



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 09:05 pm GMT

PDB ID : 4FE4  
Title : Crystal structure of apo E. coli XylR  
Authors : Schumacher, M.A.; Ni, L.  
Deposited on : 2012-05-29  
Resolution : 3.45 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

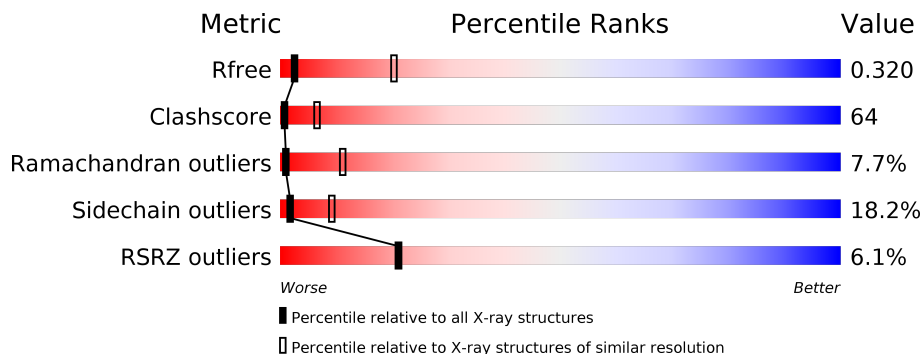
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.45 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 111664                      | 1091 (3.52-3.40)                                      |
| Clashscore            | 122126                      | 1166 (3.52-3.40)                                      |
| Ramachandran outliers | 120053                      | 1135 (3.52-3.40)                                      |
| Sidechain outliers    | 120020                      | 1136 (3.52-3.40)                                      |
| RSRZ outliers         | 108989                      | 1015 (3.52-3.40)                                      |

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 392    | <div> <div>5%</div> <div>22% 57% 16%</div> <div>• •</div> </div>  |
| 1   | B     | 392    | <div> <div>3%</div> <div>26% 55% 15%</div> <div>• •</div> </div>  |
| 1   | C     | 392    | <div> <div>10%</div> <div>25% 56% 14%</div> <div>• •</div> </div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9189 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

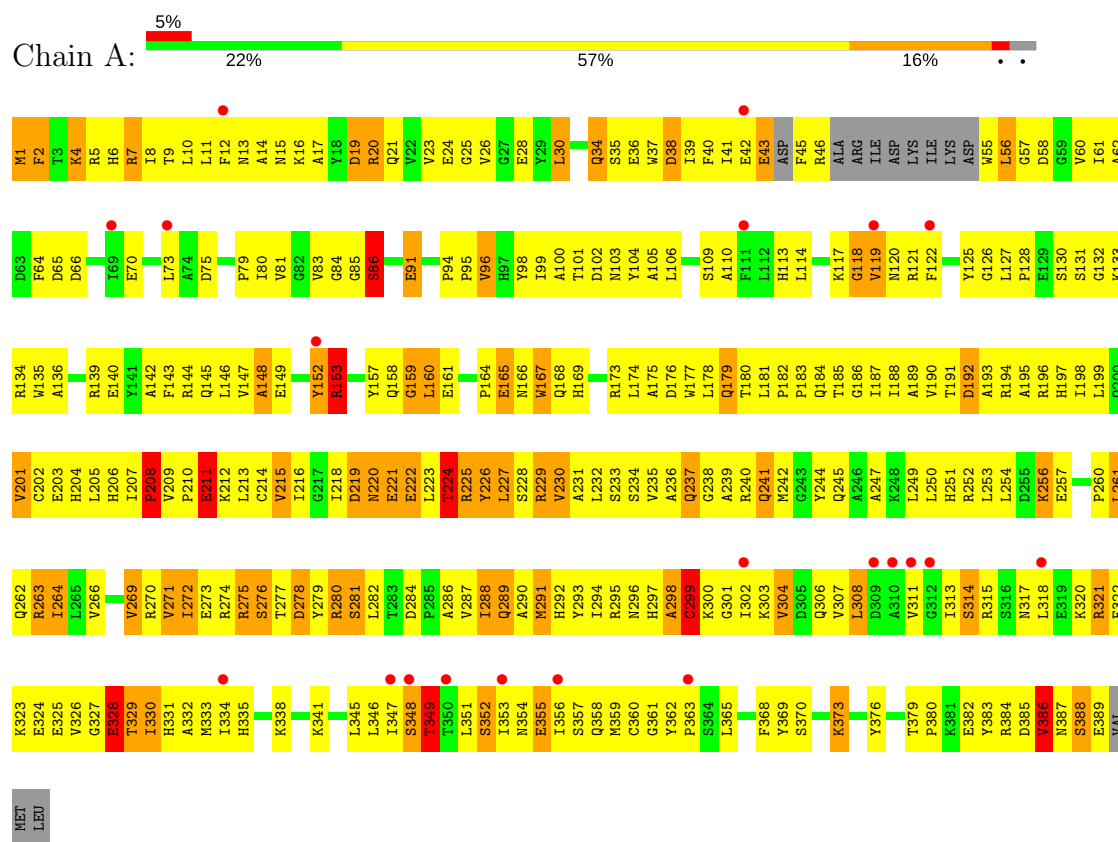
- Molecule 1 is a protein called Xylose operon regulatory protein.

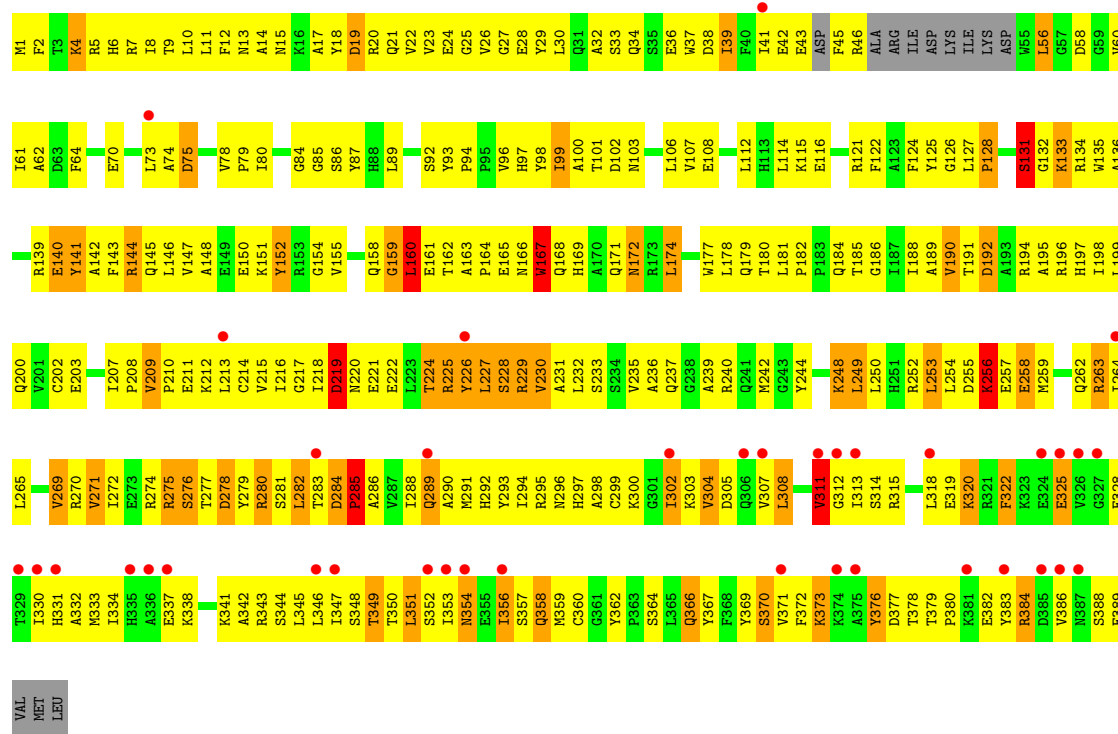
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 380      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3063  | 1946 | 538 | 569 | 10 |         |         |       |
| 1   | B     | 380      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3063  | 1946 | 538 | 569 | 10 |         |         |       |
| 1   | C     | 380      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3063  | 1946 | 538 | 569 | 10 |         |         |       |

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

#### • Molecule 1: Xylose operon regulatory protein





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 32 2 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 124.50Å 124.50Å 189.80Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)  | 107.80 – 3.45<br>107.82 – 3.45                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.3 (107.80-3.45)<br>96.3 (107.82-3.45)                    | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.71 (at 3.49Å)   | Xtriage          |
| Refinement program  | CNS 1.2   | Depositor        |
| R, $R_{free}$   | 0.289 , 0.318<br>0.290 , 0.320                              | Depositor<br>DCC |
| $R_{free}$ test set   | 1222 reflections (5.52%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 97.2  | Xtriage          |
| Anisotropy  | 0.592   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 79.9   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$ | Xtriage          |
| Estimated twinning fraction   | 0.109 for -h,-k,l   | Xtriage          |
| $F_o, F_c$ correlation  | 0.90  | EDS              |
| Total number of atoms   | 9189  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 115.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$    |
| 1   | A     | 0.55         | 1/3129 (0.0%) | 0.79        | 2/4238 (0.0%)  |
| 1   | B     | 0.58         | 0/3129        | 0.76        | 1/4238 (0.0%)  |
| 1   | C     | 0.62         | 2/3129 (0.1%) | 0.80        | 2/4238 (0.0%)  |
| All | All   | 0.58         | 3/9387 (0.0%) | 0.78        | 5/12714 (0.0%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 140 | GLU  | CG-CD  | -6.95 | 1.41        | 1.51     |
| 1   | C     | 311 | VAL  | CB-CG1 | -5.92 | 1.40        | 1.52     |
| 1   | A     | 386 | VAL  | CB-CG2 | -5.58 | 1.41        | 1.52     |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 235 | VAL  | CB-CA-C   | -7.39 | 97.36       | 111.40   |
| 1   | A     | 325 | GLU  | N-CA-C    | 6.39  | 128.25      | 111.00   |
| 1   | C     | 99  | ILE  | N-CA-C    | -5.61 | 95.85       | 111.00   |
| 1   | A     | 324 | GLU  | N-CA-C    | 5.35  | 125.44      | 111.00   |
| 1   | C     | 219 | ASP  | CB-CG-OD2 | -5.32 | 113.51      | 118.30   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3063  | 0        | 3028     | 426     | 0            |
| 1   | B     | 3063  | 0        | 3028     | 346     | 0            |
| 1   | C     | 3063  | 0        | 3028     | 424     | 1            |
| All | All   | 9189  | 0        | 9084     | 1169    | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 64.

