 0.49 |
| 1:J:212:ARG:HH11 | 1:J:212:ARG:HG3 | 1.76 | 0.49 |
| 1:J:173:ASN:OD1 | 1:J:284:PHE:HD1 | 1.94 | 0.49 |
| 1:K:223:ILE:HG12 | 1:K:332:ILE:HG23 | 1.94 | 0.49 |
| 1:D:182:LYS:HZ1 | 1:D:349:ARG:HD3 | 1.78 | 0.49 |
| 1:I:254:ASP:OD1 | 1:I:255:ARG:HG3 | 2.11 | 0.49 |
| 1:E:202:ILE:HG21 | 1:E:269:LEU:HD23 | 1.93 | 0.49 |
| 1:B:183:ARG:NH1 | 1:B:185:MET:SD | 2.84 | 0.49 |
| 1:J:183:ARG:NH1 | 1:J:185:MET:SD | 2.85 | 0.49 |
| 1:L:212:ARG:HH11 | 1:L:212:ARG:HG3 | 1.75 | 0.49 |
| 1:B:173:ASN:OD1 | 1:B:284:PHE:HD1 | 1.93 | 0.49 |
| 1:K:123:ASP:O | 1:K:127:LEU:HB2 | 2.12 | 0.49 |
| 1:L:202:ILE:HG21 | 1:L:269:LEU:HD23 | 1.93 | 0.49 |
| 1:G:349:ARG:HH11 | 1:G:349:ARG:CB | 2.18 | 0.49 |
| 1:J:286:LEU:N | 1:J:286:LEU:CD1 | 2.32 | 0.49 |
| 1:F:223:ILE:HG12 | 1:F:332:ILE:HG23 | 1.95 | 0.49 |
| 1:H:123:ASP:O | 1:H:127:LEU:HB2 | 2.12 | 0.49 |
| 1:J:202:ILE:HG21 | 1:J:269:LEU:HD23 | 1.94 | 0.49 |
| 1:L:281:LYS:O | 1:L:282:GLU:CB | 2.57 | 0.49 |
| 1:D:223:ILE:HD11 | 1:D:335:LEU:CD1 | 2.40 | 0.49 |
| 1:J:123:ASP:O | 1:J:127:LEU:HB2 | 2.13 | 0.49 |
| 1:G:123:ASP:O | 1:G:127:LEU:HB2 | 2.13 | 0.49 |
| 1:J:25:LYS:HE2 | 1:J:49:TYR:OH | 2.11 | 0.49 |
| 1:F:183:ARG:NH1 | 1:F:185:MET:SD | 2.85 | 0.49 |
| 1:H:173:ASN:OD1 | 1:H:284:PHE:HD1 | 1.96 | 0.49 |
| 1:G:223:ILE:HG12 | 1:G:332:ILE:HG23 | 1.95 | 0.49 |
| 1:C:163:LYS:HA | 1:I:156:ASN:OD1 | 2.12 | 0.49 |
| 1:B:201:LEU:O | 1:B:231:LEU:HD12 | 2.13 | 0.49 |
| 1:I:173:ASN:OD1 | 1:I:284:PHE:HD1 | 1.95 | 0.49 |
| 1:J:281:LYS:CB | 1:J:281:LYS:HZ3 | 2.25 | 0.49 |
| 1:A:312:HIS:HD2 | 1:A:313:GLY:N | 2.11 | 0.49 |
| 1:E:223:ILE:HG12 | 1:E:332:ILE:HG23 | 1.95 | 0.49 |
| 1:D:312:HIS:HD2 | 1:D:313:GLY:N | 2.11 | 0.49 |
| 1:E:123:ASP:O | 1:E:127:LEU:HB2 | 2.13 | 0.49 |
| 1:C:201:LEU:O | 1:C:231:LEU:HD12 | 2.13 | 0.49 |
| 1:C:363:SER:O | 1:C:367:THR:HG23 | 2.13 | 0.49 |
| 1:D:281:LYS:HZ3 | 1:D:281:LYS:CB | 2.26 | 0.49 |
| 1:I:312:HIS:HD2 | 1:I:313:GLY:N | 2.11 | 0.49 |
| 1:C:123:ASP:O | 1:C:127:LEU:HB2 | 2.13 | 0.49 |
| 1:J:121:GLY:O | 1:J:125:THR:OG1 | 2.19 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:363:SER:O | 1:B:367:THR:HG23 | 2.13 | 0.49 |
| 1:L:281:LYS:HA | 1:L:303:VAL:CG1 | 2.32 | 0.48 |
| 1:L:312:HIS:HD2 | 1:L:313:GLY:N | 2.10 | 0.48 |
| 1:B:223:ILE:HG12 | 1:B:332:ILE:HG23 | 1.94 | 0.48 |
| 1:D:223:ILE:HG12 | 1:D:332:ILE:HG23 | 1.94 | 0.48 |
| 1:D:123:ASP:O | 1:D:127:LEU:HB2 | 2.13 | 0.48 |
| 1:I:123:ASP:O | 1:I:127:LEU:HB2 | 2.13 | 0.48 |
| 1:H:113:ILE:HD13 | 1:H:114:LYS:N | 2.28 | 0.48 |
| 1:A:201:LEU:O | 1:A:231:LEU:HD12 | 2.13 | 0.48 |
| 1:L:201:LEU:O | 1:L:231:LEU:HD12 | 2.13 | 0.48 |
| 1:K:173:ASN:OD1 | 1:K:284:PHE:HD1 | 1.96 | 0.48 |
| 1:J:281:LYS:HA | 1:J:303:VAL:CG1 | 2.32 | 0.48 |
| 1:C:312:HIS:HD2 | 1:C:313:GLY:N | 2.11 | 0.48 |
| 1:A:123:ASP:O | 1:A:127:LEU:HB2 | 2.13 | 0.48 |
| 1:B:123:ASP:O | 1:B:127:LEU:HB2 | 2.13 | 0.48 |
| 1:I:122:THR:HG22 | 1:I:126:VAL:HG12 | 1.95 | 0.48 |
| 1:G:363:SER:O | 1:G:367:THR:HG23 | 2.13 | 0.48 |
| 1:H:363:SER:O | 1:H:367:THR:HG23 | 2.13 | 0.48 |
| 1:H:223:ILE:HG12 | 1:H:332:ILE:HG23 | 1.95 | 0.48 |
| 1:B:182:LYS:HZ2 | 1:B:349:ARG:CD | 2.26 | 0.48 |
| 1:J:89:ILE:HD11 | 1:J:373:LEU:HD11 | 1.95 | 0.48 |
| 1:E:363:SER:O | 1:E:367:THR:HG23 | 2.13 | 0.48 |
| 1:I:201:LEU:O | 1:I:231:LEU:HD12 | 2.14 | 0.48 |
| 1:A:65:PHE:HZ | 1:B:96:ILE:CG2 | 2.26 | 0.48 |
| 1:I:182:LYS:HZ1 | 1:I:349:ARG:HD3 | 1.78 | 0.48 |
| 1:D:122:THR:HG22 | 1:D:126:VAL:HG12 | 1.95 | 0.48 |
| 1:F:122:THR:HG22 | 1:F:126:VAL:HG12 | 1.95 | 0.48 |
| 1:I:223:ILE:HG12 | 1:I:332:ILE:HG23 | 1.95 | 0.48 |
| 1:E:122:THR:HG22 | 1:E:126:VAL:HG12 | 1.95 | 0.48 |
| 1:K:89:ILE:HD11 | 1:K:373:LEU:HD11 | 1.95 | 0.48 |
| 1:H:201:LEU:O | 1:H:231:LEU:HD12 | 2.13 | 0.48 |
| 1:I:363:SER:O | 1:I:367:THR:HG23 | 2.14 | 0.48 |
| 1:H:312:HIS:HD2 | 1:H:313:GLY:N | 2.11 | 0.48 |
| 1:B:312:HIS:HD2 | 1:B:313:GLY:N | 2.11 | 0.48 |
| 1:J:312:HIS:HD2 | 1:J:313:GLY:N | 2.12 | 0.48 |
| 1:J:223:ILE:HG12 | 1:J:332:ILE:HG23 | 1.95 | 0.48 |
| 1:D:113:ILE:HD13 | 1:D:114:LYS:N | 2.29 | 0.48 |
| 1:L:363:SER:O | 1:L:367:THR:HG23 | 2.14 | 0.48 |
| 1:K:257:LEU:N | 1:K:257:LEU:HD13 | 2.28 | 0.48 |
| 1:C:223:ILE:HG12 | 1:C:332:ILE:HG23 | 1.95 | 0.48 |
| 1:A:199:LYS:HB2 | 1:A:229:ALA:CB | 2.35 | 0.48 |
| 1:L:199:LYS:HB2 | 1:L:229:ALA:CB | 2.35 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:K:139:PHE:CG | 1:L:108:MET:HG2 | 2.49 | 0.48 |
| 1:K:261:LYS:HG3 | 1:K:261:LYS:O | 2.14 | 0.48 |
| 1:G:312:HIS:HD2 | 1:G:313:GLY:N | 2.12 | 0.48 |
| 1:I:89:ILE:HD11 | 1:I:373:LEU:HD11 | 1.96 | 0.48 |
| 1:B:89:ILE:HD11 | 1:B:373:LEU:HD11 | 1.96 | 0.48 |
| 1:C:113:ILE:HD13 | 1:C:114:LYS:N | 2.29 | 0.48 |
| 1:K:201:LEU:O | 1:K:231:LEU:HD12 | 2.14 | 0.48 |
| 1:B:281:LYS:O | 1:B:282:GLU:CB | 2.57 | 0.48 |
| 1:C:287:VAL:HG22 | 1:C:288:LEU:N | 2.29 | 0.48 |
| 1:E:288:LEU:HA | 1:E:288:LEU:HD23 | 1.62 | 0.48 |
| 1:A:223:ILE:HG12 | 1:A:332:ILE:HG23 | 1.95 | 0.48 |
| 1:L:123:ASP:O | 1:L:127:LEU:HB2 | 2.13 | 0.48 |
| 1:F:123:ASP:O | 1:F:127:LEU:HB2 | 2.13 | 0.48 |
| 1:L:122:THR:HG22 | 1:L:126:VAL:HG12 | 1.95 | 0.48 |
| 1:I:113:ILE:HD13 | 1:I:114:LYS:N | 2.29 | 0.48 |
| 1:F:201:LEU:O | 1:F:231:LEU:HD12 | 2.13 | 0.48 |
| 1:G:173:ASN:HB2 | 1:G:284:PHE:CE1 | 2.49 | 0.48 |
| 1:G:284:PHE:CB | 1:G:285:GLY:HA2 | 2.31 | 0.48 |
| 1:C:122:THR:HG22 | 1:C:126:VAL:HG12 | 1.95 | 0.48 |
| 1:D:89:ILE:HD11 | 1:D:373:LEU:HD11 | 1.96 | 0.48 |
| 1:G:122:THR:HG22 | 1:G:126:VAL:HG12 | 1.95 | 0.48 |
| 1:F:113:ILE:HD13 | 1:F:114:LYS:N | 2.29 | 0.48 |
| 1:D:201:LEU:O | 1:D:231:LEU:HD12 | 2.14 | 0.48 |
| 1:J:363:SER:O | 1:J:367:THR:HG23 | 2.14 | 0.48 |
| 1:G:173:ASN:OD1 | 1:G:284:PHE:HD1 | 1.95 | 0.47 |
| 1:I:173:ASN:HB2 | 1:I:284:PHE:CE1 | 2.49 | 0.47 |
| 1:B:173:ASN:HB2 | 1:B:284:PHE:CE1 | 2.49 | 0.47 |
| 1:J:122:THR:HG22 | 1:J:126:VAL:HG12 | 1.95 | 0.47 |
| 1:L:89:ILE:HD11 | 1:L:373:LEU:HD11 | 1.96 | 0.47 |
| 1:L:223:ILE:HG12 | 1:L:332:ILE:HG23 | 1.95 | 0.47 |
| 1:E:89:ILE:HD11 | 1:E:373:LEU:HD11 | 1.96 | 0.47 |
| 1:A:113:ILE:HD13 | 1:A:114:LYS:N | 2.29 | 0.47 |
| 1:A:287:VAL:HG22 | 1:A:288:LEU:N | 2.29 | 0.47 |
| 1:E:257:LEU:N | 1:E:257:LEU:HD13 | 2.28 | 0.47 |
| 1:E:312:HIS:HD2 | 1:E:313:GLY:N | 2.11 | 0.47 |
| 1:E:199:LYS:HB2 | 1:E:229:ALA:CB | 2.34 | 0.47 |
| 1:B:122:THR:HG22 | 1:B:126:VAL:HG12 | 1.95 | 0.47 |
| 1:G:89:ILE:HD11 | 1:G:373:LEU:HD11 | 1.96 | 0.47 |
| 1:I:281:LYS:HA | 1:I:303:VAL:CG1 | 2.31 | 0.47 |
| 1:G:287:VAL:HG22 | 1:G:288:LEU:N | 2.29 | 0.47 |
| 1:A:261:LYS:O | 1:A:261:LYS:HG3 | 2.15 | 0.47 |
| 1:E:113:ILE:HD13 | 1:E:114:LYS:N | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:89:ILE:HD11 | 1:A:373:LEU:HD11 | 1.96 | 0.47 |
| 1:A:363:SER:O | 1:A:367:THR:HG23 | 2.13 | 0.47 |
| 1:H:281:LYS:O | 1:H:282:GLU:CB | 2.57 | 0.47 |
| 1:F:173:ASN:HB2 | 1:F:284:PHE:CE1 | 2.49 | 0.47 |
| 1:H:199:LYS:HB2 | 1:H:229:ALA:CB | 2.34 | 0.47 |
| 1:C:199:LYS:HB2 | 1:C:229:ALA:CB | 2.35 | 0.47 |
| 1:B:113:ILE:HD13 | 1:B:114:LYS:N | 2.28 | 0.47 |
| 1:G:261:LYS:O | 1:G:261:LYS:HG3 | 2.15 | 0.47 |
| 1:D:363:SER:O | 1:D:367:THR:HG23 | 2.13 | 0.47 |
| 1:C:173:ASN:HB2 | 1:C:284:PHE:CE1 | 2.49 | 0.47 |
| 1:C:257:LEU:HD13 | 1:C:257:LEU:N | 2.28 | 0.47 |
| 1:F:312:HIS:HD2 | 1:F:313:GLY:N | 2.12 | 0.47 |
| 1:F:89:ILE:HD11 | 1:F:373:LEU:HD11 | 1.96 | 0.47 |