All (1169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:320:LYS:O    | 1:B:323:LYS:HE2  | 1.42                     | 1.18              |
| 1:A:280:ARG:HG2  | 1:A:282:LEU:HD12 | 1.28                     | 1.12              |
| 1:A:282:LEU:HD21 | 1:A:326:VAL:HG21 | 1.12                     | 1.11              |
| 1:A:280:ARG:HG2  | 1:A:282:LEU:CD1  | 1.81                     | 1.09              |
| 1:B:320:LYS:O    | 1:B:323:LYS:CE   | 2.01                     | 1.07              |
| 1:A:272:ILE:H    | 1:A:272:ILE:HD12 | 1.15                     | 1.06              |
| 1:A:382:GLU:O    | 1:A:386:VAL:HG23 | 1.58                     | 1.03              |
| 1:B:98:TYR:HD2   | 1:B:100:ALA:HB2  | 1.24                     | 1.01              |
| 1:A:223:LEU:HD12 | 1:C:24:GLU:HG3   | 1.41                     | 1.01              |
| 1:A:308:LEU:HA   | 1:A:318:LEU:HG   | 1.43                     | 1.00              |
| 1:C:79:PRO:HB3   | 1:C:253:LEU:HD22 | 1.42                     | 1.00              |
| 1:A:210:PRO:HD2  | 1:A:295:ARG:NH1  | 1.78                     | 0.99              |
| 1:A:282:LEU:CD2  | 1:A:326:VAL:HG21 | 1.93                     | 0.98              |
| 1:B:225:ARG:NH2  | 1:B:389:GLU:O    | 1.94                     | 0.98              |
| 1:C:190:VAL:HG23 | 1:C:191:THR:HG23 | 1.45                     | 0.98              |
| 1:A:207:ILE:HG23 | 1:A:212:LYS:HD2  | 1.43                     | 0.98              |
| 1:C:298:ALA:HA   | 1:C:302:ILE:HD11 | 1.39                     | 0.98              |
| 1:B:79:PRO:HB3   | 1:B:253:LEU:HD23 | 1.46                     | 0.97              |
| 1:A:4:LYS:HZ3    | 1:A:4:LYS:HA     | 1.28                     | 0.96              |
| 1:C:11:LEU:HB3   | 1:C:43:GLU:OE1   | 1.65                     | 0.96              |
| 1:A:269:VAL:HG12 | 1:A:270:ARG:HG3  | 1.49                     | 0.94              |
| 1:B:354:ASN:HA   | 1:B:365:LEU:HD13 | 1.47                     | 0.94              |
| 1:A:210:PRO:HD2  | 1:A:295:ARG:HH12 | 1.31                     | 0.94              |
| 1:B:98:TYR:CD2   | 1:B:100:ALA:HB2  | 2.02                     | 0.94              |
| 1:A:382:GLU:O    | 1:A:386:VAL:CG2  | 2.14                     | 0.93              |
| 1:A:282:LEU:HD21 | 1:A:326:VAL:CG2  | 1.99                     | 0.93              |
| 1:A:280:ARG:CG   | 1:A:282:LEU:CD1  | 2.47                     | 0.93              |
| 1:A:346:LEU:HD23 | 1:A:384:ARG:HH11 | 1.34                     | 0.92              |
| 1:A:280:ARG:CG   | 1:A:282:LEU:HD11 | 2.00                     | 0.91              |
| 1:C:275:ARG:HG2  | 1:C:295:ARG:HH11 | 1.34                     | 0.91              |
| 1:A:280:ARG:HG3  | 1:A:282:LEU:HD11 | 1.53                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:4:LYS:HA     | 1:A:4:LYS:NZ     | 1.84                     | 0.91              |
| 1:B:37:TRP:HZ2   | 1:B:251:HIS:HB2  | 1.33                     | 0.90              |
| 1:C:225:ARG:HE   | 1:C:274:ARG:NH2  | 1.69                     | 0.90              |
| 1:B:242:MET:HA   | 1:B:266:VAL:HG21 | 1.53                     | 0.90              |
| 1:C:160:LEU:H    | 1:C:194:ARG:HH12 | 1.17                     | 0.89              |
| 1:A:274:ARG:HG3  | 1:A:274:ARG:HH11 | 1.34                     | 0.89              |
| 1:C:311:VAL:HB   | 1:C:318:LEU:HD11 | 1.56                     | 0.88              |
| 1:A:303:LYS:O    | 1:A:307:VAL:HG23 | 1.72                     | 0.88              |
| 1:C:60:VAL:HB    | 1:C:80:ILE:HD13  | 1.53                     | 0.88              |
| 1:A:10:LEU:HD22  | 1:A:61:ILE:HB    | 1.54                     | 0.88              |
| 1:A:60:VAL:HB    | 1:A:80:ILE:HG22  | 1.55                     | 0.88              |
| 1:C:224:THR:HA   | 1:C:227:LEU:HD12 | 1.54                     | 0.88              |
| 1:C:283:THR:O    | 1:C:285:PRO:HD3  | 1.74                     | 0.87              |
| 1:C:286:ALA:O    | 1:C:311:VAL:HG11 | 1.73                     | 0.87              |
| 1:C:192:ASP:HB2  | 1:C:219:ASP:HB2  | 1.56                     | 0.87              |
| 1:C:161:GLU:HB3  | 1:C:164:PRO:HB3  | 1.56                     | 0.86              |
| 1:A:160:LEU:HD22 | 1:A:164:PRO:HB3  | 1.55                     | 0.86              |
| 1:B:323:LYS:N    | 1:B:323:LYS:HD3  | 1.90                     | 0.86              |
| 1:C:269:VAL:HG23 | 1:C:270:ARG:H    | 1.40                     | 0.86              |
| 1:C:150:GLU:HG3  | 1:C:151:LYS:H    | 1.38                     | 0.86              |
| 1:A:73:LEU:HD21  | 1:A:80:ILE:HG21  | 1.56                     | 0.85              |
| 1:C:286:ALA:O    | 1:C:311:VAL:CG1  | 2.25                     | 0.85              |
| 1:B:345:LEU:HA   | 1:B:349:THR:HG23 | 1.56                     | 0.85              |
| 1:A:328:GLU:HG3  | 1:A:332:ALA:HB1  | 1.58                     | 0.84              |
| 1:A:354:ASN:ND2  | 1:A:365:LEU:HD13 | 1.93                     | 0.84              |
| 1:A:351:LEU:H    | 1:A:384:ARG:NH2  | 1.75                     | 0.84              |
| 1:C:290:ALA:O    | 1:C:294:ILE:HG13 | 1.78                     | 0.83              |
| 1:C:239:ALA:HA   | 1:C:242:MET:HG3  | 1.60                     | 0.83              |
| 1:C:225:ARG:HE   | 1:C:274:ARG:HH22 | 1.27                     | 0.83              |
| 1:A:230:VAL:HG12 | 1:A:275:ARG:HD2  | 1.59                     | 0.83              |
| 1:B:17:ALA:O     | 1:B:21:GLN:HG3   | 1.79                     | 0.82              |
| 1:C:235:VAL:HA   | 1:C:271:VAL:HG13 | 1.61                     | 0.82              |
| 1:B:275:ARG:NH2  | 1:B:295:ARG:HD2  | 1.94                     | 0.82              |
| 1:A:79:PRO:HG3   | 1:A:253:LEU:HD22 | 1.61                     | 0.82              |
| 1:A:386:VAL:HG12 | 1:A:387:ASN:OD1  | 1.79                     | 0.82              |
| 1:A:275:ARG:HH11 | 1:A:275:ARG:HG3  | 1.43                     | 0.81              |
| 1:A:347:ILE:HG23 | 1:A:389:GLU:H    | 1.45                     | 0.81              |
| 1:B:128:PRO:HB2  | 1:B:130:SER:HB3  | 1.62                     | 0.81              |
| 1:A:346:LEU:HD23 | 1:A:384:ARG:NH1  | 1.96                     | 0.81              |
| 1:B:96:VAL:HG22  | 1:B:97:HIS:H     | 1.46                     | 0.81              |
| 1:B:304:VAL:O    | 1:B:307:VAL:HG23 | 1.80                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:167:TRP:CZ3  | 1:A:168:GLN:HB2  | 2.16                     | 0.80              |
| 1:A:313:ILE:HG23 | 1:A:317:ASN:HD22 | 1.44                     | 0.80              |
| 1:C:218:ILE:HG22 | 1:C:218:ILE:O    | 1.80                     | 0.80              |
| 1:B:275:ARG:HH21 | 1:B:295:ARG:HD2  | 1.44                     | 0.80              |
| 1:B:311:VAL:HG21 | 1:B:318:LEU:HD11 | 1.63                     | 0.80              |
| 1:B:56:LEU:HG    | 1:B:57:GLY:H     | 1.44                     | 0.80              |
| 1:B:308:LEU:HD23 | 1:B:318:LEU:HD13 | 1.64                     | 0.79              |
| 1:C:308:LEU:O    | 1:C:318:LEU:CD1  | 2.31                     | 0.79              |
| 1:A:196:ARG:NH2  | 1:A:225:ARG:HA   | 1.97                     | 0.79              |
| 1:B:307:VAL:O    | 1:B:311:VAL:HG23 | 1.82                     | 0.79              |
| 1:C:125:TYR:HE2  | 1:C:194:ARG:HB3  | 1.47                     | 0.79              |
| 1:C:308:LEU:O    | 1:C:318:LEU:HD13 | 1.83                     | 0.79              |
| 1:A:8:ILE:HD12   | 1:A:37:TRP:CE3   | 2.17                     | 0.78              |
| 1:C:151:LYS:HB3  | 1:C:152:TYR:HD1  | 1.48                     | 0.78              |
| 1:C:192:ASP:HB2  | 1:C:219:ASP:CB   | 2.13                     | 0.78              |
| 1:B:166:ASN:HB2  | 1:B:169:HIS:HB3  | 1.66                     | 0.78              |
| 1:B:186:GLY:HA2  | 1:B:214:CYS:HB2  | 1.66                     | 0.78              |
| 1:C:73:LEU:HD13  | 1:C:80:ILE:HD12  | 1.66                     | 0.78              |
| 1:A:160:LEU:HD13 | 1:A:164:PRO:HG3  | 1.64                     | 0.77              |
| 1:C:107:VAL:HG22 | 1:C:139:ARG:HG2  | 1.65                     | 0.77              |
| 1:A:282:LEU:CD2  | 1:A:326:VAL:CG2  | 2.60                     | 0.77              |
| 1:A:313:ILE:HB   | 1:A:318:LEU:HD23 | 1.66                     | 0.77              |
| 1:A:373:LYS:HA   | 1:A:376:TYR:O    | 1.84                     | 0.77              |
| 1:B:262:GLN:C    | 1:B:263:ARG:HD2  | 2.04                     | 0.77              |
| 1:B:42:GLU:O     | 1:B:43:GLU:HB2   | 1.82                     | 0.77              |
| 1:A:215:VAL:HG23 | 1:A:276:SER:HB2  | 1.67                     | 0.77              |
| 1:B:124:PHE:CZ   | 1:B:190:VAL:HG13 | 2.20                     | 0.77              |
| 1:B:191:THR:HG22 | 1:B:193:ALA:H    | 1.49                     | 0.77              |
| 1:A:229:ARG:HH12 | 1:A:296:ASN:HB3  | 1.48                     | 0.77              |
| 1:B:210:PRO:HD2  | 1:B:295:ARG:HH12 | 1.49                     | 0.77              |
| 1:B:311:VAL:CG2  | 1:B:318:LEU:HD11 | 2.15                     | 0.77              |
| 1:C:14:ALA:O     | 1:C:20:ARG:HD2   | 1.84                     | 0.77              |
| 1:C:79:PRO:CB    | 1:C:253:LEU:HD22 | 2.15                     | 0.77              |
| 1:A:179:GLN:HE22 | 1:A:207:ILE:HD11 | 1.50                     | 0.76              |
| 1:B:133:LYS:HD2  | 1:B:133:LYS:H    | 1.50                     | 0.76              |
| 1:C:297:HIS:HB3  | 1:C:300:LYS:HD2  | 1.66                     | 0.76              |
| 1:C:380:PRO:O    | 1:C:384:ARG:HB2  | 1.86                     | 0.76              |
| 1:A:359:MET:SD   | 1:C:32:ALA:HB1   | 2.25                     | 0.76              |
| 1:C:112:LEU:O    | 1:C:116:GLU:HG3  | 1.84                     | 0.76              |