| 1:G:201:LEU:O | 1:G:231:LEU:HD12 | 2.14 | 0.47 |
| 1:J:201:LEU:O | 1:J:231:LEU:HD12 | 2.14 | 0.47 |
| 1:E:201:LEU:O | 1:E:231:LEU:HD12 | 2.13 | 0.47 |
| 1:F:281:LYS:HA | 1:F:303:VAL:CG1 | 2.31 | 0.47 |
| 1:D:281:LYS:HA | 1:D:303:VAL:CG1 | 2.31 | 0.47 |
| 1:K:312:HIS:HD2 | 1:K:313:GLY:N | 2.12 | 0.47 |
| 1:G:139:PHE:CG | 1:H:108:MET:HG2 | 2.49 | 0.47 |
| 1:F:363:SER:O | 1:F:367:THR:HG23 | 2.14 | 0.47 |
| 1:I:261:LYS:HG3 | 1:I:261:LYS:O | 2.15 | 0.47 |
| 1:J:261:LYS:O | 1:J:261:LYS:HG3 | 2.14 | 0.47 |
| 1:H:173:ASN:HB2 | 1:H:284:PHE:CE1 | 2.49 | 0.47 |
| 1:A:122:THR:HG22 | 1:A:126:VAL:HG12 | 1.95 | 0.47 |
| 1:C:156:ASN:OD1 | 1:I:159:HIS:O | 2.33 | 0.47 |
| 1:L:261:LYS:HG3 | 1:L:261:LYS:O | 2.15 | 0.47 |
| 1:G:199:LYS:HB2 | 1:G:229:ALA:CB | 2.34 | 0.47 |
| 1:H:122:THR:HG22 | 1:H:126:VAL:HG12 | 1.95 | 0.47 |
| 1:C:89:ILE:HD11 | 1:C:373:LEU:HD11 | 1.96 | 0.47 |
| 1:G:113:ILE:HD13 | 1:G:114:LYS:N | 2.29 | 0.47 |
| 1:C:121:GLY:O | 1:C:125:THR:OG1 | 2.20 | 0.47 |
| 1:A:121:GLY:O | 1:A:125:THR:OG1 | 2.20 | 0.47 |
| 1:K:339:GLU:HA | 1:K:339:GLU:OE1 | 2.15 | 0.47 |
| 1:E:136:LEU:HD21 | 1:F:72:LEU:CB | 2.42 | 0.46 |
| 1:K:177:GLU:HG3 | 1:K:357:ARG:HH11 | 1.80 | 0.46 |
| 1:H:89:ILE:HD11 | 1:H:373:LEU:HD11 | 1.97 | 0.46 |
| 1:K:363:SER:O | 1:K:367:THR:HG23 | 2.15 | 0.46 |
| 1:A:173:ASN:HB2 | 1:A:284:PHE:CE1 | 2.49 | 0.46 |
| 1:J:173:ASN:HB2 | 1:J:284:PHE:CE1 | 2.50 | 0.46 |
| 1:E:136:LEU:CD2 | 1:F:72:LEU:HB3 | 2.43 | 0.46 |
| 1:L:113:ILE:HD13 | 1:L:114:LYS:N | 2.29 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:K:113:ILE:HD13 | 1:K:114:LYS:N | 2.29 | 0.46 |
| 1:F:261:LYS:HG3 | 1:F:261:LYS:O | 2.14 | 0.46 |
| 1:E:173:ASN:HB2 | 1:E:284:PHE:CE1 | 2.49 | 0.46 |
| 1:H:281:LYS:HA | 1:H:303:VAL:CG1 | 2.31 | 0.46 |
| 1:K:287:VAL:HG22 | 1:K:288:LEU:N | 2.29 | 0.46 |
| 1:D:261:LYS:O | 1:D:261:LYS:HG3 | 2.15 | 0.46 |
| 1:C:339:GLU:HA | 1:C:339:GLU:OE1 | 2.16 | 0.46 |
| 1:B:261:LYS:HG3 | 1:B:261:LYS:O | 2.15 | 0.46 |
| 1:E:48:VAL:HG23 | 1:H:262:GLN:OE1 | 2.16 | 0.46 |
| 1:K:175:ILE:HA | 1:K:175:ILE:HD13 | 1.79 | 0.46 |
| 1:E:261:LYS:HG3 | 1:E:261:LYS:O | 2.14 | 0.46 |
| 1:C:261:LYS:HG3 | 1:C:261:LYS:O | 2.15 | 0.46 |
| 1:K:281:LYS:O | 1:K:282:GLU:CB | 2.57 | 0.46 |
| 1:L:173:ASN:HB2 | 1:L:284:PHE:CE1 | 2.50 | 0.46 |
| 1:J:287:VAL:HG22 | 1:J:288:LEU:N | 2.28 | 0.46 |
| 1:A:288:LEU:HD23 | 1:A:288:LEU:HA | 1.62 | 0.46 |
| 1:C:281:LYS:CB | 1:C:281:LYS:HZ3 | 2.28 | 0.46 |
| 1:D:173:ASN:HB2 | 1:D:284:PHE:CE1 | 2.50 | 0.46 |
| 1:K:122:THR:HG22 | 1:K:126:VAL:HG12 | 1.97 | 0.46 |
| 1:C:282:GLU:HG3 | 1:C:284:PHE:H | 1.81 | 0.46 |
| 1:F:287:VAL:HG22 | 1:F:288:LEU:N | 2.29 | 0.46 |
| 1:H:212:ARG:HG3 | 1:H:212:ARG:NH1 | 2.31 | 0.46 |
| 1:J:113:ILE:HD13 | 1:J:114:LYS:N | 2.30 | 0.46 |
| 1:I:339:GLU:OE1 | 1:I:339:GLU:HA | 2.16 | 0.46 |
| 1:E:173:ASN:OD1 | 1:E:284:PHE:HD1 | 1.96 | 0.46 |
| 1:D:287:VAL:HG22 | 1:D:288:LEU:N | 2.29 | 0.46 |
| 1:A:257:LEU:N | 1:A:257:LEU:HD13 | 2.28 | 0.46 |
| 1:L:332:ILE:O | 1:L:336:LYS:HG2 | 2.16 | 0.46 |
| 1:E:182:LYS:HZ1 | 1:E:349:ARG:HD3 | 1.80 | 0.46 |
| 1:H:282:GLU:HG3 | 1:H:284:PHE:H | 1.81 | 0.46 |
| 1:F:281:LYS:O | 1:F:282:GLU:CB | 2.58 | 0.46 |
| 1:A:332:ILE:O | 1:A:336:LYS:HG2 | 2.16 | 0.46 |
| 1:E:212:ARG:HG3 | 1:E:212:ARG:NH1 | 2.31 | 0.45 |
| 1:C:212:ARG:HG3 | 1:C:212:ARG:NH1 | 2.31 | 0.45 |
| 1:L:282:GLU:HG3 | 1:L:284:PHE:H | 1.81 | 0.45 |
| 1:I:287:VAL:HG22 | 1:I:288:LEU:N | 2.29 | 0.45 |
| 1:F:212:ARG:NH1 | 1:F:212:ARG:HG3 | 2.31 | 0.45 |
| 1:F:284:PHE:CB | 1:F:285:GLY:HA2 | 2.32 | 0.45 |
| 1:A:76:SER:HB2 | 1:B:136:LEU:HD22 | 1.98 | 0.45 |
| 1:K:212:ARG:NH1 | 1:K:212:ARG:HG3 | 2.31 | 0.45 |
| 1:K:282:GLU:HG3 | 1:K:284:PHE:H | 1.81 | 0.45 |
| 1:B:282:GLU:HG3 | 1:B:284:PHE:H | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:F:332:ILE:O | 1:F:336:LYS:HG2 | 2.16 | 0.45 |
| 1:C:175:ILE:HD13 | 1:C:175:ILE:HA | 1.79 | 0.45 |
| 1:K:199:LYS:O | 1:K:229:ALA:HB1 | 2.17 | 0.45 |
| 1:A:339:GLU:OE1 | 1:A:339:GLU:HA | 2.16 | 0.45 |
| 1:H:175:ILE:HA | 1:H:175:ILE:HD13 | 1.79 | 0.45 |
| 1:D:339:GLU:HA | 1:D:339:GLU:OE1 | 2.15 | 0.45 |
| 1:E:339:GLU:OE1 | 1:E:339:GLU:HA | 2.16 | 0.45 |
| 1:E:281:LYS:O | 1:E:282:GLU:CB | 2.58 | 0.45 |
| 1:B:212:ARG:HG3 | 1:B:212:ARG:NH1 | 2.31 | 0.45 |
| 1:F:282:GLU:HG3 | 1:F:284:PHE:H | 1.82 | 0.45 |
| 1:D:212:ARG:NH1 | 1:D:212:ARG:HG3 | 2.32 | 0.45 |
| 1:H:275:MET:SD | 1:H:287:VAL:HG23 | 2.57 | 0.45 |
| 1:B:332:ILE:O | 1:B:336:LYS:HG2 | 2.16 | 0.45 |
| 1:F:177:GLU:HG3 | 1:F:357:ARG:HH11 | 1.81 | 0.45 |
| 1:H:339:GLU:OE1 | 1:H:339:GLU:HA | 2.16 | 0.45 |
| 1:A:275:MET:SD | 1:A:287:VAL:HG23 | 2.57 | 0.45 |
| 1:A:212:ARG:NH1 | 1:A:212:ARG:HG3 | 2.31 | 0.45 |
| 1:H:287:VAL:HG22 | 1:H:288:LEU:N | 2.30 | 0.45 |
| 1:C:332:ILE:O | 1:C:336:LYS:HG2 | 2.16 | 0.45 |
| 1:H:112:ARG:NH2 | 1:H:112:ARG:HB3 | 2.32 | 0.45 |
| 1:B:112:ARG:HB3 | 1:B:112:ARG:NH2 | 2.32 | 0.45 |
| 1:K:112:ARG:NH2 | 1:K:112:ARG:HB3 | 2.32 | 0.45 |
| 1:D:282:GLU:HG3 | 1:D:284:PHE:H | 1.82 | 0.45 |
| 1:L:275:MET:SD | 1:L:287:VAL:HG23 | 2.57 | 0.45 |
| 1:J:336:LYS:HB3 | 1:J:336:LYS:HE2 | 1.86 | 0.45 |
| 1:D:175:ILE:HA | 1:D:175:ILE:HD13 | 1.79 | 0.45 |
| 1:C:112:ARG:NH2 | 1:C:112:ARG:HB3 | 2.32 | 0.45 |
| 1:J:112:ARG:NH2 | 1:J:112:ARG:HB3 | 2.32 | 0.45 |
| 1:D:112:ARG:HB3 | 1:D:112:ARG:NH2 | 2.32 | 0.45 |
| 1:H:332:ILE:O | 1:H:336:LYS:HG2 | 2.16 | 0.45 |
| 1:G:332:ILE:O | 1:G:336:LYS:HG2 | 2.16 | 0.45 |
| 1:C:136:LEU:CD2 | 1:D:72:LEU:HB3 | 2.43 | 0.45 |
| 1:A:177:GLU:HG3 | 1:A:357:ARG:HH11 | 1.81 | 0.45 |
| 1:B:339:GLU:HA | 1:B:339:GLU:OE1 | 2.16 | 0.45 |
| 1:H:261:LYS:O | 1:H:261:LYS:HG3 | 2.15 | 0.45 |
| 1:L:112:ARG:NH2 | 1:L:112:ARG:HB3 | 2.32 | 0.45 |
| 1:F:112:ARG:HB3 | 1:F:112:ARG:NH2 | 2.32 | 0.45 |
| 1:J:339:GLU:OE1 | 1:J:339:GLU:HA | 2.16 | 0.45 |
| 1:G:212:ARG:HG3 | 1:G:212:ARG:NH1 | 2.31 | 0.45 |
| 1:L:212:ARG:NH1 | 1:L:212:ARG:HG3 | 2.31 | 0.45 |
| 1:F:288:LEU:HD23 | 1:F:288:LEU:HA | 1.62 | 0.45 |
| 1:J:332:ILE:O | 1:J:336:LYS:HG2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:177:GLU:HG3 | 1:D:357:ARG:HH11 | 1.81 | 0.45 |
| 1:G:339:GLU:OE1 | 1:G:339:GLU:HA | 2.16 | 0.45 |
| 1:E:287:VAL:HG22 | 1:E:288:LEU:N | 2.29 | 0.45 |
| 1:B:334:LEU:HD11 | 1:B:341:HIS:HA | 1.99 | 0.45 |
| 1:G:199:LYS:O | 1:G:229:ALA:HB1 | 2.17 | 0.45 |
| 1:A:79:ALA:CB | 1:A:108:MET:HE2 | 2.46 | 0.45 |
| 1:F:277:LEU:O | 1:F:300:GLY:HA2 | 2.17 | 0.45 |
| 1:I:212:ARG:HG3 | 1:I:212:ARG:NH1 | 2.32 | 0.45 |
| 1:D:275:MET:SD | 1:D:287:VAL:HG23 | 2.57 | 0.45 |
| 1:J:199:LYS:O | 1:J:229:ALA:HB1 | 2.17 | 0.45 |
| 1:L:339:GLU:OE1 | 1:L:339:GLU:HA | 2.16 | 0.45 |
| 1:F:339:GLU:OE1 | 1:F:339:GLU:HA | 2.16 | 0.45 |
| 1:I:112:ARG:HB3 | 1:I:112:ARG:NH2 | 2.32 | 0.45 |
| 1:G:104:LEU:HD23 | 1:G:104:LEU:HA | 1.84 | 0.45 |
| 1:G:112:ARG:HB3 | 1:G:112:ARG:NH2 | 2.32 | 0.45 |
| 1:G:155:ILE:HG22 | 1:L:156:ASN:HD21 | 1.82 | 0.45 |
| 1:G:282:GLU:HG3 | 1:G:284:PHE:H | 1.82 | 0.44 |
| 1:I:282:GLU:HG3 | 1:I:284:PHE:H | 1.82 | 0.44 |
| 1:I:284:PHE:CB | 1:I:285:GLY:HA2 | 2.32 | 0.44 |
| 1:J:212:ARG:HG3 | 1:J:212:ARG:NH1 | 2.32 | 0.44 |
| 1:J:284:PHE:CB | 1:J:285:GLY:HA2 | 2.30 | 0.44 |
| 1:D:199:LYS:O | 1:D:229:ALA:HB1 | 2.18 | 0.44 |
| 1:E:177:GLU:HG3 | 1:E:357:ARG:HH11 | 1.82 | 0.44 |
| 1:I:177:GLU:HG3 | 1:I:357:ARG:HH11 | 1.81 | 0.44 |