| 1:B:303:LYS:H    | 1:B:306:GLN:HB2  | 1.51                     | 0.76              |
| 1:B:37:TRP:CZ2   | 1:B:251:HIS:HB2  | 2.21                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:127:LEU:HA   | 1:C:194:ARG:HH21 | 1.51                     | 0.76              |
| 1:C:290:ALA:HA   | 1:C:311:VAL:HG22 | 1.66                     | 0.76              |
| 1:C:25:GLY:HA2   | 1:C:28:GLU:HG3   | 1.68                     | 0.76              |
| 1:B:10:LEU:HD23  | 1:B:61:ILE:HB    | 1.66                     | 0.75              |
| 1:C:79:PRO:HB3   | 1:C:253:LEU:CD2  | 2.17                     | 0.75              |
| 1:A:354:ASN:HD21 | 1:A:365:LEU:HD13 | 1.47                     | 0.75              |
| 1:B:8:ILE:HD13   | 1:B:37:TRP:HB3   | 1.68                     | 0.75              |
| 1:C:5:ARG:HA     | 1:C:36:GLU:O     | 1.85                     | 0.75              |
| 1:C:160:LEU:N    | 1:C:194:ARG:HH12 | 1.85                     | 0.75              |
| 1:B:345:LEU:HA   | 1:B:349:THR:CG2  | 2.16                     | 0.75              |
| 1:C:151:LYS:HB3  | 1:C:152:TYR:CD1  | 2.22                     | 0.74              |
| 1:B:192:ASP:OD1  | 1:B:219:ASP:N    | 2.20                     | 0.74              |
| 1:B:292:HIS:CE1  | 1:B:296:ASN:HD21 | 2.06                     | 0.74              |
| 1:C:289:GLN:HB3  | 1:C:311:VAL:HA   | 1.66                     | 0.74              |
| 1:B:272:ILE:HG21 | 1:B:274:ARG:HE   | 1.51                     | 0.74              |
| 1:B:314:SER:O    | 1:B:318:LEU:HB2  | 1.87                     | 0.74              |
| 1:C:89:LEU:O     | 1:C:92:SER:HB2   | 1.88                     | 0.73              |
| 1:A:313:ILE:HG22 | 1:A:317:ASN:HB3  | 1.71                     | 0.73              |
| 1:B:17:ALA:HB2   | 1:B:221:GLU:HA   | 1.70                     | 0.73              |
| 1:B:294:ILE:HG22 | 1:B:298:ALA:HB2  | 1.70                     | 0.73              |
| 1:C:378:THR:HG1  | 1:C:383:TYR:HD1  | 1.36                     | 0.73              |
| 1:A:189:ALA:HB3  | 1:A:195:ALA:HB2  | 1.69                     | 0.73              |
| 1:B:23:VAL:HG21  | 1:B:41:ILE:HD11  | 1.68                     | 0.73              |
| 1:A:223:LEU:HD12 | 1:C:24:GLU:CG    | 2.18                     | 0.73              |
| 1:B:308:LEU:CD2  | 1:B:318:LEU:HD13 | 2.18                     | 0.73              |
| 1:A:41:ILE:O     | 1:A:41:ILE:HG22  | 1.88                     | 0.73              |
| 1:B:249:LEU:O    | 1:B:249:LEU:HD23 | 1.88                     | 0.73              |
| 1:C:208:PRO:HB3  | 1:C:211:GLU:HB2  | 1.70                     | 0.73              |
| 1:B:367:TYR:O    | 1:B:370:SER:HB3  | 1.89                     | 0.73              |
| 1:A:275:ARG:NH1  | 1:A:275:ARG:HG3  | 2.04                     | 0.73              |
| 1:A:277:THR:O    | 1:A:279:TYR:N    | 2.21                     | 0.73              |
| 1:A:216:ILE:HD12 | 1:A:233:SER:O    | 1.89                     | 0.72              |
| 1:B:114:LEU:O    | 1:B:119:VAL:HB   | 1.89                     | 0.72              |
| 1:B:262:GLN:O    | 1:B:263:ARG:HD2  | 1.90                     | 0.72              |
| 1:B:343:ARG:HG2  | 1:B:383:TYR:CE2  | 2.24                     | 0.72              |
| 1:B:343:ARG:HH11 | 1:B:383:TYR:HE2  | 1.35                     | 0.72              |
| 1:C:131:SER:O    | 1:C:133:LYS:N    | 2.21                     | 0.72              |
| 1:A:230:VAL:CG1  | 1:A:275:ARG:HD2  | 2.18                     | 0.72              |
| 1:A:227:LEU:HB3  | 1:C:27:GLY:CA    | 2.19                     | 0.72              |
| 1:A:101:THR:HB   | 1:A:242:MET:CE   | 2.19                     | 0.72              |
| 1:C:328:GLU:HB2  | 1:C:332:ALA:HB3  | 1.71                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:363:PRO:HD2  | 1:B:367:TYR:CD2  | 2.24                     | 0.72              |
| 1:A:179:GLN:NE2  | 1:A:207:ILE:HD11 | 2.04                     | 0.72              |
| 1:A:46:ARG:NH1   | 1:A:46:ARG:HB2   | 2.04                     | 0.71              |
| 1:B:67:LYS:HE2   | 1:B:134:ARG:NH1  | 2.05                     | 0.71              |
| 1:B:11:LEU:HB2   | 1:B:62:ALA:CB    | 2.20                     | 0.71              |
| 1:C:292:HIS:O    | 1:C:296:ASN:HB2  | 1.89                     | 0.71              |
| 1:A:11:LEU:HB2   | 1:A:62:ALA:HB2   | 1.72                     | 0.71              |
| 1:C:155:VAL:HG11 | 1:C:177:TRP:HE1  | 1.56                     | 0.71              |
| 1:A:175:ALA:HA   | 1:A:178:LEU:HD13 | 1.72                     | 0.71              |
| 1:C:56:LEU:HD21  | 1:C:60:VAL:HG21  | 1.72                     | 0.71              |
| 1:A:34:GLN:NE2   | 1:C:229:ARG:HD2  | 2.06                     | 0.71              |
| 1:C:160:LEU:H    | 1:C:194:ARG:NH1  | 1.88                     | 0.71              |
| 1:A:212:LYS:HG2  | 1:A:213:LEU:HG   | 1.72                     | 0.71              |
| 1:B:188:ILE:HA   | 1:B:216:ILE:HG22 | 1.73                     | 0.71              |
| 1:B:89:LEU:HB3   | 1:B:91:GLU:OE1   | 1.91                     | 0.71              |
| 1:A:199:LEU:HD21 | 1:A:215:VAL:HG21 | 1.71                     | 0.70              |
| 1:A:6:HIS:O      | 1:A:8:ILE:HG13   | 1.91                     | 0.70              |
| 1:A:133:LYS:H    | 1:A:133:LYS:HD2  | 1.55                     | 0.70              |
| 1:A:20:ARG:O     | 1:A:24:GLU:HG3   | 1.91                     | 0.70              |
| 1:C:108:GLU:O    | 1:C:112:LEU:HD12 | 1.92                     | 0.70              |
| 1:A:272:ILE:H    | 1:A:272:ILE:CD1  | 1.93                     | 0.70              |
| 1:A:60:VAL:HG12  | 1:A:61:ILE:H     | 1.56                     | 0.70              |
| 1:C:131:SER:C    | 1:C:133:LYS:H    | 1.95                     | 0.70              |
| 1:C:362:TYR:HD1  | 1:C:367:TYR:HD2  | 1.39                     | 0.70              |
| 1:A:133:LYS:HD2  | 1:A:133:LYS:N    | 2.06                     | 0.69              |
| 1:C:364:SER:HB2  | 1:C:366:GLN:HG3  | 1.74                     | 0.69              |
| 1:A:11:LEU:HB2   | 1:A:62:ALA:CB    | 2.22                     | 0.69              |
| 1:B:284:ASP:HB3  | 1:B:325:GLU:OE1  | 1.92                     | 0.69              |
| 1:B:317:ASN:HB3  | 1:B:321:ARG:HD2  | 1.74                     | 0.69              |
| 1:B:335:HIS:HA   | 1:B:338:LYS:HE2  | 1.74                     | 0.69              |
| 1:C:196:ARG:HG3  | 1:C:224:THR:HG21 | 1.74                     | 0.69              |
| 1:A:15:ASN:CG    | 1:A:16:LYS:H     | 1.94                     | 0.69              |
| 1:A:160:LEU:H    | 1:A:194:ARG:HH22 | 1.39                     | 0.69              |
| 1:A:225:ARG:HH21 | 1:A:274:ARG:CZ   | 2.05                     | 0.69              |
| 1:B:183:PRO:HG3  | 1:B:212:LYS:HE2  | 1.74                     | 0.69              |
| 1:B:7:ARG:HD3    | 1:B:57:GLY:HA2   | 1.75                     | 0.69              |
| 1:A:240:ARG:HD3  | 1:C:350:THR:HG21 | 1.73                     | 0.69              |
| 1:A:25:GLY:O     | 1:A:28:GLU:HB3   | 1.91                     | 0.69              |
| 1:A:225:ARG:HE   | 1:A:274:ARG:NH1  | 1.91                     | 0.69              |
| 1:A:34:GLN:HE21  | 1:C:229:ARG:HD2  | 1.58                     | 0.69              |
| 1:C:299:CYS:HA   | 1:C:338:LYS:CG   | 2.23                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:342:ALA:HB2  | 1:C:360:CYS:SG   | 2.33                     | 0.69              |
| 1:A:328:GLU:HB3  | 1:A:333:MET:HG2  | 1.75                     | 0.68              |
| 1:B:123:ALA:HB2  | 1:B:181:LEU:HD21 | 1.73                     | 0.68              |
| 1:C:21:GLN:HB3   | 1:C:239:ALA:HB3  | 1.74                     | 0.68              |
| 1:A:121:ARG:HG2  | 1:A:152:TYR:CD1  | 2.29                     | 0.68              |
| 1:B:133:LYS:HD2  | 1:B:133:LYS:N    | 2.08                     | 0.68              |
| 1:C:311:VAL:CB   | 1:C:318:LEU:HD11 | 2.23                     | 0.68              |
| 1:A:13:ASN:O     | 1:A:19:ASP:HB3   | 1.92                     | 0.68              |
| 1:A:42:GLU:O     | 1:A:43:GLU:HB2   | 1.93                     | 0.68              |
| 1:A:95:PRO:O     | 1:A:96:VAL:HB    | 1.92                     | 0.68              |
| 1:B:369:TYR:CZ   | 1:B:373:LYS:HD2  | 2.28                     | 0.67              |
| 1:A:348:SER:O    | 1:A:349:THR:HG23 | 1.94                     | 0.67              |
| 1:C:197:HIS:N    | 1:C:200:GLN:HE21 | 1.92                     | 0.67              |
| 1:C:197:HIS:HA   | 1:C:200:GLN:NE2  | 2.10                     | 0.67              |
| 1:C:70:GLU:OE2   | 1:C:94:PRO:HB3   | 1.94                     | 0.67              |
| 1:B:210:PRO:HD2  | 1:B:295:ARG:NH1  | 2.10                     | 0.67              |
| 1:B:343:ARG:HB3  | 1:B:343:ARG:CZ   | 2.24                     | 0.67              |
| 1:C:161:GLU:HB3  | 1:C:164:PRO:CB   | 2.24                     | 0.67              |
| 1:C:313:ILE:HG22 | 1:C:314:SER:H    | 1.60                     | 0.67              |
| 1:A:167:TRP:CE3  | 1:A:168:GLN:HB2  | 2.29                     | 0.67              |
| 1:A:61:ILE:HD13  | 1:A:81:VAL:HB    | 1.77                     | 0.67              |
| 1:A:26:VAL:HG13  | 1:A:247:ALA:HB2  | 1.76                     | 0.67              |
| 1:B:5:ARG:HA     | 1:B:36:GLU:O     | 1.95                     | 0.67              |
| 1:B:30:LEU:HD23  | 1:B:30:LEU:O     | 1.94                     | 0.67              |
| 1:C:299:CYS:HA   | 1:C:338:LYS:HG3  | 1.76                     | 0.67              |
| 1:B:218:ILE:HA   | 1:B:235:VAL:HG23 | 1.76                     | 0.66              |
| 1:A:185:THR:HG22 | 1:A:186:GLY:N    | 2.11                     | 0.66              |
| 1:A:253:LEU:O    | 1:A:253:LEU:HD23 | 1.94                     | 0.66              |
| 1:B:56:LEU:CD2   | 1:B:78:VAL:HG21  | 2.24                     | 0.66              |
| 1:A:43:GLU:HG2   | 1:A:45:PHE:O     | 1.96                     | 0.66              |
| 1:C:293:TYR:HE2  | 1:C:302:ILE:HG13 | 1.59                     | 0.66              |
| 1:C:33:SER:O     | 1:C:34:GLN:HB2   | 1.95                     | 0.66              |
| 1:B:135:TRP:HE3  | 1:B:139:ARG:NH2  | 1.94                     | 0.66              |
| 1:A:304:VAL:HG12 | 1:A:308:LEU:HD21 | 1.78                     | 0.66              |
| 1:B:345:LEU:HB3  | 1:B:356:ILE:HD12 | 1.77                     | 0.66              |
| 1:A:160:LEU:HD23 | 1:A:161:GLU:H    | 1.61                     | 0.65              |
| 1:B:43:GLU:HG2   | 1:B:45:PHE:O     | 1.96                     | 0.65              |
| 1:C:362:TYR:HD1  | 1:C:367:TYR:CD2  | 2.13                     | 0.65              |
| 1:A:254:LEU:C    | 1:A:256:LYS:H    | 2.00                     | 0.65              |
| 1:C:56:LEU:CD2   | 1:C:60:VAL:HG21  | 2.26                     | 0.65              |
| 1:C:378:THR:HG22 | 1:C:382:GLU:OE1  | 1.96                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:122:PHE:O    | 1:C:154:GLY:HA2  | 1.97                     | 0.65              |
| 1:A:227:LEU:HB3  | 1:C:27:GLY:HA3   | 1.79                     | 0.65              |
| 1:A:7:ARG:HH12   | 1:A:57:GLY:HA2   | 1.60                     | 0.65              |
| 1:B:363:PRO:HD2  | 1:B:367:TYR:CE2  | 2.32                     | 0.65              |
| 1:C:127:LEU:HA   | 1:C:194:ARG:NH2  | 2.11                     | 0.65              |
| 1:A:286:ALA:HA   | 1:A:311:VAL:HG11 | 1.79                     | 0.65              |
| 1:C:125:TYR:CE2  | 1:C:194:ARG:HB3  | 2.31                     | 0.65              |
| 1:C:384:ARG:O    | 1:C:388:SER:HB2  | 1.96                     | 0.65              |
| 1:A:175:ALA:HB1  | 1:A:205:LEU:HD21 | 1.79                     | 0.65              |
| 1:A:303:LYS:O    | 1:A:307:VAL:CG2  | 2.43                     | 0.65              |
| 1:B:124:PHE:HZ   | 1:B:190:VAL:HG13 | 1.60                     | 0.65              |
| 1:B:162:THR:HG23 | 1:B:163:ALA:N    | 2.11                     | 0.65              |
| 1:C:366:GLN:O    | 1:C:369:TYR:HB3  | 1.97                     | 0.65              |
| 1:A:106:LEU:O    | 1:A:109:SER:HB3  | 1.97                     | 0.65              |
| 1:A:101:THR:HB   | 1:A:242:MET:HE1  | 1.79                     | 0.65              |
| 1:B:195:ALA:HB3  | 1:B:232:LEU:HD11 | 1.79                     | 0.65              |
| 1:A:272:ILE:HG21 | 1:A:274:ARG:HH21 | 1.62                     | 0.64              |
| 1:C:272:ILE:HG21 | 1:C:274:ARG:CZ   | 2.27                     | 0.64              |
| 1:A:160:LEU:HD22 | 1:A:164:PRO:CB   | 2.28                     | 0.64              |
| 1:C:12:PHE:HD2   | 1:C:23:VAL:HG22  | 1.61                     | 0.64              |
| 1:A:121:ARG:HG2  | 1:A:152:TYR:HD1  | 1.61                     | 0.64              |
| 1:A:199:LEU:CD2  | 1:A:215:VAL:HG21 | 2.26                     | 0.64              |
| 1:B:108:GLU:HG2  | 1:B:112:LEU:HD12 | 1.79                     | 0.64              |
| 1:C:93:TYR:OH    | 1:C:265:LEU:HD21 | 1.96                     | 0.64              |
| 1:A:272:ILE:HD12 | 1:A:272:ILE:N    | 2.01                     | 0.64              |
| 1:A:99:ILE:HD12  | 1:A:264:ILE:HG12 | 1.77                     | 0.64              |
| 1:B:143:PHE:CE2  | 1:B:147:VAL:HG11 | 2.32                     | 0.64              |
| 1:C:185:THR:HB   | 1:C:213:LEU:HD22 | 1.79                     | 0.64              |
| 1:C:225:ARG:NE   | 1:C:274:ARG:NH2  | 2.44                     | 0.64              |
| 1:B:311:VAL:HG21 | 1:B:318:LEU:HD21 | 1.79                     | 0.64              |
| 1:B:354:ASN:O    | 1:B:357:SER:HB3  | 1.98                     | 0.64              |
| 1:B:355:GLU:O    | 1:B:359:MET:HB3  | 1.97                     | 0.64              |
| 1:C:184:GLN:NE2  | 1:C:211:GLU:O    | 2.31                     | 0.64              |
| 1:C:299:CYS:HB3  | 1:C:341:LYS:HB2  | 1.79                     | 0.64              |
| 1:B:133:LYS:HB3  | 1:B:135:TRP:CD1  | 2.33                     | 0.64              |
| 1:C:155:VAL:CG1  | 1:C:177:TRP:HE1  | 2.10                     | 0.64              |
| 1:C:17:ALA:HB2   | 1:C:221:GLU:OE1  | 1.98                     | 0.64              |
| 1:A:86:SER:HB3   | 1:A:102:ASP:HA   | 1.80                     | 0.63              |
| 1:C:220:ASN:ND2  | 1:C:225:ARG:HH22 | 1.96                     | 0.63              |
| 1:B:345:LEU:CA   | 1:B:349:THR:HG23 | 2.27                     | 0.63              |
| 1:C:131:SER:HB2  | 1:C:133:LYS:HD2  | 1.80                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:386:VAL:HG12 | 1:A:387:ASN:N    | 2.13                     | 0.63              |
| 1:B:230:VAL:HG12 | 1:B:275:ARG:HD3  | 1.81                     | 0.63              |
| 1:C:302:ILE:H    | 1:C:302:ILE:HD13 | 1.63                     | 0.63              |
| 1:B:143:PHE:CZ   | 1:B:147:VAL:HG21 | 2.34                     | 0.63              |
| 1:C:262:GLN:O    | 1:C:263:ARG:HD2  | 1.97                     | 0.63              |
| 1:B:84:GLY:O     | 1:B:101:THR:HG22 | 1.99                     | 0.63              |
| 1:A:302:ILE:HG13 | 1:A:334:ILE:CD1  | 2.29                     | 0.63              |
| 1:A:298:ALA:HB3  | 1:A:341:LYS:HD2  | 1.81                     | 0.63              |
| 1:A:169:HIS:NE2  | 1:A:173:ARG:HD2  | 2.13                     | 0.63              |
| 1:A:346:LEU:HA   | 1:A:384:ARG:NH1  | 2.14                     | 0.63              |
| 1:A:43:GLU:HA    | 1:A:45:PHE:O     | 1.99                     | 0.63              |
| 1:B:292:HIS:O    | 1:B:295:ARG:N    | 2.32                     | 0.63              |
| 1:C:174:LEU:HD11 | 1:C:178:LEU:HD11 | 1.81                     | 0.62              |
| 1:C:308:LEU:HD13 | 1:C:315:ARG:HB2  | 1.81                     | 0.62              |
| 1:C:328:GLU:HB2  | 1:C:332:ALA:CB   | 2.28                     | 0.62              |
| 1:A:279:TYR:CE2  | 1:A:281:SER:HA   | 2.33                     | 0.62              |
| 1:B:347:ILE:O    | 1:B:389:GLU:N    | 2.31                     | 0.62              |
| 1:C:286:ALA:HA   | 1:C:311:VAL:CG1  | 2.29                     | 0.62              |
| 1:B:151:LYS:HB3  | 1:B:152:TYR:CE1  | 2.34                     | 0.62              |
| 1:C:296:ASN:HB3  | 1:C:297:HIS:ND1  | 2.15                     | 0.62              |
| 1:B:292:HIS:HA   | 1:B:295:ARG:HG3  | 1.82                     | 0.62              |
| 1:B:225:ARG:HH12 | 1:B:389:GLU:C    | 2.03                     | 0.62              |
| 1:C:13:ASN:O     | 1:C:19:ASP:HB2   | 1.99                     | 0.62              |
| 1:A:232:LEU:HD23 | 1:A:233:SER:O    | 2.00                     | 0.62              |
| 1:C:302:ILE:HD13 | 1:C:302:ILE:N    | 2.14                     | 0.62              |
| 1:A:240:ARG:HD3  | 1:C:350:THR:CB   | 2.29                     | 0.62              |
| 1:C:4:LYS:NZ     | 1:C:4:LYS:HA     | 2.15                     | 0.62              |
| 1:A:121:ARG:HH11 | 1:A:121:ARG:HG3  | 1.65                     | 0.61              |
| 1:A:292:HIS:CD2  | 1:A:296:ASN:HD21 | 2.18                     | 0.61              |
| 1:C:290:ALA:CA   | 1:C:311:VAL:HG22 | 2.30                     | 0.61              |
| 1:A:15:ASN:CG    | 1:A:16:LYS:N     | 2.54                     | 0.61              |
| 1:A:10:LEU:CD2   | 1:A:61:ILE:HB    | 2.29                     | 0.61              |
| 1:B:131:SER:O    | 1:B:133:LYS:N    | 2.33                     | 0.61              |
| 1:B:135:TRP:HE3  | 1:B:139:ARG:CZ   | 2.13                     | 0.61              |
| 1:B:308:LEU:HA   | 1:B:318:LEU:CD1  | 2.30                     | 0.61              |
| 1:B:347:ILE:HG13 | 1:B:387:ASN:O    | 1.99                     | 0.61              |
| 1:A:382:GLU:O    | 1:A:386:VAL:HG21 | 2.00                     | 0.61              |
| 1:C:342:ALA:HB1  | 1:C:356:ILE:HG22 | 1.81                     | 0.61              |
| 1:C:39:ILE:HD12  | 1:C:39:ILE:H     | 1.65                     | 0.61              |
| 1:B:207:ILE:O    | 1:B:209:VAL:HG23 | 1.99                     | 0.61              |
| 1:B:211:GLU:OE2  | 1:B:211:GLU:HA   | 1.99                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:269:VAL:HG12 | 1:A:270:ARG:N    | 2.14                     | 0.61              |
| 1:A:64:PHE:CD2   | 1:A:70:GLU:HB2   | 2.34                     | 0.61              |
| 1:B:333:MET:O    | 1:B:337:GLU:N    | 2.33                     | 0.61              |
| 1:B:43:GLU:HA    | 1:B:45:PHE:N     | 2.16                     | 0.61              |
| 1:B:96:VAL:HG22  | 1:B:97:HIS:N     | 2.13                     | 0.61              |
| 1:A:286:ALA:HB3  | 1:A:321:ARG:HG2  | 1.82                     | 0.61              |
| 1:B:144:ARG:HH11 | 1:B:144:ARG:HG3  | 1.65                     | 0.61              |
| 1:B:313:ILE:HG13 | 1:B:321:ARG:HH12 | 1.66                     | 0.61              |
| 1:B:220:ASN:HD21 | 1:B:272:ILE:HG13 | 1.66                     | 0.61              |
| 1:C:185:THR:HB   | 1:C:213:LEU:CD2  | 2.31                     | 0.61              |
| 1:A:160:LEU:CD2  | 1:A:161:GLU:H    | 2.14                     | 0.61              |
| 1:C:150:GLU:CG   | 1:C:151:LYS:H    | 2.12                     | 0.60              |
| 1:C:345:LEU:HD23 | 1:C:349:THR:HG21 | 1.83                     | 0.60              |
| 1:C:388:SER:O    | 1:C:389:GLU:HB3  | 2.00                     | 0.60              |
| 1:C:87:TYR:HD2   | 1:C:92:SER:HB3   | 1.66                     | 0.60              |
| 1:A:144:ARG:O    | 1:A:147:VAL:HG12 | 2.02                     | 0.60              |
| 1:A:227:LEU:HB3  | 1:C:27:GLY:HA2   | 1.83                     | 0.60              |