| 1:E:277:LEU:O | 1:E:300:GLY:HA2 | 2.17 | 0.44 |
| 1:C:277:LEU:O | 1:C:300:GLY:HA2 | 2.17 | 0.44 |
| 1:E:112:ARG:HB3 | 1:E:112:ARG:NH2 | 2.32 | 0.44 |
| 1:B:275:MET:SD | 1:B:287:VAL:HG23 | 2.57 | 0.44 |
| 1:F:275:MET:SD | 1:F:287:VAL:HG23 | 2.57 | 0.44 |
| 1:L:257:LEU:HD13 | 1:L:257:LEU:N | 2.28 | 0.44 |
| 1:K:332:ILE:O | 1:K:336:LYS:HG2 | 2.17 | 0.44 |
| 1:I:332:ILE:O | 1:I:336:LYS:HG2 | 2.16 | 0.44 |
| 1:E:332:ILE:O | 1:E:336:LYS:HG2 | 2.16 | 0.44 |
| 1:D:332:ILE:O | 1:D:336:LYS:HG2 | 2.16 | 0.44 |
| 1:F:199:LYS:O | 1:F:229:ALA:HB1 | 2.17 | 0.44 |
| 1:F:252:ILE:HG22 | 1:F:255:ARG:HB2 | 1.99 | 0.44 |
| 1:I:277:LEU:O | 1:I:300:GLY:HA2 | 2.17 | 0.44 |
| 1:A:281:LYS:O | 1:A:282:GLU:CB | 2.57 | 0.44 |
| 1:I:334:LEU:HD11 | 1:I:341:HIS:HA | 2.00 | 0.44 |
| 1:L:199:LYS:O | 1:L:229:ALA:HB1 | 2.18 | 0.44 |
| 1:B:114:LYS:HG3 | 1:B:373:LEU:HD23 | 2.00 | 0.44 |
| 1:A:277:LEU:O | 1:A:300:GLY:HA2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:G:65:PHE:HZ | 1:H:96:ILE:HG21 | 1.83 | 0.44 |
| 1:E:108:MET:CE | 1:F:135:ASN:ND2 | 2.80 | 0.44 |
| 1:F:239:GLU:O | 1:F:243:ILE:HG12 | 2.18 | 0.44 |
| 1:K:275:MET:SD | 1:K:287:VAL:HG23 | 2.58 | 0.44 |
| 1:A:199:LYS:O | 1:A:229:ALA:HB1 | 2.17 | 0.44 |
| 1:L:177:GLU:HG3 | 1:L:357:ARG:HH11 | 1.81 | 0.44 |
| 1:G:177:GLU:HG3 | 1:G:357:ARG:HH11 | 1.81 | 0.44 |
| 1:E:250:LEU:HB3 | 1:E:252:ILE:HG13 | 2.00 | 0.44 |
| 1:A:112:ARG:HB3 | 1:A:112:ARG:NH2 | 2.32 | 0.44 |
| 1:C:284:PHE:CB | 1:C:285:GLY:HA2 | 2.32 | 0.44 |
| 1:I:288:LEU:HA | 1:I:288:LEU:HD23 | 1.62 | 0.44 |
| 1:E:275:MET:SD | 1:E:287:VAL:HG23 | 2.57 | 0.44 |
| 1:G:275:MET:SD | 1:G:287:VAL:HG23 | 2.57 | 0.44 |
| 1:B:199:LYS:O | 1:B:229:ALA:HB1 | 2.18 | 0.44 |
| 1:A:306:ILE:H | 1:A:307:PRO:HD2 | 1.83 | 0.44 |
| 1:B:177:GLU:HG3 | 1:B:357:ARG:HH11 | 1.81 | 0.44 |
| 1:F:250:LEU:HB3 | 1:F:252:ILE:HG13 | 2.00 | 0.44 |
| 1:E:199:LYS:O | 1:E:229:ALA:HB1 | 2.18 | 0.44 |
| 1:C:127:LEU:HA | 1:C:127:LEU:HD23 | 1.81 | 0.44 |
| 1:C:186:THR:HA | 1:C:189:LYS:CD | 2.44 | 0.44 |
| 1:G:250:LEU:HB3 | 1:G:252:ILE:HG13 | 2.00 | 0.44 |
| 1:L:252:ILE:HG22 | 1:L:255:ARG:HB2 | 2.00 | 0.44 |
| 1:G:122:THR:HA | 1:G:126:VAL:HG12 | 2.00 | 0.44 |
| 1:B:252:ILE:HG22 | 1:B:255:ARG:HB2 | 1.99 | 0.44 |
| 1:E:239:GLU:O | 1:E:243:ILE:HG12 | 2.18 | 0.44 |
| 1:K:34:ILE:HD12 | 1:K:34:ILE:N | 2.33 | 0.44 |
| 1:A:281:LYS:HA | 1:A:303:VAL:CG1 | 2.32 | 0.44 |
| 1:A:282:GLU:HG3 | 1:A:284:PHE:H | 1.82 | 0.44 |
| 1:E:282:GLU:HG3 | 1:E:284:PHE:H | 1.82 | 0.44 |
| 1:L:334:LEU:HD11 | 1:L:341:HIS:HA | 2.00 | 0.44 |
| 1:H:186:THR:HA | 1:H:189:LYS:CD | 2.45 | 0.44 |
| 1:J:177:GLU:HG3 | 1:J:357:ARG:HH11 | 1.82 | 0.44 |
| 1:A:72:LEU:CD2 | 1:B:97:PRO:HB3 | 2.47 | 0.44 |
| 1:A:250:LEU:HB3 | 1:A:252:ILE:HG13 | 2.00 | 0.44 |
| 1:D:250:LEU:HB3 | 1:D:252:ILE:HG13 | 2.00 | 0.44 |
| 1:D:252:ILE:HG22 | 1:D:255:ARG:HB2 | 2.00 | 0.44 |
| 1:F:114:LYS:HG3 | 1:F:373:LEU:HD23 | 2.00 | 0.44 |
| 1:B:175:ILE:HD13 | 1:B:175:ILE:HA | 1.80 | 0.44 |
| 1:J:175:ILE:HA | 1:J:175:ILE:HD13 | 1.78 | 0.44 |
| 1:G:277:LEU:O | 1:G:300:GLY:HA2 | 2.17 | 0.44 |
| 1:G:300:GLY:O | 1:G:318:LEU:HA | 2.18 | 0.44 |
| 1:H:277:LEU:O | 1:H:300:GLY:HA2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:C:275:MET:SD | 1:C:287:VAL:HG23 | 2.57 | 0.44 |
| 1:G:257:LEU:HD13 | 1:G:257:LEU:N | 2.28 | 0.44 |
| 1:F:122:THR:HA | 1:F:126:VAL:HG12 | 2.00 | 0.44 |
| 1:J:250:LEU:HB3 | 1:J:252:ILE:HG13 | 2.00 | 0.44 |
| 1:K:122:THR:HA | 1:K:126:VAL:HG12 | 2.00 | 0.44 |
| 1:E:252:ILE:HG22 | 1:E:255:ARG:HB2 | 2.00 | 0.44 |
| 1:G:97:PRO:HB3 | 1:H:72:LEU:HD21 | 2.00 | 0.44 |
| 1:I:239:GLU:O | 1:I:243:ILE:HG12 | 2.18 | 0.44 |
| 1:C:239:GLU:O | 1:C:243:ILE:HG12 | 2.17 | 0.44 |
| 1:D:104:LEU:HA | 1:D:104:LEU:HD23 | 1.84 | 0.44 |
| 1:K:104:LEU:HA | 1:K:104:LEU:HD23 | 1.83 | 0.44 |
| 1:G:281:LYS:O | 1:G:282:GLU:CB | 2.57 | 0.44 |
| 1:H:289:LEU:N | 1:H:289:LEU:HD12 | 2.33 | 0.44 |
| 1:A:312:HIS:CD2 | 1:A:313:GLY:N | 2.86 | 0.44 |
| 1:F:199:LYS:HB2 | 1:F:229:ALA:CB | 2.35 | 0.44 |
| 1:A:252:ILE:HG22 | 1:A:255:ARG:HB2 | 2.00 | 0.44 |
| 1:H:250:LEU:HB3 | 1:H:252:ILE:HG13 | 2.00 | 0.44 |
| 1:B:277:LEU:O | 1:B:300:GLY:HA2 | 2.17 | 0.44 |
| 1:L:312:HIS:CD2 | 1:L:313:GLY:N | 2.86 | 0.43 |
| 1:D:334:LEU:HD11 | 1:D:341:HIS:HA | 1.99 | 0.43 |
| 1:I:250:LEU:HB3 | 1:I:252:ILE:HG13 | 2.00 | 0.43 |
| 1:L:250:LEU:HB3 | 1:L:252:ILE:HG13 | 2.00 | 0.43 |
| 1:L:114:LYS:HG3 | 1:L:373:LEU:HD23 | 2.00 | 0.43 |
| 1:C:114:LYS:HG3 | 1:C:373:LEU:HD23 | 2.00 | 0.43 |
| 1:G:239:GLU:O | 1:G:243:ILE:HG12 | 2.18 | 0.43 |
| 1:B:77:LYS:O | 1:B:81:VAL:HG23 | 2.18 | 0.43 |
| 1:G:79:ALA:CB | 1:G:108:MET:HE2 | 2.48 | 0.43 |
| 1:K:277:LEU:O | 1:K:300:GLY:HA2 | 2.17 | 0.43 |
| 1:J:239:GLU:O | 1:J:243:ILE:HG12 | 2.17 | 0.43 |
| 1:L:287:VAL:HG22 | 1:L:288:LEU:N | 2.29 | 0.43 |
| 1:C:334:LEU:HD11 | 1:C:341:HIS:HA | 1.99 | 0.43 |
| 1:F:306:ILE:H | 1:F:307:PRO:HD2 | 1.83 | 0.43 |
| 1:G:252:ILE:HG22 | 1:G:255:ARG:HB2 | 1.99 | 0.43 |
| 1:B:250:LEU:HB3 | 1:B:252:ILE:HG13 | 2.00 | 0.43 |
| 1:C:300:GLY:O | 1:C:318:LEU:HA | 2.18 | 0.43 |
| 1:D:277:LEU:O | 1:D:300:GLY:HA2 | 2.17 | 0.43 |
| 1:D:239:GLU:O | 1:D:243:ILE:HG12 | 2.18 | 0.43 |
| 1:G:77:LYS:O | 1:G:81:VAL:HG23 | 2.19 | 0.43 |
| 1:A:97:PRO:HB3 | 1:B:72:LEU:CD2 | 2.48 | 0.43 |
| 1:C:173:ASN:OD1 | 1:C:284:PHE:HD1 | 2.00 | 0.43 |
| 1:I:275:MET:SD | 1:I:287:VAL:HG23 | 2.58 | 0.43 |
| 1:B:312:HIS:CD2 | 1:B:313:GLY:N | 2.86 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:H:177:GLU:HG3 | 1:H:357:ARG:HH11 | 1.81 | 0.43 |
| 1:J:252:ILE:HG22 | 1:J:255:ARG:HB2 | 2.00 | 0.43 |
| 1:D:77:LYS:O | 1:D:81:VAL:HG23 | 2.19 | 0.43 |
| 1:L:277:LEU:O | 1:L:300:GLY:HA2 | 2.17 | 0.43 |
| 1:L:300:GLY:O | 1:L:318:LEU:HA | 2.19 | 0.43 |
| 1:J:212:ARG:HD3 | 1:J:280:GLU:OE1 | 2.18 | 0.43 |
| 1:C:288:LEU:HD23 | 1:C:288:LEU:HA | 1.62 | 0.43 |
| 1:H:257:LEU:HA | 1:H:257:LEU:HD12 | 1.63 | 0.43 |
| 1:I:257:LEU:N | 1:I:257:LEU:HD13 | 2.28 | 0.43 |
| 1:A:114:LYS:HG3 | 1:A:373:LEU:HD23 | 2.00 | 0.43 |
| 1:G:136:LEU:HD22 | 1:H:76:SER:HB2 | 1.99 | 0.43 |
| 1:A:77:LYS:O | 1:A:81:VAL:HG23 | 2.19 | 0.43 |
| 1:B:239:GLU:O | 1:B:243:ILE:HG12 | 2.18 | 0.43 |
| 1:F:34:ILE:N | 1:F:34:ILE:HD12 | 2.34 | 0.43 |
| 1:K:173:ASN:HB2 | 1:K:284:PHE:CE1 | 2.52 | 0.43 |
| 1:F:257:LEU:HD13 | 1:F:257:LEU:N | 2.28 | 0.43 |
| 1:K:257:LEU:O | 1:K:259:LEU:N | 2.52 | 0.43 |
| 1:C:312:HIS:CD2 | 1:C:313:GLY:N | 2.87 | 0.43 |
| 1:F:334:LEU:HD11 | 1:F:341:HIS:HA | 1.99 | 0.43 |
| 1:D:312:HIS:CD2 | 1:D:313:GLY:N | 2.86 | 0.43 |
| 1:H:199:LYS:O | 1:H:229:ALA:HB1 | 2.18 | 0.43 |
| 1:B:182:LYS:HZ2 | 1:B:349:ARG:HD3 | 1.81 | 0.43 |
| 1:C:306:ILE:H | 1:C:307:PRO:HD2 | 1.83 | 0.43 |
| 1:I:306:ILE:H | 1:I:307:PRO:HD2 | 1.84 | 0.43 |
| 1:K:250:LEU:HB3 | 1:K:252:ILE:HG13 | 2.01 | 0.43 |
| 1:E:122:THR:HA | 1:E:126:VAL:HG12 | 2.00 | 0.43 |
| 1:I:122:THR:HA | 1:I:126:VAL:HG12 | 2.00 | 0.43 |
| 1:D:114:LYS:HG3 | 1:D:373:LEU:HD23 | 2.00 | 0.43 |
| 1:B:300:GLY:O | 1:B:318:LEU:HA | 2.19 | 0.43 |
| 1:C:311:GLN:HG3 | 1:C:314:ASP:HB3 | 2.01 | 0.43 |
| 1:L:77:LYS:O | 1:L:81:VAL:HG23 | 2.19 | 0.43 |
| 1:F:346:GLU:O | 1:F:350:GLU:HG3 | 2.19 | 0.43 |
| 1:K:346:GLU:O | 1:K:350:GLU:HG3 | 2.18 | 0.43 |
| 1:L:289:LEU:N | 1:L:289:LEU:HD12 | 2.34 | 0.43 |
| 1:I:312:HIS:CD2 | 1:I:313:GLY:N | 2.87 | 0.43 |