| 1:B:175:ALA:CB   | 1:B:205:LEU:HD21 | 2.31                     | 0.60              |
| 1:B:294:ILE:O    | 1:B:298:ALA:CB   | 2.49                     | 0.60              |
| 1:B:56:LEU:HG    | 1:B:57:GLY:N     | 2.15                     | 0.60              |
| 1:C:42:GLU:HA    | 1:C:45:PHE:HZ    | 1.64                     | 0.60              |
| 1:A:274:ARG:HG3  | 1:A:274:ARG:NH1  | 2.12                     | 0.60              |
| 1:C:342:ALA:O    | 1:C:356:ILE:HG21 | 2.01                     | 0.60              |
| 1:A:328:GLU:HG2  | 1:A:333:MET:SD   | 2.41                     | 0.60              |
| 1:B:1:MET:HA     | 1:B:1:MET:CE     | 2.31                     | 0.60              |
| 1:B:358:GLN:HG3  | 1:B:359:MET:H    | 1.66                     | 0.60              |
| 1:C:298:ALA:N    | 1:C:341:LYS:NZ   | 2.50                     | 0.60              |
| 1:C:135:TRP:HB2  | 1:C:139:ARG:HH21 | 1.66                     | 0.60              |
| 1:C:235:VAL:O    | 1:C:235:VAL:HG12 | 2.00                     | 0.60              |
| 1:C:311:VAL:CG2  | 1:C:318:LEU:HD11 | 2.32                     | 0.60              |
| 1:A:7:ARG:HB3    | 1:A:7:ARG:CZ     | 2.32                     | 0.60              |
| 1:B:223:LEU:H    | 1:B:223:LEU:HD23 | 1.67                     | 0.60              |
| 1:A:229:ARG:NH1  | 1:A:296:ASN:HB3  | 2.16                     | 0.60              |
| 1:C:197:HIS:CA   | 1:C:200:GLN:HE21 | 2.15                     | 0.60              |
| 1:C:319:GLU:O    | 1:C:322:PHE:HB2  | 2.02                     | 0.60              |
| 1:A:158:GLN:O    | 1:A:159:GLY:O    | 2.19                     | 0.60              |
| 1:B:328:GLU:HA   | 1:B:328:GLU:OE1  | 2.01                     | 0.60              |
| 1:C:304:VAL:O    | 1:C:304:VAL:HG12 | 2.02                     | 0.60              |
| 1:A:238:GLY:O    | 1:A:242:MET:HB2  | 2.02                     | 0.59              |
| 1:A:315:ARG:HH11 | 1:A:315:ARG:HG3  | 1.65                     | 0.59              |
| 1:A:269:VAL:CG1  | 1:A:270:ARG:HG3  | 2.28                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:97:HIS:NE2   | 1:B:261:LEU:HA   | 2.17                     | 0.59              |
| 1:A:353:ILE:HD11 | 1:A:384:ARG:HD3  | 1.85                     | 0.59              |
| 1:B:336:ALA:O    | 1:B:339:LEU:HB2  | 2.02                     | 0.59              |
| 1:C:97:HIS:CD2   | 1:C:262:GLN:H    | 2.20                     | 0.59              |
| 1:A:222:GLU:OE2  | 1:C:20:ARG:NH2   | 2.33                     | 0.59              |
| 1:B:311:VAL:HG12 | 1:B:312:GLY:N    | 2.17                     | 0.59              |
| 1:B:11:LEU:HB2   | 1:B:62:ALA:HB2   | 1.84                     | 0.59              |
| 1:A:212:LYS:O    | 1:A:213:LEU:HD23 | 2.02                     | 0.59              |
| 1:A:298:ALA:O    | 1:A:338:LYS:HE2  | 2.02                     | 0.59              |
| 1:B:85:GLY:O     | 1:B:87:TYR:HD1   | 1.85                     | 0.59              |
| 1:C:174:LEU:HD11 | 1:C:178:LEU:CD1  | 2.32                     | 0.59              |
| 1:A:240:ARG:HD3  | 1:C:350:THR:CG2  | 2.32                     | 0.59              |
| 1:A:351:LEU:H    | 1:A:384:ARG:HH22 | 1.46                     | 0.59              |
| 1:C:98:TYR:CD2   | 1:C:100:ALA:HB2  | 2.38                     | 0.59              |
| 1:A:121:ARG:HD3  | 1:A:182:PRO:HB2  | 1.84                     | 0.59              |
| 1:A:303:LYS:HG2  | 1:A:306:GLN:NE2  | 2.18                     | 0.59              |
| 1:B:133:LYS:CG   | 1:B:135:TRP:HE1  | 2.16                     | 0.59              |
| 1:C:299:CYS:HB3  | 1:C:341:LYS:HD3  | 1.83                     | 0.59              |
| 1:A:262:GLN:O    | 1:A:263:ARG:HG3  | 2.03                     | 0.59              |
| 1:A:302:ILE:H    | 1:A:334:ILE:HD11 | 1.68                     | 0.59              |
| 1:B:162:THR:HG23 | 1:B:163:ALA:H    | 1.67                     | 0.59              |
| 1:A:190:VAL:HG23 | 1:A:191:THR:N    | 2.17                     | 0.59              |
| 1:A:188:ILE:HG12 | 1:A:216:ILE:HG23 | 1.84                     | 0.59              |
| 1:A:34:GLN:HG3   | 1:C:300:LYS:HZ2  | 1.67                     | 0.59              |
| 1:B:126:GLY:HA2  | 1:B:190:VAL:HG22 | 1.85                     | 0.59              |
| 1:B:86:SER:HB3   | 1:B:265:LEU:HD22 | 1.85                     | 0.59              |
| 1:B:275:ARG:O    | 1:B:277:THR:N    | 2.35                     | 0.59              |
| 1:C:376:TYR:O    | 1:C:378:THR:N    | 2.35                     | 0.59              |
| 1:A:224:THR:O    | 1:A:226:TYR:N    | 2.36                     | 0.58              |
| 1:A:300:LYS:HE2  | 1:C:2:PHE:HZ     | 1.68                     | 0.58              |
| 1:A:240:ARG:HG2  | 1:C:350:THR:HG21 | 1.85                     | 0.58              |
| 1:B:221:GLU:HG2  | 1:B:223:LEU:HD21 | 1.86                     | 0.58              |
| 1:C:10:LEU:CD2   | 1:C:61:ILE:HD12  | 2.32                     | 0.58              |
| 1:A:355:GLU:HA   | 1:A:358:GLN:OE1  | 2.03                     | 0.58              |
| 1:B:185:THR:HB   | 1:B:213:LEU:HD22 | 1.85                     | 0.58              |
| 1:C:231:ALA:HB1  | 1:C:274:ARG:HG2  | 1.85                     | 0.58              |
| 1:C:313:ILE:HB   | 1:C:318:LEU:HB2  | 1.83                     | 0.58              |
| 1:B:30:LEU:HD12  | 1:B:39:ILE:HD13  | 1.84                     | 0.58              |
| 1:B:88:HIS:HB2   | 1:B:138:GLU:OE1  | 2.03                     | 0.58              |
| 1:A:226:TYR:HB3  | 1:A:227:LEU:HD23 | 1.86                     | 0.58              |
| 1:A:238:GLY:O    | 1:A:266:VAL:HG11 | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:55:TRP:O     | 1:B:56:LEU:O     | 2.22                     | 0.58              |
| 1:A:4:LYS:CA     | 1:A:4:LYS:NZ     | 2.63                     | 0.58              |
| 1:B:119:VAL:HG12 | 1:B:122:PHE:CE2  | 2.38                     | 0.58              |
| 1:B:124:PHE:CD2  | 1:B:124:PHE:C    | 2.78                     | 0.58              |
| 1:C:286:ALA:O    | 1:C:311:VAL:HG13 | 2.01                     | 0.58              |
| 1:C:220:ASN:HB2  | 1:C:236:ALA:HA   | 1.85                     | 0.58              |
| 1:B:290:ALA:O    | 1:B:294:ILE:HG12 | 2.04                     | 0.57              |
| 1:C:64:PHE:HB2   | 1:C:98:TYR:HE1   | 1.68                     | 0.57              |
| 1:B:86:SER:OG    | 1:B:103:ASN:N    | 2.36                     | 0.57              |
| 1:B:113:HIS:HE1  | 1:B:273:GLU:OE1  | 1.87                     | 0.57              |
| 1:B:17:ALA:CB    | 1:B:221:GLU:HA   | 2.34                     | 0.57              |
| 1:A:135:TRP:O    | 1:A:139:ARG:HG3  | 2.02                     | 0.57              |
| 1:B:308:LEU:HD13 | 1:B:315:ARG:HB2  | 1.84                     | 0.57              |
| 1:C:135:TRP:CE3  | 1:C:136:ALA:N    | 2.72                     | 0.57              |
| 1:B:155:VAL:HG11 | 1:B:177:TRP:HE1  | 1.68                     | 0.57              |
| 1:C:191:THR:O    | 1:C:195:ALA:HB2  | 2.04                     | 0.57              |
| 1:C:11:LEU:CB    | 1:C:43:GLU:OE1   | 2.45                     | 0.57              |
| 1:A:140:GLU:O    | 1:A:144:ARG:HG2  | 2.03                     | 0.57              |
| 1:A:249:LEU:C    | 1:A:249:LEU:HD23 | 2.25                     | 0.57              |
| 1:C:224:THR:O    | 1:C:225:ARG:C    | 2.43                     | 0.57              |
| 1:C:73:LEU:HD13  | 1:C:80:ILE:CD1   | 2.34                     | 0.57              |
| 1:A:34:GLN:HE21  | 1:C:229:ARG:CD   | 2.17                     | 0.57              |
| 1:B:292:HIS:O    | 1:B:294:ILE:N    | 2.38                     | 0.57              |
| 1:C:197:HIS:HA   | 1:C:200:GLN:HE21 | 1.69                     | 0.57              |
| 1:C:293:TYR:CE1  | 1:C:297:HIS:HB2  | 2.40                     | 0.57              |
| 1:A:126:GLY:HA2  | 1:A:190:VAL:HG13 | 1.86                     | 0.57              |
| 1:B:24:GLU:HB3   | 1:B:240:ARG:NH2  | 2.20                     | 0.57              |
| 1:C:220:ASN:OD1  | 1:C:272:ILE:HD12 | 2.03                     | 0.57              |
| 1:A:12:PHE:HD2   | 1:A:23:VAL:HG23  | 1.70                     | 0.57              |
| 1:A:244:TYR:HD1  | 1:A:245:GLN:HE21 | 1.53                     | 0.57              |
| 1:A:330:ILE:HG22 | 1:A:331:HIS:N    | 2.19                     | 0.57              |
| 1:B:251:HIS:O    | 1:B:254:LEU:HB2  | 2.04                     | 0.57              |
| 1:C:8:ILE:HG13   | 1:C:37:TRP:CE3   | 2.40                     | 0.57              |
| 1:C:96:VAL:HG22  | 1:C:97:HIS:H     | 1.68                     | 0.57              |
| 1:A:286:ALA:O    | 1:A:290:ALA:HB2  | 2.04                     | 0.57              |
| 1:B:107:VAL:HG12 | 1:B:146:LEU:HD11 | 1.86                     | 0.57              |
| 1:A:261:LEU:HB3  | 1:A:263:ARG:HH21 | 1.70                     | 0.57              |
| 1:A:356:ILE:O    | 1:A:360:CYS:HB2  | 2.05                     | 0.57              |
| 1:B:264:ILE:HD12 | 1:B:265:LEU:N    | 2.20                     | 0.57              |
| 1:C:263:ARG:HG2  | 1:C:263:ARG:HH11 | 1.70                     | 0.57              |
| 1:A:110:ALA:O    | 1:A:113:HIS:HB3  | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:79:PRO:CG    | 1:A:253:LEU:HD22 | 2.32                     | 0.56              |
| 1:A:46:ARG:HH11  | 1:A:46:ARG:HB2   | 1.69                     | 0.56              |
| 1:B:174:LEU:HG   | 1:B:178:LEU:HD13 | 1.87                     | 0.56              |
| 1:C:85:GLY:HA2   | 1:C:101:THR:HG22 | 1.87                     | 0.56              |
| 1:C:328:GLU:HG3  | 1:C:332:ALA:O    | 2.05                     | 0.56              |
| 1:A:43:GLU:C     | 1:A:45:PHE:N     | 2.58                     | 0.56              |
| 1:C:308:LEU:HB2  | 1:C:314:SER:O    | 2.05                     | 0.56              |
| 1:A:289:GLN:HB3  | 1:A:311:VAL:HG13 | 1.87                     | 0.56              |
| 1:B:124:PHE:C    | 1:B:124:PHE:HD2  | 2.09                     | 0.56              |
| 1:C:85:GLY:HA2   | 1:C:101:THR:CG2  | 2.35                     | 0.56              |
| 1:C:256:LYS:HE3  | 1:C:256:LYS:N    | 2.20                     | 0.56              |
| 1:B:343:ARG:NH1  | 1:B:383:TYR:OH   | 2.38                     | 0.56              |
| 1:C:126:GLY:O    | 1:C:158:GLN:HA   | 2.05                     | 0.56              |
| 1:C:252:ARG:NH2  | 1:C:259:MET:CE   | 2.68                     | 0.56              |
| 1:C:87:TYR:CD2   | 1:C:92:SER:HB3   | 2.40                     | 0.56              |
| 1:A:221:GLU:O    | 1:A:225:ARG:HG2  | 2.04                     | 0.56              |
| 1:B:151:LYS:HG2  | 1:B:151:LYS:O    | 2.05                     | 0.56              |
| 1:B:311:VAL:CB   | 1:B:318:LEU:HD11 | 2.36                     | 0.56              |
| 1:C:232:LEU:HD22 | 1:C:233:SER:N    | 2.20                     | 0.56              |
| 1:C:103:ASN:O    | 1:C:107:VAL:HG23 | 2.05                     | 0.56              |
| 1:C:152:TYR:N    | 1:C:152:TYR:CD1  | 2.73                     | 0.56              |
| 1:C:259:MET:HG2  | 1:C:262:GLN:NE2  | 2.20                     | 0.56              |
| 1:A:291:MET:O    | 1:A:292:HIS:C    | 2.42                     | 0.56              |
| 1:B:269:VAL:HG12 | 1:B:270:ARG:HD3  | 1.87                     | 0.56              |
| 1:C:147:VAL:HG21 | 1:C:154:GLY:H    | 1.70                     | 0.56              |
| 1:A:127:LEU:CD1  | 1:A:194:ARG:NE   | 2.69                     | 0.55              |
| 1:B:81:VAL:HG21  | 1:B:249:LEU:HD22 | 1.88                     | 0.55              |
| 1:B:11:LEU:HB2   | 1:B:62:ALA:HB1   | 1.88                     | 0.55              |
| 1:C:79:PRO:HB3   | 1:C:253:LEU:HD13 | 1.86                     | 0.55              |
| 1:A:7:ARG:HA     | 1:A:38:ASP:HB3   | 1.88                     | 0.55              |
| 1:B:211:GLU:OE1  | 1:B:295:ARG:NH2  | 2.38                     | 0.55              |
| 1:B:358:GLN:O    | 1:B:359:MET:C    | 2.45                     | 0.55              |
| 1:C:79:PRO:CG    | 1:C:253:LEU:HD22 | 2.36                     | 0.55              |
| 1:B:320:LYS:O    | 1:B:323:LYS:CD   | 2.54                     | 0.55              |
| 1:C:345:LEU:HA   | 1:C:349:THR:HG21 | 1.87                     | 0.55              |
| 1:C:286:ALA:HA   | 1:C:311:VAL:HG12 | 1.89                     | 0.55              |
| 1:B:221:GLU:HG2  | 1:B:223:LEU:CD2  | 2.36                     | 0.55              |
| 1:C:12:PHE:O     | 1:C:43:GLU:HB3   | 2.07                     | 0.55              |
| 1:A:146:LEU:HD12 | 1:A:147:VAL:N    | 2.21                     | 0.55              |
| 1:B:135:TRP:CE3  | 1:B:139:ARG:NH2  | 2.74                     | 0.55              |
| 1:C:282:LEU:HD22 | 1:C:325:GLU:HG3  | 1.87                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:135:TRP:CE3  | 1:A:136:ALA:N    | 2.74                     | 0.55              |
| 1:A:272:ILE:HG21 | 1:A:274:ARG:NH2  | 2.21                     | 0.55              |
| 1:A:280:ARG:HB3  | 1:A:280:ARG:CZ   | 2.36                     | 0.55              |
| 1:A:274:ARG:HH11 | 1:A:274:ARG:CG   | 2.10                     | 0.55              |
| 1:A:347:ILE:CG2  | 1:A:389:GLU:H    | 2.18                     | 0.55              |
| 1:B:108:GLU:HG2  | 1:B:112:LEU:CD1  | 2.36                     | 0.55              |
| 1:B:13:ASN:O     | 1:B:15:ASN:N     | 2.39                     | 0.55              |
| 1:C:18:TYR:O     | 1:C:21:GLN:HB2   | 2.07                     | 0.55              |
| 1:C:382:GLU:HG2  | 1:C:382:GLU:O    | 2.05                     | 0.55              |
| 1:A:286:ALA:HA   | 1:A:311:VAL:CG1  | 2.36                     | 0.54              |
| 1:A:313:ILE:CG2  | 1:A:317:ASN:HB3  | 2.37                     | 0.54              |
| 1:A:235:VAL:HA   | 1:A:271:VAL:HG13 | 1.89                     | 0.54              |
| 1:A:60:VAL:O     | 1:A:61:ILE:HG12  | 2.07                     | 0.54              |
| 1:B:320:LYS:O    | 1:B:323:LYS:NZ   | 2.39                     | 0.54              |
| 1:C:345:LEU:HA   | 1:C:349:THR:CG2  | 2.37                     | 0.54              |
| 1:A:160:LEU:N    | 1:A:194:ARG:HH22 | 2.04                     | 0.54              |
| 1:A:329:THR:N    | 1:A:332:ALA:HB3  | 2.22                     | 0.54              |
| 1:C:150:GLU:HG3  | 1:C:151:LYS:N    | 2.17                     | 0.54              |
| 1:C:174:LEU:CD1  | 1:C:178:LEU:CD1  | 2.85                     | 0.54              |
| 1:C:232:LEU:HD22 | 1:C:233:SER:H    | 1.73                     | 0.54              |
| 1:A:126:GLY:HA2  | 1:A:190:VAL:CG1  | 2.37                     | 0.54              |
| 1:C:151:LYS:HD2  | 1:C:152:TYR:CE1  | 2.43                     | 0.54              |
| 1:C:162:THR:HG23 | 1:C:163:ALA:N    | 2.23                     | 0.54              |
| 1:C:372:PHE:O    | 1:C:372:PHE:HD2  | 1.90                     | 0.54              |
| 1:B:313:ILE:HG13 | 1:B:321:ARG:NH1  | 2.22                     | 0.54              |
| 1:B:351:LEU:H    | 1:B:384:ARG:NH2  | 2.05                     | 0.54              |
| 1:A:165:GLU:HG2  | 1:A:166:ASN:H    | 1.72                     | 0.54              |
| 1:A:178:LEU:HD23 | 1:A:202:CYS:SG   | 2.48                     | 0.54              |
| 1:A:240:ARG:CD   | 1:C:350:THR:HG21 | 2.37                     | 0.54              |
| 1:A:347:ILE:HD11 | 1:A:383:TYR:CZ   | 2.43                     | 0.54              |
| 1:A:388:SER:O    | 1:A:389:GLU:HB2  | 2.07                     | 0.54              |
| 1:B:275:ARG:HH21 | 1:B:295:ARG:HH11 | 1.56                     | 0.54              |
| 1:B:6:HIS:ND1    | 1:B:6:HIS:N      | 2.56                     | 0.54              |
| 1:A:100:ALA:O    | 1:A:266:VAL:HG23 | 2.08                     | 0.54              |
| 1:A:314:SER:O    | 1:A:318:LEU:HB2  | 2.06                     | 0.54              |
| 1:B:23:VAL:CG1   | 1:B:24:GLU:N     | 2.70                     | 0.54              |
| 1:B:275:ARG:C    | 1:B:277:THR:H    | 2.11                     | 0.54              |
| 1:C:127:LEU:CD2  | 1:C:190:VAL:HG21 | 2.38                     | 0.54              |
| 1:C:139:ARG:HD3  | 1:C:218:ILE:HD12 | 1.89                     | 0.54              |
| 1:C:24:GLU:HB3   | 1:C:240:ARG:NH1  | 2.22                     | 0.54              |
| 1:A:30:LEU:CD2   | 1:A:39:ILE:HD11  | 2.38                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:99:ILE:HD12  | 1:A:264:ILE:CG1  | 2.38                     | 0.54              |
| 1:B:159:GLY:HA3  | 1:B:194:ARG:NH2  | 2.22                     | 0.54              |
| 1:B:85:GLY:O     | 1:B:87:TYR:CD1   | 2.61                     | 0.54              |
| 1:C:87:TYR:HE2   | 1:C:134:ARG:HE   | 1.55                     | 0.54              |
| 1:A:104:TYR:HA   | 1:A:142:ALA:HB1  | 1.89                     | 0.54              |
| 1:A:188:ILE:HG12 | 1:A:216:ILE:CG2  | 2.38                     | 0.54              |
| 1:A:30:LEU:HD21  | 1:A:39:ILE:HD11  | 1.90                     | 0.54              |
| 1:B:356:ILE:O    | 1:B:360:CYS:HB2  | 2.08                     | 0.54              |
| 1:C:345:LEU:HD22 | 1:C:351:LEU:HD12 | 1.88                     | 0.54              |
| 1:C:42:GLU:O     | 1:C:43:GLU:HB2   | 2.07                     | 0.54              |
| 1:C:11:LEU:HD12  | 1:C:62:ALA:HB2   | 1.90                     | 0.54              |
| 1:A:159:GLY:HA3  | 1:A:194:ARG:HH21 | 1.73                     | 0.53              |
| 1:A:24:GLU:OE1   | 1:A:240:ARG:NH2  | 2.33                     | 0.53              |
| 1:A:328:GLU:HG3  | 1:A:332:ALA:CB   | 2.35                     | 0.53              |
| 1:B:149:GLU:O    | 1:B:149:GLU:HG2  | 2.06                     | 0.53              |
| 1:B:9:THR:O      | 1:B:60:VAL:HG12  | 2.08                     | 0.53              |
| 1:B:97:HIS:CE1   | 1:B:262:GLN:H    | 2.26                     | 0.53              |
| 1:C:192:ASP:H    | 1:C:219:ASP:HB2  | 1.73                     | 0.53              |
| 1:C:218:ILE:HA   | 1:C:235:VAL:HB   | 1.90                     | 0.53              |
| 1:A:311:VAL:CG2  | 1:A:318:LEU:HD21 | 2.39                     | 0.53              |
| 1:B:182:PRO:O    | 1:B:213:LEU:HD21 | 2.09                     | 0.53              |
| 1:C:128:PRO:HG2  | 1:C:160:LEU:O    | 2.08                     | 0.53              |
| 1:A:195:ALA:HB3  | 1:A:232:LEU:HD11 | 1.90                     | 0.53              |
| 1:A:178:LEU:HD22 | 1:A:201:VAL:HG12 | 1.90                     | 0.53              |
| 1:A:227:LEU:HD23 | 1:A:227:LEU:H    | 1.72                     | 0.53              |
| 1:A:326:VAL:O    | 1:A:326:VAL:HG12 | 2.09                     | 0.53              |
| 1:A:1:MET:HG2    | 1:A:2:PHE:N      | 2.24                     | 0.53              |
| 1:A:353:ILE:CD1  | 1:A:384:ARG:HD3  | 2.39                     | 0.53              |
| 1:B:272:ILE:CG2  | 1:B:274:ARG:HE   | 2.18                     | 0.53              |
| 1:C:131:SER:C    | 1:C:133:LYS:N    | 2.61                     | 0.53              |
| 1:C:218:ILE:O    | 1:C:218:ILE:CG2  | 2.53                     | 0.53              |
| 1:A:225:ARG:HE   | 1:A:274:ARG:HH12 | 1.55                     | 0.53              |
| 1:B:233:SER:HA   | 1:B:274:ARG:HG2  | 1.89                     | 0.53              |
| 1:B:319:GLU:O    | 1:B:323:LYS:HD2  | 2.08                     | 0.53              |
| 1:C:220:ASN:C    | 1:C:225:ARG:HH12 | 2.12                     | 0.53              |
| 1:A:169:HIS:CE1  | 1:A:173:ARG:HD2  | 2.44                     | 0.53              |