| 1:H:312:HIS:CD2 | 1:H:313:GLY:N | 2.86 | 0.43 |
| 1:E:334:LEU:HD11 | 1:E:341:HIS:HA | 1.99 | 0.43 |
| 1:J:186:THR:HA | 1:J:189:LYS:CD | 2.45 | 0.43 |
| 1:E:300:GLY:O | 1:E:318:LEU:HA | 2.19 | 0.43 |
| 1:A:239:GLU:O | 1:A:243:ILE:HG12 | 2.18 | 0.43 |
| 1:B:311:GLN:HG3 | 1:B:314:ASP:HB3 | 2.01 | 0.43 |
| 1:B:287:VAL:HG22 | 1:B:288:LEU:N | 2.29 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:289:LEU:HD12 | 1:B:289:LEU:N | 2.33 | 0.43 |
| 1:C:281:LYS:HZ2 | 1:C:281:LYS:HB2 | 1.83 | 0.43 |
| 1:D:281:LYS:O | 1:D:282:GLU:CB | 2.58 | 0.43 |
| 1:G:257:LEU:O | 1:G:259:LEU:N | 2.52 | 0.43 |
| 1:K:334:LEU:HD11 | 1:K:341:HIS:HA | 1.99 | 0.43 |
| 1:G:313:GLY:N | 1:G:316:GLY:O | 2.38 | 0.43 |
| 1:H:122:THR:HA | 1:H:126:VAL:HG12 | 2.00 | 0.43 |
| 1:C:122:THR:HA | 1:C:126:VAL:HG12 | 2.00 | 0.43 |
| 1:H:252:ILE:HG22 | 1:H:255:ARG:HB2 | 2.00 | 0.43 |
| 1:H:300:GLY:O | 1:H:318:LEU:HA | 2.18 | 0.43 |
| 1:D:300:GLY:O | 1:D:318:LEU:HA | 2.18 | 0.43 |
| 1:I:311:GLN:HG3 | 1:I:314:ASP:HB3 | 2.01 | 0.43 |
| 1:J:277:LEU:O | 1:J:300:GLY:HA2 | 2.18 | 0.43 |
| 1:K:239:GLU:O | 1:K:243:ILE:HG12 | 2.18 | 0.43 |
| 1:B:34:ILE:N | 1:B:34:ILE:HD12 | 2.34 | 0.43 |
| 1:C:34:ILE:HD12 | 1:C:34:ILE:N | 2.34 | 0.43 |
| 1:I:289:LEU:HD12 | 1:I:289:LEU:N | 2.34 | 0.43 |
| 1:G:288:LEU:HD23 | 1:G:288:LEU:HA | 1.62 | 0.43 |
| 1:C:257:LEU:O | 1:C:259:LEU:N | 2.52 | 0.43 |
| 1:I:257:LEU:O | 1:I:259:LEU:N | 2.52 | 0.43 |
| 1:B:257:LEU:HD13 | 1:B:257:LEU:N | 2.28 | 0.43 |
| 1:F:312:HIS:CD2 | 1:F:313:GLY:N | 2.87 | 0.43 |
| 1:E:312:HIS:CD2 | 1:E:313:GLY:N | 2.87 | 0.43 |
| 1:K:252:ILE:HG22 | 1:K:255:ARG:HB2 | 2.00 | 0.43 |
| 1:D:122:THR:HA | 1:D:126:VAL:HG12 | 2.00 | 0.43 |
| 1:I:252:ILE:HG22 | 1:I:255:ARG:HB2 | 2.00 | 0.43 |
| 1:I:114:LYS:HG3 | 1:I:373:LEU:HD23 | 2.00 | 0.43 |
| 1:K:96:ILE:HG22 | 1:L:65:PHE:CZ | 2.54 | 0.43 |
| 1:E:119:LEU:HD22 | 1:E:124:ILE:CD1 | 2.49 | 0.43 |
| 1:H:239:GLU:O | 1:H:243:ILE:HG12 | 2.18 | 0.43 |
| 1:E:77:LYS:O | 1:E:81:VAL:HG23 | 2.19 | 0.43 |
| 1:A:34:ILE:N | 1:A:34:ILE:HD12 | 2.34 | 0.43 |
| 1:A:311:GLN:HG3 | 1:A:314:ASP:HB3 | 2.01 | 0.43 |
| 1:B:281:LYS:HA | 1:B:303:VAL:CG1 | 2.32 | 0.43 |
| 1:J:275:MET:SD | 1:J:287:VAL:HG23 | 2.59 | 0.43 |
| 1:D:313:GLY:N | 1:D:316:GLY:O | 2.38 | 0.43 |
| 1:J:312:HIS:CD2 | 1:J:313:GLY:N | 2.87 | 0.43 |
| 1:J:334:LEU:HD11 | 1:J:341:HIS:HA | 2.00 | 0.43 |
| 1:C:199:LYS:O | 1:C:229:ALA:HB1 | 2.18 | 0.43 |
| 1:E:182:LYS:HZ2 | 1:E:349:ARG:CD | 2.31 | 0.43 |
| 1:K:136:LEU:HD22 | 1:L:76:SER:HB2 | 1.99 | 0.43 |
| 1:B:186:THR:HA | 1:B:189:LYS:CD | 2.45 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:J:114:LYS:HG3 | 1:J:373:LEU:HD23 | 2.01 | 0.43 |
| 1:F:300:GLY:O | 1:F:318:LEU:HA | 2.18 | 0.43 |
| 1:K:274:LEU:HD11 | 1:K:299:ILE:HG13 | 2.01 | 0.43 |
| 1:G:346:GLU:O | 1:G:350:GLU:HG3 | 2.19 | 0.43 |
| 1:J:311:GLN:HG3 | 1:J:314:ASP:HB3 | 2.00 | 0.43 |
| 1:F:77:LYS:O | 1:F:81:VAL:HG23 | 2.18 | 0.43 |
| 1:L:311:GLN:HG3 | 1:L:314:ASP:HB3 | 2.01 | 0.43 |
| 1:J:34:ILE:HD12 | 1:J:34:ILE:N | 2.34 | 0.43 |
| 1:E:289:LEU:N | 1:E:289:LEU:HD12 | 2.34 | 0.43 |
| 1:D:127:LEU:HD23 | 1:D:127:LEU:HA | 1.81 | 0.43 |
| 1:I:186:THR:HA | 1:I:189:LYS:CD | 2.45 | 0.43 |
| 1:L:119:LEU:HD22 | 1:L:124:ILE:CD1 | 2.49 | 0.43 |
| 1:K:121:GLY:O | 1:K:125:THR:CB | 2.66 | 0.43 |
| 1:B:346:GLU:O | 1:B:350:GLU:HG3 | 2.19 | 0.43 |
| 1:H:346:GLU:O | 1:H:350:GLU:HG3 | 2.18 | 0.43 |
| 1:F:138:ARG:O | 1:F:142:GLU:HG3 | 2.19 | 0.43 |
| 1:A:274:LEU:HD11 | 1:A:299:ILE:HG13 | 2.01 | 0.43 |
| 1:F:275:MET:SD | 1:F:287:VAL:HG21 | 2.59 | 0.42 |
| 1:H:336:LYS:HE2 | 1:H:336:LYS:HB3 | 1.85 | 0.42 |
| 1:J:306:ILE:H | 1:J:307:PRO:HD2 | 1.84 | 0.42 |
| 1:C:177:GLU:HG3 | 1:C:357:ARG:HH11 | 1.81 | 0.42 |
| 1:C:250:LEU:HB3 | 1:C:252:ILE:HG13 | 2.00 | 0.42 |
| 1:A:122:THR:HA | 1:A:126:VAL:HG12 | 2.00 | 0.42 |
| 1:E:114:LYS:HG3 | 1:E:373:LEU:HD23 | 2.00 | 0.42 |
| 1:K:114:LYS:HG3 | 1:K:373:LEU:HD23 | 2.01 | 0.42 |
| 1:G:121:GLY:O | 1:G:125:THR:CB | 2.67 | 0.42 |
| 1:J:300:GLY:O | 1:J:318:LEU:HA | 2.18 | 0.42 |
| 1:A:138:ARG:O | 1:A:142:GLU:HG3 | 2.19 | 0.42 |
| 1:K:311:GLN:HG3 | 1:K:314:ASP:HB3 | 2.01 | 0.42 |
| 1:B:104:LEU:HA | 1:B:104:LEU:HD23 | 1.83 | 0.42 |
| 1:E:34:ILE:HD12 | 1:E:34:ILE:N | 2.34 | 0.42 |
| 1:A:275:MET:SD | 1:A:287:VAL:HG21 | 2.59 | 0.42 |
| 1:I:212:ARG:HD3 | 1:I:280:GLU:OE1 | 2.20 | 0.42 |
| 1:E:286:LEU:N | 1:E:286:LEU:CD1 | 2.31 | 0.42 |
| 1:G:275:MET:SD | 1:G:287:VAL:HG21 | 2.59 | 0.42 |
| 1:A:334:LEU:HD11 | 1:A:341:HIS:HA | 1.99 | 0.42 |
| 1:J:313:GLY:N | 1:J:316:GLY:O | 2.38 | 0.42 |
| 1:A:300:GLY:O | 1:A:318:LEU:HA | 2.18 | 0.42 |
| 1:C:77:LYS:O | 1:C:81:VAL:HG23 | 2.19 | 0.42 |
| 1:H:34:ILE:N | 1:H:34:ILE:HD12 | 2.34 | 0.42 |
| 1:I:34:ILE:HD12 | 1:I:34:ILE:N | 2.34 | 0.42 |
| 1:A:289:LEU:HD12 | 1:A:289:LEU:N | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:J:257:LEU:O | 1:J:259:LEU:N | 2.52 | 0.42 |
| 1:G:334:LEU:HD11 | 1:G:341:HIS:HA | 1.99 | 0.42 |
| 1:B:267:GLU:OE1 | 1:D:48:VAL:CG1 | 2.67 | 0.42 |
| 1:B:122:THR:HA | 1:B:126:VAL:HG12 | 2.00 | 0.42 |
| 1:H:114:LYS:HG3 | 1:H:373:LEU:HD23 | 2.00 | 0.42 |
| 1:B:119:LEU:HD22 | 1:B:124:ILE:CD1 | 2.50 | 0.42 |
| 1:C:119:LEU:HD22 | 1:C:124:ILE:CD1 | 2.50 | 0.42 |
| 1:G:155:ILE:CG2 | 1:L:156:ASN:HD21 | 2.32 | 0.42 |
| 1:I:300:GLY:O | 1:I:318:LEU:HA | 2.19 | 0.42 |
| 1:H:138:ARG:O | 1:H:142:GLU:HG3 | 2.20 | 0.42 |
| 1:D:346:GLU:O | 1:D:350:GLU:HG3 | 2.19 | 0.42 |
| 1:C:284:PHE:CD2 | 1:C:284:PHE:O | 2.72 | 0.42 |
| 1:L:212:ARG:HD3 | 1:L:280:GLU:OE1 | 2.20 | 0.42 |
| 1:D:212:ARG:HD3 | 1:D:280:GLU:OE1 | 2.20 | 0.42 |
| 1:F:257:LEU:O | 1:F:259:LEU:N | 2.52 | 0.42 |
| 1:I:257:LEU:HA | 1:I:257:LEU:HD12 | 1.63 | 0.42 |
| 1:F:336:LYS:HE2 | 1:F:336:LYS:HB3 | 1.85 | 0.42 |
| 1:I:199:LYS:O | 1:I:229:ALA:HB1 | 2.17 | 0.42 |
| 1:C:252:ILE:HG22 | 1:C:255:ARG:HB2 | 2.00 | 0.42 |
| 1:A:119:LEU:HD22 | 1:A:124:ILE:CD1 | 2.50 | 0.42 |
| 1:A:136:LEU:HD21 | 1:B:72:LEU:HB3 | 2.01 | 0.42 |
| 1:E:138:ARG:O | 1:E:142:GLU:HG3 | 2.20 | 0.42 |
| 1:K:138:ARG:O | 1:K:142:GLU:HG3 | 2.19 | 0.42 |
| 1:C:274:LEU:HD11 | 1:C:299:ILE:HG13 | 2.02 | 0.42 |
| 1:E:104:LEU:HD23 | 1:E:104:LEU:HA | 1.84 | 0.42 |
| 1:J:90:LEU:HD12 | 1:J:90:LEU:HA | 1.86 | 0.42 |
| 1:G:284:PHE:O | 1:G:284:PHE:CD2 | 2.73 | 0.42 |
| 1:B:212:ARG:HD3 | 1:B:280:GLU:OE1 | 2.20 | 0.42 |
| 1:H:275:MET:SD | 1:H:287:VAL:HG21 | 2.59 | 0.42 |
| 1:A:257:LEU:O | 1:A:259:LEU:N | 2.52 | 0.42 |
| 1:K:313:GLY:N | 1:K:316:GLY:O | 2.38 | 0.42 |
| 1:H:334:LEU:HD11 | 1:H:341:HIS:HA | 2.00 | 0.42 |
| 1:F:313:GLY:N | 1:F:316:GLY:O | 2.38 | 0.42 |
| 1:J:122:THR:HA | 1:J:126:VAL:HG12 | 2.00 | 0.42 |
| 1:L:122:THR:HA | 1:L:126:VAL:HG12 | 2.00 | 0.42 |
| 1:G:114:LYS:HG3 | 1:G:373:LEU:HD23 | 2.00 | 0.42 |
| 1:K:119:LEU:HD22 | 1:K:124:ILE:CD1 | 2.49 | 0.42 |
| 1:H:104:LEU:HA | 1:H:104:LEU:HD23 | 1.83 | 0.42 |
| 1:G:311:GLN:HG3 | 1:G:314:ASP:HB3 | 2.01 | 0.42 |
| 1:B:275:MET:SD | 1:B:287:VAL:HG21 | 2.60 | 0.42 |
| 1:H:284:PHE:O | 1:H:284:PHE:CD2 | 2.72 | 0.42 |
| 1:C:289:LEU:N | 1:C:289:LEU:HD12 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:284:PHE:CD2 | 1:D:284:PHE:O | 2.73 | 0.42 |
| 1:G:312:HIS:CD2 | 1:G:313:GLY:N | 2.87 | 0.42 |
| 1:K:49:TYR:HA | 1:K:50:PRO:HD3 | 1.86 | 0.42 |
| 1:K:274:LEU:HD21 | 1:K:299:ILE:HD12 | 2.01 | 0.42 |
| 1:L:346:GLU:O | 1:L:350:GLU:HG3 | 2.19 | 0.42 |