| 1:C:275:ARG:HG2  | 1:C:295:ARG:NH1  | 2.13                     | 0.53              |
| 1:A:225:ARG:NH2  | 1:A:274:ARG:CZ   | 2.72                     | 0.53              |
| 1:A:73:LEU:CD2   | 1:A:80:ILE:HD13  | 2.38                     | 0.53              |
| 1:C:161:GLU:HG2  | 1:C:164:PRO:HA   | 1.89                     | 0.53              |
| 1:C:220:ASN:HD21 | 1:C:225:ARG:HH22 | 1.56                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:269:VAL:HG23 | 1:C:270:ARG:N    | 2.18                     | 0.53              |
| 1:A:190:VAL:O    | 1:A:218:ILE:HD13 | 2.09                     | 0.53              |
| 1:A:235:VAL:HG12 | 1:A:236:ALA:H    | 1.74                     | 0.53              |
| 1:C:11:LEU:HA    | 1:C:42:GLU:O     | 2.09                     | 0.53              |
| 1:C:196:ARG:C    | 1:C:200:GLN:HE21 | 2.13                     | 0.52              |
| 1:A:61:ILE:HD11  | 1:A:250:LEU:HD22 | 1.92                     | 0.52              |
| 1:B:126:GLY:HA2  | 1:B:190:VAL:CG2  | 2.39                     | 0.52              |
| 1:B:175:ALA:HB2  | 1:B:205:LEU:HD21 | 1.90                     | 0.52              |
| 1:C:142:ALA:O    | 1:C:146:LEU:HG   | 2.09                     | 0.52              |
| 1:C:174:LEU:O    | 1:C:178:LEU:HB2  | 2.08                     | 0.52              |
| 1:C:26:VAL:C     | 1:C:28:GLU:H     | 2.12                     | 0.52              |
| 1:A:128:PRO:C    | 1:A:130:SER:H    | 2.12                     | 0.52              |
| 1:A:177:TRP:NE1  | 1:A:181:LEU:HD21 | 2.25                     | 0.52              |
| 1:C:99:ILE:HD13  | 1:C:264:ILE:CG2  | 2.40                     | 0.52              |
| 1:A:98:TYR:O     | 1:A:263:ARG:HA   | 2.09                     | 0.52              |
| 1:B:187:ILE:O    | 1:B:216:ILE:HG22 | 2.09                     | 0.52              |
| 1:B:369:TYR:O    | 1:B:373:LYS:HG3  | 2.10                     | 0.52              |
| 1:C:275:ARG:HH22 | 1:C:296:ASN:HD21 | 1.57                     | 0.52              |
| 1:B:135:TRP:CE3  | 1:B:139:ARG:CZ   | 2.92                     | 0.52              |
| 1:C:353:ILE:HD11 | 1:C:384:ARG:HG3  | 1.91                     | 0.52              |
| 1:A:299:CYS:HA   | 1:A:338:LYS:HG3  | 1.91                     | 0.52              |
| 1:B:205:LEU:HD12 | 1:B:205:LEU:N    | 2.25                     | 0.52              |
| 1:C:159:GLY:HA3  | 1:C:194:ARG:NH1  | 2.25                     | 0.52              |
| 1:C:42:GLU:HA    | 1:C:45:PHE:CZ    | 2.44                     | 0.52              |
| 1:A:192:ASP:OD2  | 1:A:232:LEU:HD22 | 2.10                     | 0.52              |
| 1:A:345:LEU:HA   | 1:A:349:THR:OG1  | 2.10                     | 0.52              |
| 1:A:61:ILE:CD1   | 1:A:81:VAL:HB    | 2.40                     | 0.52              |
| 1:A:7:ARG:HA     | 1:A:38:ASP:CB    | 2.40                     | 0.52              |
| 1:A:91:GLU:HG2   | 1:A:91:GLU:O     | 2.10                     | 0.52              |
| 1:A:83:VAL:HA    | 1:A:99:ILE:O     | 2.09                     | 0.52              |
| 1:C:280:ARG:O    | 1:C:282:LEU:HG   | 2.10                     | 0.52              |
| 1:C:369:TYR:HE1  | 1:C:379:THR:HG22 | 1.75                     | 0.52              |
| 1:C:376:TYR:C    | 1:C:378:THR:H    | 2.14                     | 0.52              |
| 1:C:89:LEU:HB2   | 1:C:92:SER:OG    | 2.10                     | 0.52              |
| 1:A:102:ASP:OD2  | 1:A:105:ALA:HB2  | 2.10                     | 0.52              |
| 1:A:182:PRO:O    | 1:A:185:THR:OG1  | 2.27                     | 0.52              |
| 1:C:291:MET:HG2  | 1:C:291:MET:O    | 2.10                     | 0.52              |
| 1:A:254:LEU:C    | 1:A:256:LYS:N    | 2.63                     | 0.51              |
| 1:A:299:CYS:HB2  | 1:A:360:CYS:HA   | 1.92                     | 0.51              |
| 1:A:308:LEU:HD22 | 1:A:315:ARG:HA   | 1.91                     | 0.51              |
| 1:A:174:LEU:HD12 | 1:A:178:LEU:HD13 | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:241:GLN:O    | 1:A:245:GLN:HG2  | 2.10                     | 0.51              |
| 1:B:311:VAL:HB   | 1:B:318:LEU:HD11 | 1.93                     | 0.51              |
| 1:B:66:ASP:OD2   | 1:B:69:ILE:HD13  | 2.09                     | 0.51              |
| 1:C:198:ILE:HG21 | 1:C:215:VAL:HG13 | 1.93                     | 0.51              |
| 1:A:174:LEU:HD12 | 1:A:178:LEU:CD1  | 2.39                     | 0.51              |
| 1:A:347:ILE:HG23 | 1:A:387:ASN:O    | 2.10                     | 0.51              |
| 1:A:240:ARG:CG   | 1:C:350:THR:HG21 | 2.40                     | 0.51              |
| 1:C:256:LYS:HE3  | 1:C:256:LYS:H    | 1.74                     | 0.51              |
| 1:C:296:ASN:HB3  | 1:C:297:HIS:CE1  | 2.46                     | 0.51              |
| 1:A:210:PRO:CD   | 1:A:295:ARG:HH12 | 2.14                     | 0.51              |
| 1:B:135:TRP:H    | 1:B:135:TRP:HD1  | 1.59                     | 0.51              |
| 1:C:298:ALA:HA   | 1:C:302:ILE:CD1  | 2.27                     | 0.51              |
| 1:C:86:SER:HB3   | 1:C:102:ASP:HA   | 1.91                     | 0.51              |
| 1:A:157:TYR:CZ   | 1:A:174:LEU:HA   | 2.46                     | 0.51              |
| 1:A:347:ILE:HG23 | 1:A:388:SER:HA   | 1.93                     | 0.51              |
| 1:B:126:GLY:O    | 1:B:127:LEU:HD12 | 2.10                     | 0.51              |
| 1:B:119:VAL:HG23 | 1:B:279:TYR:CD2  | 2.46                     | 0.51              |
| 1:B:384:ARG:O    | 1:B:388:SER:HB2  | 2.11                     | 0.51              |
| 1:B:67:LYS:HE2   | 1:B:134:ARG:HH12 | 1.76                     | 0.51              |
| 1:A:13:ASN:O     | 1:A:19:ASP:CB    | 2.59                     | 0.50              |
| 1:A:311:VAL:HG21 | 1:A:318:LEU:HD21 | 1.93                     | 0.50              |
| 1:B:294:ILE:HG22 | 1:B:298:ALA:CB   | 2.39                     | 0.50              |
| 1:B:6:HIS:CD2    | 1:B:254:LEU:HD13 | 2.47                     | 0.50              |
| 1:C:199:LEU:HD22 | 1:C:230:VAL:HG21 | 1.92                     | 0.50              |
| 1:A:193:ALA:O    | 1:A:196:ARG:HB2  | 2.11                     | 0.50              |
| 1:A:110:ALA:HB2  | 1:A:235:VAL:CG2  | 2.41                     | 0.50              |
| 1:B:191:THR:HG22 | 1:B:193:ALA:N    | 2.22                     | 0.50              |
| 1:B:351:LEU:H    | 1:B:384:ARG:HH22 | 1.59                     | 0.50              |
| 1:C:345:LEU:HD13 | 1:C:356:ILE:HD12 | 1.93                     | 0.50              |
| 1:C:378:THR:OG1  | 1:C:383:TYR:HD1  | 1.93                     | 0.50              |
| 1:B:124:PHE:CE2  | 1:B:190:VAL:HG13 | 2.45                     | 0.50              |
| 1:B:183:PRO:O    | 1:B:184:GLN:HG2  | 2.11                     | 0.50              |
| 1:C:86:SER:C     | 1:C:87:TYR:CD1   | 2.84                     | 0.50              |
| 1:C:84:GLY:HA3   | 1:C:98:TYR:OH    | 2.12                     | 0.50              |
| 1:A:282:LEU:HD23 | 1:A:326:VAL:CG2  | 2.40                     | 0.50              |
| 1:A:290:ALA:O    | 1:A:294:ILE:HG13 | 2.12                     | 0.50              |
| 1:B:101:THR:HA   | 1:B:242:MET:HE2  | 1.93                     | 0.50              |
| 1:C:347:ILE:HD12 | 1:C:347:ILE:H    | 1.77                     | 0.50              |
| 1:C:357:SER:O    | 1:C:362:TYR:N    | 2.44                     | 0.50              |
| 1:A:174:LEU:C    | 1:A:174:LEU:HD12 | 2.32                     | 0.50              |
| 1:B:133:LYS:HG3  | 1:B:135:TRP:HE1  | 1.76                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:358:GLN:O    | 1:B:361:GLY:N    | 2.44                     | 0.50              |
| 1:B:10:LEU:CD2   | 1:B:61:ILE:HB    | 2.39                     | 0.50              |
| 1:C:97:HIS:HB3   | 1:C:262:GLN:HB2  | 1.94                     | 0.50              |
| 1:C:298:ALA:H    | 1:C:341:LYS:NZ   | 2.08                     | 0.50              |
| 1:B:347:ILE:HA   | 1:B:388:SER:HA   | 1.93                     | 0.50              |
| 1:C:133:LYS:HD2  | 1:C:133:LYS:H    | 1.77                     | 0.50              |
| 1:A:304:VAL:O    | 1:A:308:LEU:HG   | 2.12                     | 0.50              |
| 1:A:313:ILE:CG2  | 1:A:317:ASN:HD22 | 2.18                     | 0.50              |
| 1:C:192:ASP:OD1  | 1:C:217:GLY:HA3  | 2.11                     | 0.50              |
| 1:A:104:TYR:CD1  | 1:A:142:ALA:HA   | 2.47                     | 0.50              |
| 1:B:112:LEU:O    | 1:B:116:GLU:HB2  | 2.12                     | 0.50              |
| 1:C:4:LYS:C      | 1:C:4:LYS:HD3    | 2.32                     | 0.50              |
| 1:A:346:LEU:CD2  | 1:A:384:ARG:HH11 | 2.14                     | 0.49              |
| 1:B:162:THR:CG2  | 1:B:163:ALA:H    | 2.25                     | 0.49              |
| 1:B:99:ILE:HG21  | 1:B:242:MET:O    | 2.11                     | 0.49              |
| 1:C:358:GLN:HE22 | 1:C:359:MET:CE   | 2.24                     | 0.49              |
| 1:C:70:GLU:OE2   | 1:C:94:PRO:CB    | 2.60                     | 0.49              |
| 1:A:229:ARG:NH2  | 1:A:296:ASN:OD1  | 2.45                     | 0.49              |
| 1:B:86:SER:HB3   | 1:B:102:ASP:HA   | 1.93                     | 0.49              |
| 1:B:313:ILE:HG21 | 1:B:317:ASN:HB2  | 1.94                     | 0.49              |
| 1:B:86:SER:CB    | 1:B:265:LEU:HD22 | 2.42                     | 0.49              |
| 1:C:98:TYR:CE2   | 1:C:100:ALA:HB2  | 2.47                     | 0.49              |
| 1:C:189:ALA:O    | 1:C:191:THR:N    | 2.45                     | 0.49              |
| 1:C:74:ALA:O     | 1:C:75:ASP:HB3   | 2.12                     | 0.49              |
| 1:A:143:PHE:O    | 1:A:146:LEU:HG   | 2.12                     | 0.49              |