| 1:H:77:LYS:O | 1:H:81:VAL:HG23 | 2.19 | 0.42 |
| 1:A:346:GLU:O | 1:A:350:GLU:HG3 | 2.19 | 0.42 |
| 1:H:274:LEU:HD11 | 1:H:299:ILE:HG13 | 2.01 | 0.42 |
| 1:D:34:ILE:HD12 | 1:D:34:ILE:N | 2.34 | 0.42 |
| 1:B:90:LEU:HD12 | 1:B:90:LEU:HA | 1.87 | 0.42 |
| 1:L:239:GLU:O | 1:L:243:ILE:HG12 | 2.18 | 0.42 |
| 1:B:286:LEU:CD1 | 1:B:286:LEU:N | 2.31 | 0.42 |
| 1:C:212:ARG:HD3 | 1:C:280:GLU:OE1 | 2.19 | 0.42 |
| 1:F:289:LEU:HD12 | 1:F:289:LEU:N | 2.34 | 0.42 |
| 1:C:292:MET:C | 1:C:294:CYS:N | 2.73 | 0.42 |
| 1:D:281:LYS:HZ2 | 1:D:281:LYS:HB2 | 1.84 | 0.42 |
| 1:L:127:LEU:HD23 | 1:L:127:LEU:HA | 1.82 | 0.42 |
| 1:B:306:ILE:H | 1:B:307:PRO:HD2 | 1.83 | 0.42 |
| 1:B:127:LEU:HD23 | 1:B:127:LEU:HA | 1.81 | 0.42 |
| 1:G:186:THR:HA | 1:G:189:LYS:CD | 2.45 | 0.42 |
| 1:C:218:GLN:O | 1:C:222:LYS:HG3 | 2.20 | 0.42 |
| 1:D:138:ARG:O | 1:D:142:GLU:HG3 | 2.19 | 0.42 |
| 1:G:212:ARG:HD3 | 1:G:280:GLU:OE1 | 2.20 | 0.42 |
| 1:C:281:LYS:HA | 1:C:303:VAL:CG1 | 2.32 | 0.42 |
| 1:D:275:MET:SD | 1:D:287:VAL:HG21 | 2.59 | 0.42 |
| 1:C:275:MET:SD | 1:C:287:VAL:HG21 | 2.60 | 0.42 |
| 1:H:257:LEU:HD13 | 1:H:257:LEU:N | 2.28 | 0.42 |
| 1:D:182:LYS:HZ2 | 1:D:349:ARG:CD | 2.33 | 0.42 |
| 1:K:182:LYS:HZ2 | 1:K:349:ARG:HD3 | 1.81 | 0.42 |
| 1:D:121:GLY:O | 1:D:125:THR:CB | 2.68 | 0.42 |
| 1:F:311:GLN:HG3 | 1:F:314:ASP:HB3 | 2.01 | 0.42 |
| 1:H:218:GLN:O | 1:H:222:LYS:HG3 | 2.20 | 0.42 |
| 1:I:274:LEU:HD11 | 1:I:299:ILE:HG13 | 2.01 | 0.42 |
| 1:E:346:GLU:O | 1:E:350:GLU:HG3 | 2.19 | 0.42 |
| 1:L:275:MET:SD | 1:L:287:VAL:HG21 | 2.59 | 0.42 |
| 1:L:288:LEU:HD23 | 1:L:288:LEU:HA | 1.62 | 0.42 |
| 1:G:292:MET:C | 1:G:294:CYS:N | 2.73 | 0.42 |
| 1:K:312:HIS:CD2 | 1:K:313:GLY:N | 2.87 | 0.42 |
| 1:A:336:LYS:HB3 | 1:A:336:LYS:HE2 | 1.85 | 0.42 |
| 1:B:313:GLY:N | 1:B:316:GLY:O | 2.38 | 0.42 |
| 1:K:186:THR:HA | 1:K:189:LYS:CD | 2.45 | 0.42 |
| 1:F:314:ASP:CG | 1:F:347:ARG:HE | 2.23 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:E:311:GLN:HG3 | 1:E:314:ASP:HB3 | 2.01 | 0.42 |
| 1:B:138:ARG:O | 1:B:142:GLU:HG3 | 2.20 | 0.42 |
| 1:I:79:ALA:CB | 1:I:108:MET:HE2 | 2.49 | 0.42 |
| 1:J:104:LEU:HA | 1:J:104:LEU:HD23 | 1.85 | 0.42 |
| 1:G:218:GLN:O | 1:G:222:LYS:HG3 | 2.20 | 0.42 |
| 1:D:292:MET:C | 1:D:294:CYS:N | 2.73 | 0.42 |
| 1:B:257:LEU:O | 1:B:259:LEU:N | 2.52 | 0.42 |
| 1:C:336:LYS:HG2 | 1:C:336:LYS:H | 1.64 | 0.42 |
| 1:D:119:LEU:HD22 | 1:D:124:ILE:CD1 | 2.49 | 0.42 |
| 1:J:202:ILE:HG12 | 1:J:232:LEU:HB2 | 2.02 | 0.42 |
| 1:J:121:GLY:O | 1:J:125:THR:CB | 2.68 | 0.42 |
| 1:E:212:ARG:HD3 | 1:E:280:GLU:OE1 | 2.20 | 0.41 |
| 1:I:284:PHE:CD2 | 1:I:284:PHE:O | 2.73 | 0.41 |
| 1:F:212:ARG:HD3 | 1:F:280:GLU:OE1 | 2.20 | 0.41 |
| 1:I:182:LYS:HZ2 | 1:I:349:ARG:CD | 2.33 | 0.41 |
| 1:K:127:LEU:HA | 1:K:127:LEU:HD23 | 1.83 | 0.41 |
| 1:G:306:ILE:H | 1:G:307:PRO:HD2 | 1.83 | 0.41 |
| 1:E:189:LYS:HB3 | 1:E:194:ILE:HG23 | 2.02 | 0.41 |
| 1:G:189:LYS:HB3 | 1:G:194:ILE:HG23 | 2.02 | 0.41 |
| 1:C:189:LYS:HB3 | 1:C:194:ILE:HG23 | 2.02 | 0.41 |
| 1:G:138:ARG:O | 1:G:142:GLU:HG3 | 2.20 | 0.41 |
| 1:H:128:GLY:HA2 | 1:H:137:ILE:HD12 | 2.02 | 0.41 |
| 1:I:218:GLN:O | 1:I:222:LYS:HG3 | 2.20 | 0.41 |
| 1:C:128:GLY:HA2 | 1:C:137:ILE:HD12 | 2.02 | 0.41 |
| 1:D:218:GLN:O | 1:D:222:LYS:HG3 | 2.20 | 0.41 |
| 1:D:314:ASP:CG | 1:D:347:ARG:HE | 2.24 | 0.41 |
| 1:L:34:ILE:N | 1:L:34:ILE:HD12 | 2.35 | 0.41 |
| 1:K:284:PHE:CD2 | 1:K:284:PHE:O | 2.72 | 0.41 |
| 1:A:212:ARG:HD3 | 1:A:280:GLU:OE1 | 2.19 | 0.41 |
| 1:I:292:MET:C | 1:I:294:CYS:N | 2.73 | 0.41 |
| 1:H:212:ARG:HD3 | 1:H:280:GLU:OE1 | 2.19 | 0.41 |
| 1:K:275:MET:SD | 1:K:287:VAL:HG21 | 2.60 | 0.41 |
| 1:H:257:LEU:O | 1:H:259:LEU:N | 2.52 | 0.41 |
| 1:E:257:LEU:O | 1:E:259:LEU:N | 2.52 | 0.41 |
| 1:F:336:LYS:HG2 | 1:F:336:LYS:H | 1.64 | 0.41 |
| 1:I:127:LEU:HA | 1:I:127:LEU:HD23 | 1.81 | 0.41 |
| 1:B:314:ASP:CG | 1:B:347:ARG:HE | 2.24 | 0.41 |
| 1:J:314:ASP:CG | 1:J:347:ARG:HE | 2.24 | 0.41 |
| 1:I:274:LEU:HD21 | 1:I:299:ILE:HD12 | 2.03 | 0.41 |
| 1:B:79:ALA:CB | 1:B:108:MET:HE2 | 2.50 | 0.41 |
| 1:E:274:LEU:HD11 | 1:E:299:ILE:HG13 | 2.02 | 0.41 |
| 1:G:274:LEU:HD21 | 1:G:299:ILE:HD12 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:218:GLN:O | 1:A:222:LYS:HG3 | 2.21 | 0.41 |
| 1:J:281:LYS:HB2 | 1:J:281:LYS:HZ2 | 1.85 | 0.41 |
| 1:J:282:GLU:HG3 | 1:J:284:PHE:H | 1.85 | 0.41 |
| 1:J:288:LEU:HD23 | 1:J:288:LEU:HA | 1.62 | 0.41 |
| 1:J:289:LEU:N | 1:J:289:LEU:HD12 | 2.34 | 0.41 |
| 1:H:292:MET:C | 1:H:294:CYS:N | 2.74 | 0.41 |
| 1:H:49:TYR:HA | 1:H:50:PRO:HD3 | 1.85 | 0.41 |
| 1:A:306:ILE:N | 1:A:307:PRO:HD2 | 2.35 | 0.41 |
| 1:B:189:LYS:HB3 | 1:B:194:ILE:HG23 | 2.02 | 0.41 |
| 1:I:189:LYS:HB3 | 1:I:194:ILE:HG23 | 2.02 | 0.41 |
| 1:G:119:LEU:HD22 | 1:G:124:ILE:CD1 | 2.50 | 0.41 |
| 1:C:159:HIS:CD2 | 1:I:159:HIS:CD2 | 3.08 | 0.41 |
| 1:I:119:LEU:HD22 | 1:I:124:ILE:CD1 | 2.50 | 0.41 |
| 1:C:121:GLY:O | 1:C:125:THR:CB | 2.68 | 0.41 |
| 1:A:121:GLY:O | 1:A:125:THR:CB | 2.68 | 0.41 |
| 1:L:314:ASP:CG | 1:L:347:ARG:HE | 2.23 | 0.41 |
| 1:B:128:GLY:HA2 | 1:B:137:ILE:HD12 | 2.02 | 0.41 |
| 1:C:346:GLU:O | 1:C:350:GLU:HG3 | 2.19 | 0.41 |
| 1:F:104:LEU:HA | 1:F:104:LEU:HD23 | 1.84 | 0.41 |
| 1:L:257:LEU:O | 1:L:259:LEU:N | 2.53 | 0.41 |
| 1:H:336:LYS:HG2 | 1:H:336:LYS:H | 1.64 | 0.41 |
| 1:G:182:LYS:HZ2 | 1:G:349:ARG:CD | 2.34 | 0.41 |
| 1:B:306:ILE:N | 1:B:307:PRO:HD2 | 2.35 | 0.41 |
| 1:G:202:ILE:HG12 | 1:G:232:LEU:HB2 | 2.02 | 0.41 |
| 1:H:121:GLY:O | 1:H:125:THR:CB | 2.68 | 0.41 |
| 1:F:202:ILE:HG12 | 1:F:232:LEU:HB2 | 2.03 | 0.41 |
| 1:A:314:ASP:CG | 1:A:347:ARG:HE | 2.24 | 0.41 |
| 1:H:311:GLN:HG3 | 1:H:314:ASP:HB3 | 2.01 | 0.41 |
| 1:D:311:GLN:HG3 | 1:D:314:ASP:HB3 | 2.01 | 0.41 |
| 1:I:77:LYS:O | 1:I:81:VAL:HG23 | 2.19 | 0.41 |
| 1:L:274:LEU:HD11 | 1:L:299:ILE:HG13 | 2.01 | 0.41 |
| 1:F:274:LEU:HD11 | 1:F:299:ILE:HG13 | 2.02 | 0.41 |
| 1:C:138:ARG:O | 1:C:142:GLU:HG3 | 2.19 | 0.41 |
| 1:B:274:LEU:HD11 | 1:B:299:ILE:HG13 | 2.01 | 0.41 |
| 1:B:274:LEU:HD21 | 1:B:299:ILE:HD12 | 2.02 | 0.41 |
| 1:D:274:LEU:HD21 | 1:D:299:ILE:HD12 | 2.03 | 0.41 |
| 1:K:289:LEU:HD12 | 1:K:289:LEU:N | 2.34 | 0.41 |
| 1:J:309:VAL:HG12 | 1:J:356:PHE:CZ | 2.56 | 0.41 |
| 1:B:309:VAL:HG12 | 1:B:356:PHE:CZ | 2.56 | 0.41 |
| 1:C:306:ILE:N | 1:C:307:PRO:HD2 | 2.36 | 0.41 |
| 1:C:136:LEU:HD21 | 1:D:72:LEU:CB | 2.42 | 0.41 |
| 1:H:189:LYS:HB3 | 1:H:194:ILE:HG23 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:L:189:LYS:HB3 | 1:L:194:ILE:HG23 | 2.02 | 0.41 |
| 1:E:121:GLY:O | 1:E:125:THR:CB | 2.68 | 0.41 |
| 1:E:314:ASP:CG | 1:E:347:ARG:HE | 2.24 | 0.41 |
| 1:L:274:LEU:HD21 | 1:L:299:ILE:HD12 | 2.03 | 0.41 |
| 1:F:175:ILE:HD13 | 1:F:175:ILE:HA | 1.79 | 0.41 |
| 1:B:284:PHE:O | 1:B:284:PHE:CD2 | 2.74 | 0.41 |
| 1:D:257:LEU:O | 1:D:259:LEU:N | 2.52 | 0.41 |
| 1:I:306:ILE:N | 1:I:307:PRO:HD2 | 2.36 | 0.41 |
| 1:F:189:LYS:HB3 | 1:F:194:ILE:HG23 | 2.02 | 0.41 |
| 1:C:202:ILE:HG12 | 1:C:232:LEU:HB2 | 2.03 | 0.41 |
| 1:K:300:GLY:O | 1:K:318:LEU:HA | 2.19 | 0.41 |
| 1:G:274:LEU:HD11 | 1:G:299:ILE:HG13 | 2.01 | 0.41 |
| 1:I:128:GLY:HA2 | 1:I:137:ILE:HD12 | 2.03 | 0.41 |
| 1:I:138:ARG:O | 1:I:142:GLU:HG3 | 2.20 | 0.41 |
| 1:F:218:GLN:O | 1:F:222:LYS:HG3 | 2.20 | 0.41 |
| 1:I:275:MET:SD | 1:I:287:VAL:HG21 | 2.60 | 0.41 |
| 1:K:287:VAL:O | 1:K:288:LEU:C | 2.55 | 0.41 |
| 1:J:250:LEU:HB3 | 1:J:252:ILE:CD1 | 2.51 | 0.41 |
| 1:H:314:ASP:CG | 1:H:347:ARG:HE | 2.24 | 0.41 |
| 1:J:218:GLN:O | 1:J:222:LYS:HG3 | 2.20 | 0.41 |
| 1:J:138:ARG:O | 1:J:142:GLU:HG3 | 2.20 | 0.41 |
| 1:E:128:GLY:HA2 | 1:E:137:ILE:HD12 | 2.03 | 0.41 |
| 1:K:77:LYS:O | 1:K:81:VAL:HG23 | 2.20 | 0.41 |
| 1:I:346:GLU:O | 1:I:350:GLU:HG3 | 2.19 | 0.41 |
| 1:L:175:ILE:HD13 | 1:L:175:ILE:HA | 1.80 | 0.41 |
| 1:D:289:LEU:HD12 | 1:D:289:LEU:N | 2.34 | 0.41 |
| 1:F:127:LEU:HA | 1:F:127:LEU:HD23 | 1.81 | 0.41 |
| 1:L:49:TYR:HA | 1:L:50:PRO:HD3 | 1.85 | 0.41 |
| 1:H:250:LEU:HB3 | 1:H:252:ILE:CD1 | 2.51 | 0.41 |
| 1:B:250:LEU:HB3 | 1:B:252:ILE:CD1 | 2.51 | 0.41 |
| 1:H:202:ILE:HG12 | 1:H:232:LEU:HB2 | 2.02 | 0.41 |
| 1:D:274:LEU:HD11 | 1:D:299:ILE:HG13 | 2.01 | 0.41 |
| 1:K:79:ALA:CB | 1:K:108:MET:HE2 | 2.51 | 0.41 |
| 1:A:128:GLY:HA2 | 1:A:137:ILE:HD12 | 2.03 | 0.41 |
| 1:A:287:VAL:O | 1:A:288:LEU:C | 2.56 | 0.41 |
| 1:K:212:ARG:HD3 | 1:K:280:GLU:OE1 | 2.19 | 0.41 |
| 1:K:19:VAL:HG11 | 1:K:173:ASN:HD22 | 1.86 | 0.41 |
| 1:E:284:PHE:O | 1:E:284:PHE:CD2 | 2.73 | 0.41 |
| 1:I:281:LYS:HZ3 | 1:I:281:LYS:HB2 | 1.83 | 0.41 |
| 1:F:284:PHE:O | 1:F:284:PHE:CD2 | 2.73 | 0.41 |
| 1:J:292:MET:C | 1:J:294:CYS:N | 2.74 | 0.41 |
| 1:H:286:LEU:CD1 | 1:H:286:LEU:N | 2.31 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:G:289:LEU:N | 1:G:289:LEU:HD12 | 2.33 | 0.41 |
| 1:J:257:LEU:N | 1:J:257:LEU:HD13 | 2.28 | 0.41 |
| 1:G:72:LEU:CB | 1:H:136:LEU:HD21 | 2.43 | 0.41 |
| 1:H:309:VAL:HG12 | 1:H:356:PHE:CZ | 2.56 | 0.41 |
| 1:D:309:VAL:HG12 | 1:D:356:PHE:CZ | 2.56 | 0.41 |
| 1:E:309:VAL:HG12 | 1:E:356:PHE:CZ | 2.56 | 0.41 |
| 1:A:189:LYS:HB3 | 1:A:194:ILE:HG23 | 2.02 | 0.41 |
| 1:A:250:LEU:HB3 | 1:A:252:ILE:CD1 | 2.51 | 0.41 |
| 1:D:250:LEU:HB3 | 1:D:252:ILE:CD1 | 2.51 | 0.41 |
| 1:I:250:LEU:HB3 | 1:I:252:ILE:CD1 | 2.51 | 0.41 |
| 1:L:250:LEU:HB3 | 1:L:252:ILE:CD1 | 2.51 | 0.41 |
| 1:E:250:LEU:HB3 | 1:E:252:ILE:CD1 | 2.51 | 0.41 |
| 1:A:202:ILE:HG12 | 1:A:232:LEU:HB2 | 2.03 | 0.41 |
| 1:B:121:GLY:O | 1:B:125:THR:CB | 2.68 | 0.41 |
| 1:F:121:GLY:O | 1:F:125:THR:CB | 2.68 | 0.41 |
| 1:G:314:ASP:CG | 1:G:347:ARG:HE | 2.24 | 0.41 |
| 1:E:347:ARG:O | 1:E:350:GLU:HB2 | 2.21 | 0.41 |
| 1:F:141:ILE:HG23 | 1:F:147:VAL:HG21 | 2.03 | 0.41 |
| 1:K:128:GLY:HA2 | 1:K:137:ILE:HD12 | 2.02 | 0.41 |
| 1:E:218:GLN:O | 1:E:222:LYS:HG3 | 2.20 | 0.41 |
| 1:A:3:LEU:HA | 1:A:3:LEU:HD12 | 1.94 | 0.41 |
| 1:A:104:LEU:HD23 | 1:A:104:LEU:HA | 1.84 | 0.41 |
| 1:J:346:GLU:O | 1:J:350:GLU:HG3 | 2.20 | 0.41 |
| 1:B:288:LEU:HA | 1:B:288:LEU:HD23 | 1.61 | 0.41 |
| 1:I:281:LYS:O | 1:I:282:GLU:CB | 2.57 | 0.41 |
| 1:E:275:MET:SD | 1:E:287:VAL:HG21 | 2.60 | 0.41 |
| 1:K:336:LYS:HE2 | 1:K:336:LYS:HB3 | 1.85 | 0.41 |
| 1:L:313:GLY:N | 1:L:316:GLY:O | 2.39 | 0.41 |
| 1:J:306:ILE:N | 1:J:307:PRO:HD2 | 2.36 | 0.41 |
| 1:F:306:ILE:N | 1:F:307:PRO:HD2 | 2.36 | 0.41 |
| 1:K:182:LYS:HZ1 | 1:K:349:ARG:HD3 | 1.86 | 0.41 |
| 1:E:186:THR:HA | 1:E:189:LYS:CD | 2.45 | 0.41 |
| 1:L:121:GLY:O | 1:L:125:THR:CB | 2.68 | 0.41 |
| 1:D:202:ILE:HG12 | 1:D:232:LEU:HB2 | 2.03 | 0.41 |
| 1:F:119:LEU:HD22 | 1:F:124:ILE:CD1 | 2.49 | 0.41 |
| 1:H:347:ARG:O | 1:H:350:GLU:HB2 | 2.21 | 0.41 |
| 1:B:218:GLN:O | 1:B:222:LYS:HG3 | 2.20 | 0.41 |
| 1:L:138:ARG:O | 1:L:142:GLU:HG3 | 2.20 | 0.41 |
| 1:J:128:GLY:HA2 | 1:J:137:ILE:HD12 | 2.02 | 0.41 |
| 1:L:39:SER:HB3 | 1:L:57:VAL:HB | 2.03 | 0.41 |
| 1:E:141:ILE:HG23 | 1:E:147:VAL:HG21 | 2.03 | 0.41 |
| 1:E:175:ILE:HD13 | 1:E:175:ILE:HA | 1.79 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:G:34:ILE:N | 1:G:34:ILE:HD12 | 2.34 | 0.41 |
| 1:F:292:MET:C | 1:F:294:CYS:N | 2.73 | 0.40 |
| 1:K:288:LEU:HA | 1:K:288:LEU:HD23 | 1.60 | 0.40 |
| 1:K:292:MET:C | 1:K:294:CYS:N | 2.73 | 0.40 |
| 1:J:275:MET:SD | 1:J:287:VAL:HG21 | 2.61 | 0.40 |
| 1:E:292:MET:C | 1:E:294:CYS:N | 2.73 | 0.40 |
| 1:D:336:LYS:H | 1:D:336:LYS:HG2 | 1.64 | 0.40 |
| 1:D:336:LYS:HE2 | 1:D:336:LYS:HB3 | 1.85 | 0.40 |
| 1:F:309:VAL:HG12 | 1:F:356:PHE:CZ | 2.56 | 0.40 |
| 1:G:309:VAL:HG12 | 1:G:356:PHE:CZ | 2.55 | 0.40 |
| 1:L:202:ILE:HG12 | 1:L:232:LEU:HB2 | 2.02 | 0.40 |
| 1:H:79:ALA:CB | 1:H:108:MET:HE2 | 2.51 | 0.40 |
| 1:E:49:TYR:HA | 1:E:50:PRO:HD3 | 1.85 | 0.40 |
| 1:E:134:ASN:ND2 | 1:E:138:ARG:NH2 | 2.69 | 0.40 |
| 1:B:134:ASN:ND2 | 1:B:138:ARG:NH2 | 2.69 | 0.40 |
| 1:F:274:LEU:HD21 | 1:F:299:ILE:HD12 | 2.03 | 0.40 |
| 1:D:141:ILE:HG23 | 1:D:147:VAL:HG21 | 2.03 | 0.40 |
| 1:J:274:LEU:HD11 | 1:J:299:ILE:HG13 | 2.02 | 0.40 |
| 1:J:274:LEU:HD21 | 1:J:299:ILE:HD12 | 2.03 | 0.40 |
| 1:A:284:PHE:O | 1:A:284:PHE:CD2 | 2.74 | 0.40 |
| 1:C:281:LYS:O | 1:C:282:GLU:CB | 2.58 | 0.40 |
| 1:I:291:ALA:O | 1:I:292:MET:C | 2.60 | 0.40 |
| 1:C:287:VAL:O | 1:C:288:LEU:C | 2.56 | 0.40 |
| 1:B:336:LYS:HE2 | 1:B:336:LYS:HB3 | 1.85 | 0.40 |
| 1:C:309:VAL:HG12 | 1:C:356:PHE:CZ | 2.56 | 0.40 |
| 1:L:306:ILE:N | 1:L:307:PRO:HD2 | 2.36 | 0.40 |
| 1:K:250:LEU:HB3 | 1:K:252:ILE:CD1 | 2.51 | 0.40 |
| 1:C:250:LEU:HB3 | 1:C:252:ILE:CD1 | 2.51 | 0.40 |
| 1:I:121:GLY:O | 1:I:125:THR:CB | 2.68 | 0.40 |
| 1:C:159:HIS:O | 1:I:156:ASN:OD1 | 2.38 | 0.40 |
| 1:B:347:ARG:O | 1:B:350:GLU:HB2 | 2.21 | 0.40 |
| 1:C:274:LEU:HD21 | 1:C:299:ILE:HD12 | 2.03 | 0.40 |
| 1:I:134:ASN:ND2 | 1:I:138:ARG:NH2 | 2.69 | 0.40 |
| 1:A:141:ILE:HG23 | 1:A:147:VAL:HG21 | 2.03 | 0.40 |
| 1:I:141:ILE:HG23 | 1:I:147:VAL:HG21 | 2.03 | 0.40 |
| 1:C:141:ILE:HG23 | 1:C:147:VAL:HG21 | 2.03 | 0.40 |
| 1:J:39:SER:HB3 | 1:J:57:VAL:HB | 2.04 | 0.40 |
| 1:L:291:ALA:O | 1:L:292:MET:C | 2.60 | 0.40 |
| 1:J:182:LYS:HZ2 | 1:J:349:ARG:CD | 2.34 | 0.40 |
| 1:L:306:ILE:H | 1:L:307:PRO:HD2 | 1.83 | 0.40 |
| 1:B:106:LYS:HG3 | 1:B:113:ILE:HG22 | 2.03 | 0.40 |
| 1:K:106:LYS:HG3 | 1:K:113:ILE:HG22 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:202:ILE:HG12 | 1:B:232:LEU:HB2 | 2.02 | 0.40 |
| 1:I:202:ILE:HG12 | 1:I:232:LEU:HB2 | 2.03 | 0.40 |
| 1:E:202:ILE:HG12 | 1:E:232:LEU:HB2 | 2.03 | 0.40 |
| 1:F:347:ARG:O | 1:F:350:GLU:HB2 | 2.21 | 0.40 |
| 1:L:347:ARG:O | 1:L:350:GLU:HB2 | 2.21 | 0.40 |
| 1:A:274:LEU:HD21 | 1:A:299:ILE:HD12 | 2.03 | 0.40 |
| 1:I:347:ARG:O | 1:I:350:GLU:HB2 | 2.22 | 0.40 |
| 1:G:141:ILE:HG23 | 1:G:147:VAL:HG21 | 2.03 | 0.40 |
| 1:H:351:SER:O | 1:H:355:GLN:HG2 | 2.21 | 0.40 |
| 1:B:292:MET:C | 1:B:294:CYS:N | 2.73 | 0.40 |
| 1:K:281:LYS:HA | 1:K:303:VAL:CG1 | 2.33 | 0.40 |
| 1:G:19:VAL:HG11 | 1:G:173:ASN:HD22 | 1.87 | 0.40 |
| 1:I:286:LEU:N | 1:I:286:LEU:CD1 | 2.30 | 0.40 |
| 1:F:19:VAL:HG11 | 1:F:173:ASN:HD22 | 1.87 | 0.40 |
| 1:J:306:ILE:HB | 1:J:307:PRO:CD | 2.44 | 0.40 |
| 1:H:306:ILE:H | 1:H:307:PRO:HD2 | 1.83 | 0.40 |
| 1:L:309:VAL:HG12 | 1:L:356:PHE:CZ | 2.57 | 0.40 |
| 1:G:250:LEU:HB3 | 1:G:252:ILE:CD1 | 2.51 | 0.40 |
| 1:A:146:VAL:HG11 | 1:A:368:ILE:CG2 | 2.52 | 0.40 |
| 1:H:134:ASN:ND2 | 1:H:138:ARG:NH2 | 2.70 | 0.40 |
| 1:D:128:GLY:HA2 | 1:D:137:ILE:HD12 | 2.03 | 0.40 |
| 1:K:218:GLN:O | 1:K:222:LYS:HG3 | 2.22 | 0.40 |
| 1:D:256:VAL:HG12 | 1:D:258:PHE:CD2 | 2.57 | 0.40 |
| 1:F:47:LYS:CG | 1:F:48:VAL:N | 2.81 | 0.40 |
| 1:A:127:LEU:HD23 | 1:A:127:LEU:HA | 1.82 | 0.40 |
| 1:G:127:LEU:HD23 | 1:G:127:LEU:HA | 1.81 | 0.40 |
| 1:E:306:ILE:H | 1:E:307:PRO:HD2 | 1.84 | 0.40 |
| 1:D:189:LYS:HB3 | 1:D:194:ILE:HG23 | 2.02 | 0.40 |
| 1:J:189:LYS:HB3 | 1:J:194:ILE:HG23 | 2.03 | 0.40 |
| 1:J:255:ARG:HH21 | 1:J:255:ARG:HD2 | 1.78 | 0.40 |
| 1:K:122:THR:CA | 1:K:126:VAL:HG12 | 2.52 | 0.40 |
| 1:F:106:LYS:HG3 | 1:F:113:ILE:HG22 | 2.03 | 0.40 |
| 1:J:119:LEU:HD22 | 1:J:124:ILE:CD1 | 2.51 | 0.40 |
| 1:B:146:VAL:HG11 | 1:B:368:ILE:CG2 | 2.52 | 0.40 |
| 1:H:274:LEU:HD21 | 1:H:299:ILE:HD12 | 2.02 | 0.40 |
| 1:C:134:ASN:ND2 | 1:C:138:ARG:NH2 | 2.70 | 0.40 |
| 1:E:39:SER:HB3 | 1:E:57:VAL:HB | 2.04 | 0.40 |
| 1:L:128:GLY:HA2 | 1:L:137:ILE:HD12 | 2.02 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|----------------|------------------------|-------------|----------|
| 1:A:160:GLU:CA | 1:K:167:ASP:OD2[1_455] | 2.08 | 0.12 |

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 | 350/394 (89%) | 323 (92%) | 24 (7%) | 3 (1%) | 25 | 71 |
| 1 | B | 350/394 (89%) | 322 (92%) | 26 (7%) | 2 (1%) | 33 | 78 |
| 1 | C | 350/394 (89%) | 323 (92%) | 25 (7%) | 2 (1%) | 33 | 78 |
| 1 | D | 350/394 (89%) | 322 (92%) | 25 (7%) | 3 (1%) | 25 | 71 |
| 1 | E | 350/394 (89%) | 323 (92%) | 24 (7%) | 3 (1%) | 25 | 71 |
| 1 | F | 350/394 (89%) | 322 (92%) | 26 (7%) | 2 (1%) | 33 | 78 |
| 1 | G | 350/394 (89%) | 322 (92%) | 26 (7%) | 2 (1%) | 33 | 78 |
| 1 | H | 350/394 (89%) | 322 (92%) | 26 (7%) | 2 (1%) | 33 | 78 |
| 1 | I | 350/394 (89%) | 322 (92%) | 25 (7%) | 3 (1%) | 25 | 71 |
| 1 | J | 350/394 (89%) | 322 (92%) | 26 (7%) | 2 (1%) | 33 | 78 |
| 1 | K | 350/394 (89%) | 322 (92%) | 26 (7%) | 2 (1%) | 33 | 78 |
| 1 | L | 350/394 (89%) | 323 (92%) | 25 (7%) | 2 (1%) | 33 | 78 |
| All | All | 4200/4728 (89%) | 3868 (92%) | 304 (7%) | 28 (1%) | 30 | 76 |

All (28) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 293 | ALA |
| 1 | A | 304 | GLY |
| 1 | B | 293 | ALA |
| 1 | B | 304 | GLY |
| 1 | C | 293 | ALA |
| 1 | C | 304 | GLY |
| 1 | D | 293 | ALA |
| 1 | D | 304 | GLY |
| 1 | E | 293 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 304 | GLY |
| 1 | F | 293 | ALA |
| 1 | F | 304 | GLY |
| 1 | G | 293 | ALA |
| 1 | G | 304 | GLY |
| 1 | H | 293 | ALA |
| 1 | H | 304 | GLY |
| 1 | I | 293 | ALA |
| 1 | I | 304 | GLY |
| 1 | J | 293 | ALA |
| 1 | J | 304 | GLY |
| 1 | K | 293 | ALA |
| 1 | K | 304 | GLY |
| 1 | L | 293 | ALA |
| 1 | L | 304 | GLY |
| 1 | A | 98 | HIS |
| 1 | D | 98 | HIS |
| 1 | E | 98 | HIS |
| 1 | I | 98 | HIS |

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 | 312/346 (90%) | 287 (92%) | 25 (8%) | 17 | 55 |
| 1 | B | 312/346 (90%) | 287 (92%) | 25 (8%) | 17 | 55 |
| 1 | C | 312/346 (90%) | 287 (92%) | 25 (8%) | 17 | 55 |
| 1 | D | 312/346 (90%) | 287 (92%) | 25 (8%) | 17 | 55 |
| 1 | E | 312/346 (90%) | 287 (92%) | 25 (8%) | 17 | 55 |
| 1 | F | 312/346 (90%) | 287 (92%) | 25 (8%) | 17 | 55 |
| 1 | G | 312/346 (90%) | 287 (92%) | 25 (8%) | 17 | 55 |
| 1 | H | 312/346 (90%) | 287 (92%) | 25 (8%) | 17 | 55 |
| 1 | I | 312/346 (90%) | 287 (92%) | 25 (8%) | 17 | 55 |
| 1 | J | 312/346 (90%) | 286 (92%) | 26 (8%) | 16 | 53 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | K | 312/346 (90%) | 287 (92%) | 25 (8%) | 17 | 55 |
| 1 | L | 312/346 (90%) | 287 (92%) | 25 (8%) | 17 | 55 |
| All | All | 3744/4152 (90%) | 3443 (92%) | 301 (8%) | 17 | 55 |

All (301) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 56 | GLU |
| 1 | A | 59 | VAL |
| 1 | A | 65 | PHE |
| 1 | A | 86 | ASN |
| 1 | A | 92 | VAL |
| 1 | A | 113 | ILE |
| 1 | A | 122 | THR |
| 1 | A | 156 | ASN |
| 1 | A | 178 | ARG |
| 1 | A | 181 | PHE |
| 1 | A | 182 | LYS |
| 1 | A | 183 | ARG |
| 1 | A | 190 | LYS |
| 1 | A | 202 | ILE |
| 1 | A | 223 | ILE |
| 1 | A | 255 | ARG |
| 1 | A | 263 | ASP |
| 1 | A | 275 | MET |
| 1 | A | 278 | LEU |
| 1 | A | 279 | SER |
| 1 | A | 284 | PHE |
| 1 | A | 286 | LEU |
| 1 | A | 336 | LYS |
| 1 | A | 349 | ARG |
| 1 | A | 358 | SER |
| 1 | B | 56 | GLU |
| 1 | B | 59 | VAL |
| 1 | B | 65 | PHE |
| 1 | B | 86 | ASN |
| 1 | B | 92 | VAL |
| 1 | B | 113 | ILE |
| 1 | B | 122 | THR |
| 1 | B | 156 | ASN |
| 1 | B | 178 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 181 | PHE |
| 1 | B | 182 | LYS |
| 1 | B | 183 | ARG |
| 1 | B | 190 | LYS |
| 1 | B | 202 | ILE |
| 1 | B | 223 | ILE |
| 1 | B | 255 | ARG |
| 1 | B | 263 | ASP |
| 1 | B | 275 | MET |
| 1 | B | 278 | LEU |
| 1 | B | 279 | SER |
| 1 | B | 284 | PHE |
| 1 | B | 286 | LEU |
| 1 | B | 336 | LYS |
| 1 | B | 349 | ARG |
| 1 | B | 358 | SER |
| 1 | C | 56 | GLU |
| 1 | C | 59 | VAL |
| 1 | C | 65 | PHE |
| 1 | C | 86 | ASN |
| 1 | C | 92 | VAL |
| 1 | C | 113 | ILE |
| 1 | C | 122 | THR |
| 1 | C | 156 | ASN |
| 1 | C | 178 | ARG |
| 1 | C | 181 | PHE |
| 1 | C | 182 | LYS |
| 1 | C | 183 | ARG |
| 1 | C | 190 | LYS |
| 1 | C | 202 | ILE |
| 1 | C | 223 | ILE |
| 1 | C | 255 | ARG |
| 1 | C | 263 | ASP |
| 1 | C | 275 | MET |
| 1 | C | 278 | LEU |
| 1 | C | 279 | SER |
| 1 | C | 284 | PHE |
| 1 | C | 286 | LEU |
| 1 | C | 336 | LYS |
| 1 | C | 349 | ARG |
| 1 | C | 358 | SER |
| 1 | D | 56 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 59 | VAL |
| 1 | D | 65 | PHE |
| 1 | D | 86 | ASN |
| 1 | D | 92 | VAL |
| 1 | D | 113 | ILE |
| 1 | D | 122 | THR |
| 1 | D | 156 | ASN |
| 1 | D | 178 | ARG |
| 1 | D | 181 | PHE |
| 1 | D | 182 | LYS |
| 1 | D | 183 | ARG |
| 1 | D | 190 | LYS |
| 1 | D | 202 | ILE |
| 1 | D | 223 | ILE |
| 1 | D | 255 | ARG |
| 1 | D | 263 | ASP |
| 1 | D | 275 | MET |
| 1 | D | 278 | LEU |
| 1 | D | 279 | SER |
| 1 | D | 284 | PHE |
| 1 | D | 286 | LEU |
| 1 | D | 336 | LYS |
| 1 | D | 349 | ARG |
| 1 | D | 358 | SER |
| 1 | E | 56 | GLU |
| 1 | E | 59 | VAL |
| 1 | E | 65 | PHE |
| 1 | E | 86 | ASN |
| 1 | E | 92 | VAL |
| 1 | E | 113 | ILE |
| 1 | E | 122 | THR |
| 1 | E | 156 | ASN |
| 1 | E | 178 | ARG |
| 1 | E | 181 | PHE |
| 1 | E | 182 | LYS |
| 1 | E | 183 | ARG |
| 1 | E | 190 | LYS |
| 1 | E | 202 | ILE |
| 1 | E | 223 | ILE |
| 1 | E | 255 | ARG |
| 1 | E | 263 | ASP |
| 1 | E | 275 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 278 | LEU |
| 1 | E | 279 | SER |
| 1 | E | 284 | PHE |
| 1 | E | 286 | LEU |
| 1 | E | 336 | LYS |
| 1 | E | 349 | ARG |
| 1 | E | 358 | SER |
| 1 | F | 56 | GLU |
| 1 | F | 59 | VAL |
| 1 | F | 65 | PHE |
| 1 | F | 86 | ASN |
| 1 | F | 92 | VAL |
| 1 | F | 113 | ILE |
| 1 | F | 122 | THR |
| 1 | F | 156 | ASN |
| 1 | F | 178 | ARG |
| 1 | F | 181 | PHE |
| 1 | F | 182 | LYS |
| 1 | F | 183 | ARG |
| 1 | F | 190 | LYS |
| 1 | F | 202 | ILE |
| 1 | F | 223 | ILE |
| 1 | F | 255 | ARG |
| 1 | F | 263 | ASP |
| 1 | F | 275 | MET |
| 1 | F | 278 | LEU |
| 1 | F | 279 | SER |
| 1 | F | 284 | PHE |
| 1 | F | 286 | LEU |
| 1 | F | 336 | LYS |
| 1 | F | 349 | ARG |
| 1 | F | 358 | SER |
| 1 | G | 56 | GLU |
| 1 | G | 59 | VAL |
| 1 | G | 65 | PHE |
| 1 | G | 86 | ASN |
| 1 | G | 92 | VAL |
| 1 | G | 113 | ILE |
| 1 | G | 122 | THR |
| 1 | G | 156 | ASN |
| 1 | G | 178 | ARG |
| 1 | G | 181 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 182 | LYS |
| 1 | G | 183 | ARG |
| 1 | G | 190 | LYS |
| 1 | G | 202 | ILE |
| 1 | G | 223 | ILE |
| 1 | G | 255 | ARG |
| 1 | G | 263 | ASP |
| 1 | G | 275 | MET |
| 1 | G | 278 | LEU |
| 1 | G | 279 | SER |
| 1 | G | 284 | PHE |
| 1 | G | 286 | LEU |
| 1 | G | 336 | LYS |
| 1 | G | 349 | ARG |
| 1 | G | 358 | SER |
| 1 | H | 56 | GLU |
| 1 | H | 59 | VAL |
| 1 | H | 65 | PHE |
| 1 | H | 86 | ASN |
| 1 | H | 92 | VAL |
| 1 | H | 113 | ILE |
| 1 | H | 122 | THR |
| 1 | H | 156 | ASN |
| 1 | H | 178 | ARG |
| 1 | H | 181 | PHE |
| 1 | H | 182 | LYS |
| 1 | H | 183 | ARG |
| 1 | H | 190 | LYS |
| 1 | H | 202 | ILE |
| 1 | H | 223 | ILE |
| 1 | H | 255 | ARG |
| 1 | H | 263 | ASP |
| 1 | H | 275 | MET |
| 1 | H | 278 | LEU |
| 1 | H | 279 | SER |
| 1 | H | 284 | PHE |
| 1 | H | 286 | LEU |
| 1 | H | 336 | LYS |
| 1 | H | 349 | ARG |
| 1 | H | 358 | SER |
| 1 | I | 56 | GLU |
| 1 | I | 59 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 65 | PHE |
| 1 | I | 86 | ASN |
| 1 | I | 92 | VAL |
| 1 | I | 113 | ILE |
| 1 | I | 122 | THR |
| 1 | I | 156 | ASN |
| 1 | I | 178 | ARG |
| 1 | I | 181 | PHE |
| 1 | I | 182 | LYS |
| 1 | I | 183 | ARG |
| 1 | I | 190 | LYS |
| 1 | I | 202 | ILE |
| 1 | I | 223 | ILE |
| 1 | I | 255 | ARG |
| 1 | I | 263 | ASP |
| 1 | I | 275 | MET |
| 1 | I | 278 | LEU |
| 1 | I | 279 | SER |
| 1 | I | 284 | PHE |
| 1 | I | 286 | LEU |
| 1 | I | 336 | LYS |
| 1 | I | 349 | ARG |
| 1 | I | 358 | SER |
| 1 | J | 56 | GLU |
| 1 | J | 59 | VAL |
| 1 | J | 65 | PHE |
| 1 | J | 86 | ASN |
| 1 | J | 92 | VAL |
| 1 | J | 113 | ILE |
| 1 | J | 122 | THR |
| 1 | J | 156 | ASN |
| 1 | J | 178 | ARG |
| 1 | J | 181 | PHE |
| 1 | J | 182 | LYS |
| 1 | J | 183 | ARG |
| 1 | J | 190 | LYS |
| 1 | J | 195 | SER |
| 1 | J | 202 | ILE |
| 1 | J | 223 | ILE |
| 1 | J | 255 | ARG |
| 1 | J | 263 | ASP |
| 1 | J | 275 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 278 | LEU |
| 1 | J | 279 | SER |
| 1 | J | 284 | PHE |
| 1 | J | 286 | LEU |
| 1 | J | 336 | LYS |
| 1 | J | 349 | ARG |
| 1 | J | 358 | SER |
| 1 | K | 56 | GLU |
| 1 | K | 59 | VAL |
| 1 | K | 65 | PHE |
| 1 | K | 86 | ASN |
| 1 | K | 92 | VAL |
| 1 | K | 113 | ILE |
| 1 | K | 122 | THR |
| 1 | K | 156 | ASN |
| 1 | K | 178 | ARG |
| 1 | K | 181 | PHE |
| 1 | K | 182 | LYS |
| 1 | K | 183 | ARG |
| 1 | K | 190 | LYS |
| 1 | K | 202 | ILE |
| 1 | K | 223 | ILE |
| 1 | K | 255 | ARG |
| 1 | K | 263 | ASP |
| 1 | K | 275 | MET |
| 1 | K | 278 | LEU |
| 1 | K | 279 | SER |
| 1 | K | 284 | PHE |
| 1 | K | 286 | LEU |
| 1 | K | 336 | LYS |
| 1 | K | 349 | ARG |
| 1 | K | 358 | SER |
| 1 | L | 56 | GLU |
| 1 | L | 59 | VAL |
| 1 | L | 65 | PHE |
| 1 | L | 86 | ASN |
| 1 | L | 92 | VAL |
| 1 | L | 113 | ILE |
| 1 | L | 122 | THR |
| 1 | L | 156 | ASN |
| 1 | L | 178 | ARG |
| 1 | L | 181 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 182 | LYS |
| 1 | L | 183 | ARG |
| 1 | L | 190 | LYS |
| 1 | L | 202 | ILE |
| 1 | L | 223 | ILE |
| 1 | L | 255 | ARG |
| 1 | L | 263 | ASP |
| 1 | L | 275 | MET |
| 1 | L | 278 | LEU |
| 1 | L | 279 | SER |
| 1 | L | 284 | PHE |
| 1 | L | 286 | LEU |
| 1 | L | 336 | LYS |
| 1 | L | 349 | ARG |
| 1 | L | 358 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 98 | HIS |
| 1 | A | 134 | ASN |
| 1 | A | 165 | ASN |
| 1 | A | 173 | ASN |
| 1 | A | 214 | GLN |
| 1 | A | 312 | HIS |
| 1 | A | 330 | GLN |
| 1 | A | 333 | GLN |
| 1 | A | 364 | GLN |
| 1 | B | 98 | HIS |
| 1 | B | 134 | ASN |
| 1 | B | 165 | ASN |
| 1 | B | 173 | ASN |
| 1 | B | 214 | GLN |
| 1 | B | 312 | HIS |
| 1 | B | 330 | GLN |
| 1 | B | 333 | GLN |
| 1 | B | 364 | GLN |
| 1 | C | 98 | HIS |
| 1 | C | 134 | ASN |
| 1 | C | 159 | HIS |
| 1 | C | 165 | ASN |
| 1 | C | 173 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 214 | GLN |
| 1 | C | 312 | HIS |
| 1 | C | 330 | GLN |
| 1 | C | 333 | GLN |
| 1 | C | 364 | GLN |
| 1 | D | 98 | HIS |
| 1 | D | 134 | ASN |
| 1 | D | 165 | ASN |
| 1 | D | 173 | ASN |
| 1 | D | 214 | GLN |
| 1 | D | 312 | HIS |
| 1 | D | 330 | GLN |
| 1 | D | 333 | GLN |
| 1 | D | 364 | GLN |
| 1 | E | 98 | HIS |
| 1 | E | 134 | ASN |
| 1 | E | 165 | ASN |
| 1 | E | 173 | ASN |
| 1 | E | 214 | GLN |
| 1 | E | 312 | HIS |
| 1 | E | 330 | GLN |
| 1 | E | 333 | GLN |
| 1 | E | 364 | GLN |
| 1 | F | 98 | HIS |
| 1 | F | 134 | ASN |
| 1 | F | 135 | ASN |
| 1 | F | 165 | ASN |
| 1 | F | 173 | ASN |
| 1 | F | 214 | GLN |
| 1 | F | 312 | HIS |
| 1 | F | 330 | GLN |
| 1 | F | 333 | GLN |
| 1 | F | 364 | GLN |
| 1 | G | 98 | HIS |
| 1 | G | 134 | ASN |
| 1 | G | 165 | ASN |
| 1 | G | 173 | ASN |
| 1 | G | 214 | GLN |
| 1 | G | 312 | HIS |
| 1 | G | 330 | GLN |
| 1 | G | 333 | GLN |
| 1 | G | 364 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 98 | HIS |
| 1 | H | 134 | ASN |
| 1 | H | 165 | ASN |
| 1 | H | 173 | ASN |
| 1 | H | 214 | GLN |
| 1 | H | 312 | HIS |
| 1 | H | 330 | GLN |
| 1 | H | 333 | GLN |
| 1 | H | 364 | GLN |
| 1 | I | 98 | HIS |
| 1 | I | 134 | ASN |
| 1 | I | 165 | ASN |
| 1 | I | 173 | ASN |
| 1 | I | 214 | GLN |
| 1 | I | 312 | HIS |
| 1 | I | 330 | GLN |
| 1 | I | 333 | GLN |
| 1 | I | 364 | GLN |
| 1 | J | 98 | HIS |
| 1 | J | 134 | ASN |
| 1 | J | 165 | ASN |
| 1 | J | 173 | ASN |
| 1 | J | 214 | GLN |
| 1 | J | 312 | HIS |
| 1 | J | 330 | GLN |
| 1 | J | 333 | GLN |
| 1 | J | 364 | GLN |
| 1 | K | 98 | HIS |
| 1 | K | 134 | ASN |
| 1 | K | 165 | ASN |
| 1 | K | 173 | ASN |
| 1 | K | 214 | GLN |
| 1 | K | 312 | HIS |
| 1 | K | 330 | GLN |
| 1 | K | 333 | GLN |
| 1 | K | 364 | GLN |
| 1 | L | 98 | HIS |
| 1 | L | 134 | ASN |
| 1 | L | 156 | ASN |
| 1 | L | 165 | ASN |
| 1 | L | 173 | ASN |
| 1 | L | 214 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 312 | HIS |
| 1 | L | 330 | GLN |
| 1 | L | 333 | GLN |
| 1 | L | 364 | GLN |

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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 | 360/394 (91%) | -0.04 | 0 100 100 | 62, 92, 116, 125 | 0 |
| 1 | B | 360/394 (91%) | 0.11 | 1 (0%) 91 53 | 63, 94, 116, 126 | 0 |
| 1 | C | 360/394 (91%) | 0.07 | 0 100 100 | 57, 93, 116, 125 | 0 |
| 1 | D | 360/394 (91%) | 0.01 | 1 (0%) 91 53 | 58, 93, 115, 126 | 0 |
| 1 | E | 360/394 (91%) | 0.04 | 1 (0%) 91 53 | 56, 92, 116, 125 | 0 |
| 1 | F | 360/394 (91%) | 0.08 | 0 100 100 | 57, 93, 116, 125 | 0 |
| 1 | G | 360/394 (91%) | -0.00 | 0 100 100 | 62, 93, 116, 125 | 0 |
| 1 | H | 360/394 (91%) | 0.33 | 11 (3%) 47 7 | 63, 95, 117, 126 | 0 |
| 1 | I | 360/394 (91%) | 0.08 | 1 (0%) 91 53 | 57, 92, 116, 125 | 0 |
| 1 | J | 360/394 (91%) | 0.03 | 0 100 100 | 38, 87, 116, 124 | 0 |
| 1 | K | 360/394 (91%) | 0.03 | 0 100 100 | 55, 90, 116, 124 | 0 |
| 1 | L | 360/394 (91%) | -0.00 | 1 (0%) 91 53 | 61, 92, 115, 124 | 0 |
| All | All | 4320/4728 (91%) | 0.06 | 16 (0%) 90 45 | 38, 92, 116, 126 | 0 |

All (16) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | H | 177 | GLU | 3.3 |
| 1 | H | 190 | LYS | 3.2 |
| 1 | I | 182 | LYS | 3.1 |
| 1 | E | 178 | ARG | 3.1 |
| 1 | D | 182 | LYS | 2.8 |
| 1 | H | 302 | ARG | 2.4 |
| 1 | H | 339 | GLU | 2.4 |
| 1 | H | 182 | LYS | 2.4 |
| 1 | H | 340 | LEU | 2.3 |
| 1 | H | 310 | ILE | 2.3 |
| 1 | H | 185 | MET | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | H | 295 | GLY | 2.2 |
| 1 | B | 347 | ARG | 2.2 |
| 1 | H | 257 | LEU | 2.1 |
| 1 | L | 182 | LYS | 2.1 |
| 1 | H | 350 | GLU | 2.1 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.