| 1:C:330:ILE:O    | 1:C:334:ILE:HG12 | 2.13                     | 0.49              |
| 1:C:347:ILE:HD12 | 1:C:347:ILE:N    | 2.28                     | 0.49              |
| 1:C:39:ILE:CD1   | 1:C:39:ILE:H     | 2.23                     | 0.49              |
| 1:A:104:TYR:HD1  | 1:A:142:ALA:HA   | 1.77                     | 0.49              |
| 1:A:185:THR:HG22 | 1:A:186:GLY:H    | 1.78                     | 0.49              |
| 1:A:218:ILE:N    | 1:A:218:ILE:HD12 | 2.28                     | 0.49              |
| 1:A:225:ARG:HG3  | 1:A:225:ARG:HH11 | 1.77                     | 0.49              |
| 1:A:275:ARG:O    | 1:A:277:THR:N    | 2.45                     | 0.49              |
| 1:B:155:VAL:HG12 | 1:B:156:VAL:N    | 2.28                     | 0.49              |
| 1:B:158:GLN:O    | 1:B:159:GLY:O    | 2.31                     | 0.49              |
| 1:A:261:LEU:HD22 | 1:A:263:ARG:NH2  | 2.28                     | 0.49              |
| 1:B:308:LEU:HA   | 1:B:318:LEU:HD13 | 1.94                     | 0.49              |
| 1:A:184:GLN:HG2  | 1:A:279:TYR:OH   | 2.13                     | 0.49              |
| 1:B:183:PRO:O    | 1:B:184:GLN:CG   | 2.61                     | 0.49              |
| 1:B:342:ALA:O    | 1:B:346:LEU:HG   | 2.13                     | 0.49              |
| 1:A:292:HIS:O    | 1:A:295:ARG:HB2  | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:7:ARG:CZ     | 1:A:7:ARG:CB     | 2.91                     | 0.49              |
| 1:B:347:ILE:HD11 | 1:B:383:TYR:CE2  | 2.48                     | 0.49              |
| 1:C:114:LEU:HB2  | 1:C:122:PHE:CE2  | 2.47                     | 0.49              |
| 1:C:294:ILE:HA   | 1:C:298:ALA:HB2  | 1.95                     | 0.49              |
| 1:C:6:HIS:HB2    | 1:C:8:ILE:HD11   | 1.95                     | 0.49              |
| 1:A:102:ASP:O    | 1:A:103:ASN:C    | 2.51                     | 0.49              |
| 1:A:4:LYS:N      | 1:A:36:GLU:HG3   | 2.28                     | 0.49              |
| 1:B:264:ILE:HD12 | 1:B:265:LEU:H    | 1.77                     | 0.49              |
| 1:C:122:PHE:O    | 1:C:154:GLY:CA   | 2.61                     | 0.49              |
| 1:C:147:VAL:HG13 | 1:C:148:ALA:N    | 2.28                     | 0.49              |
| 1:C:169:HIS:O    | 1:C:172:ASN:HB2  | 2.11                     | 0.49              |
| 1:C:188:ILE:HA   | 1:C:216:ILE:CG2  | 2.42                     | 0.49              |
| 1:A:207:ILE:HG22 | 1:A:207:ILE:O    | 2.13                     | 0.49              |
| 1:A:260:PRO:O    | 1:A:261:LEU:C    | 2.49                     | 0.49              |
| 1:A:274:ARG:NH1  | 1:A:274:ARG:CG   | 2.71                     | 0.49              |
| 1:A:280:ARG:CG   | 1:A:282:LEU:HD12 | 2.16                     | 0.49              |
| 1:B:85:GLY:C     | 1:B:100:ALA:HB1  | 2.33                     | 0.49              |
| 1:B:368:PHE:C    | 1:B:368:PHE:CD2  | 2.86                     | 0.49              |
| 1:C:225:ARG:NE   | 1:C:274:ARG:HH22 | 2.04                     | 0.49              |
| 1:C:345:LEU:HB3  | 1:C:356:ILE:HD12 | 1.94                     | 0.49              |
| 1:A:12:PHE:CD2   | 1:A:23:VAL:HG23  | 2.48                     | 0.48              |
| 1:A:45:PHE:C     | 1:A:46:ARG:HG3   | 2.33                     | 0.48              |
| 1:B:193:ALA:O    | 1:B:196:ARG:HB2  | 2.13                     | 0.48              |
| 1:C:121:ARG:HD2  | 1:C:182:PRO:HG2  | 1.95                     | 0.48              |
| 1:C:308:LEU:HD13 | 1:C:315:ARG:HA   | 1.95                     | 0.48              |
| 1:C:4:LYS:HA     | 1:C:4:LYS:HZ3    | 1.76                     | 0.48              |
| 1:C:60:VAL:HB    | 1:C:80:ILE:CD1   | 2.36                     | 0.48              |
| 1:A:216:ILE:CD1  | 1:A:234:SER:HA   | 2.43                     | 0.48              |
| 1:C:152:TYR:HD1  | 1:C:152:TYR:N    | 2.10                     | 0.48              |
| 1:C:252:ARG:NH2  | 1:C:259:MET:HE1  | 2.27                     | 0.48              |
| 1:C:299:CYS:H    | 1:C:341:LYS:NZ   | 2.11                     | 0.48              |
| 1:A:157:TYR:CE2  | 1:A:174:LEU:HA   | 2.48                     | 0.48              |
| 1:B:121:ARG:NH1  | 1:B:184:GLN:HG3  | 2.28                     | 0.48              |
| 1:C:26:VAL:C     | 1:C:28:GLU:N     | 2.67                     | 0.48              |
| 1:A:218:ILE:HG22 | 1:A:219:ASP:N    | 2.27                     | 0.48              |
| 1:B:294:ILE:O    | 1:B:298:ALA:HB2  | 2.13                     | 0.48              |
| 1:C:11:LEU:HB3   | 1:C:43:GLU:CD    | 2.32                     | 0.48              |
| 1:B:160:LEU:HD12 | 1:B:170:ALA:HA   | 1.95                     | 0.48              |
| 1:C:135:TRP:CZ3  | 1:C:136:ALA:HB2  | 2.49                     | 0.48              |
| 1:A:242:MET:HG3  | 1:A:266:VAL:HG21 | 1.95                     | 0.48              |
| 1:A:379:THR:HB   | 1:A:380:PRO:HD2  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:226:TYR:HD2  | 1:B:348:SER:HG   | 1.58                     | 0.48              |
| 1:B:277:THR:C    | 1:B:279:TYR:H    | 2.17                     | 0.48              |
| 1:C:106:LEU:HD13 | 1:C:218:ILE:HG21 | 1.95                     | 0.48              |
| 1:A:204:HIS:C    | 1:A:206:HIS:H    | 2.17                     | 0.48              |
| 1:A:79:PRO:HG2   | 1:A:254:LEU:HD23 | 1.96                     | 0.48              |
| 1:B:118:GLY:O    | 1:B:119:VAL:C    | 2.52                     | 0.48              |
| 1:B:220:ASN:ND2  | 1:B:272:ILE:HG13 | 2.29                     | 0.48              |
| 1:B:323:LYS:HD3  | 1:B:323:LYS:H    | 1.72                     | 0.48              |
| 1:B:282:LEU:HD21 | 1:B:326:VAL:HG22 | 1.94                     | 0.48              |
| 1:C:343:ARG:O    | 1:C:343:ARG:HG2  | 2.14                     | 0.48              |
| 1:A:127:LEU:HD11 | 1:A:194:ARG:NE   | 2.29                     | 0.48              |
| 1:A:227:LEU:HD23 | 1:A:227:LEU:N    | 2.28                     | 0.48              |
| 1:A:303:LYS:CG   | 1:A:306:GLN:HE21 | 2.27                     | 0.48              |
| 1:A:70:GLU:O     | 1:A:70:GLU:HG2   | 2.14                     | 0.48              |
| 1:C:250:LEU:O    | 1:C:254:LEU:HG   | 2.13                     | 0.48              |
| 1:C:94:PRO:O     | 1:C:263:ARG:NH2  | 2.31                     | 0.48              |
| 1:A:284:ASP:O    | 1:A:288:ILE:HG13 | 2.14                     | 0.48              |
| 1:B:138:GLU:O    | 1:B:141:TYR:N    | 2.46                     | 0.48              |
| 1:B:177:TRP:CZ2  | 1:B:181:LEU:HD11 | 2.49                     | 0.48              |
| 1:B:223:LEU:H    | 1:B:223:LEU:CD2  | 2.27                     | 0.48              |
| 1:B:284:ASP:OD1  | 1:B:286:ALA:N    | 2.37                     | 0.48              |
| 1:C:161:GLU:O    | 1:C:164:PRO:HD3  | 2.13                     | 0.48              |
| 1:B:175:ALA:HB1  | 1:B:205:LEU:HD21 | 1.95                     | 0.48              |
| 1:B:343:ARG:NH1  | 1:B:383:TYR:CE2  | 2.74                     | 0.48              |
| 1:A:299:CYS:HB3  | 1:A:341:LYS:HD3  | 1.95                     | 0.47              |
| 1:A:7:ARG:NH1    | 1:A:7:ARG:HB2    | 2.28                     | 0.47              |
| 1:C:214:CYS:SG   | 1:C:279:TYR:HB2  | 2.54                     | 0.47              |
| 1:C:286:ALA:C    | 1:C:311:VAL:HG11 | 2.35                     | 0.47              |
| 1:A:302:ILE:HG13 | 1:A:334:ILE:HG13 | 1.97                     | 0.47              |
| 1:A:56:LEU:HG    | 1:A:57:GLY:N     | 2.29                     | 0.47              |
| 1:B:162:THR:CG2  | 1:B:163:ALA:N    | 2.75                     | 0.47              |
| 1:B:9:THR:HA     | 1:B:40:PHE:O     | 2.14                     | 0.47              |
| 1:C:252:ARG:NH2  | 1:C:259:MET:HE2  | 2.28                     | 0.47              |
| 1:A:261:LEU:HD22 | 1:A:263:ARG:HH21 | 1.80                     | 0.47              |
| 1:A:261:LEU:HB3  | 1:A:263:ARG:HE   | 1.78                     | 0.47              |
| 1:C:17:ALA:HB2   | 1:C:221:GLU:CD   | 2.35                     | 0.47              |
| 1:A:17:ALA:O     | 1:A:21:GLN:HG3   | 2.13                     | 0.47              |
| 1:A:294:ILE:O    | 1:A:298:ALA:HB2  | 2.15                     | 0.47              |
| 1:A:370:SER:O    | 1:A:373:LYS:HD3  | 2.14                     | 0.47              |
| 1:B:321:ARG:O    | 1:B:324:GLU:HB3  | 2.14                     | 0.47              |
| 1:B:352:SER:OG   | 1:B:355:GLU:HB3  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:133:LYS:HB3  | 1:C:135:TRP:CZ2  | 2.50                     | 0.47              |
| 1:C:199:LEU:HG   | 1:C:215:VAL:HG21 | 1.95                     | 0.47              |
| 1:A:253:LEU:O    | 1:A:253:LEU:CD2  | 2.63                     | 0.47              |
| 1:A:331:HIS:HA   | 1:A:334:ILE:HG22 | 1.96                     | 0.47              |
| 1:C:308:LEU:HD13 | 1:C:315:ARG:CA   | 2.44                     | 0.47              |
| 1:B:178:LEU:C    | 1:B:180:THR:H    | 2.18                     | 0.47              |
| 1:B:251:HIS:O    | 1:B:254:LEU:N    | 2.47                     | 0.47              |
| 1:B:292:HIS:O    | 1:B:293:TYR:C    | 2.53                     | 0.47              |
| 1:C:168:GLN:O    | 1:C:171:GLN:HB3  | 2.15                     | 0.47              |
| 1:C:253:LEU:C    | 1:C:255:ASP:H    | 2.18                     | 0.47              |
| 1:C:299:CYS:HB3  | 1:C:341:LYS:CB   | 2.44                     | 0.47              |
| 1:C:351:LEU:CD2  | 1:C:352:SER:H    | 2.28                     | 0.47              |
| 1:A:161:GLU:O    | 1:A:164:PRO:HD3  | 2.15                     | 0.47              |
| 1:A:326:VAL:O    | 1:A:326:VAL:CG1  | 2.62                     | 0.47              |
| 1:B:134:ARG:HH11 | 1:B:134:ARG:HG3  | 1.80                     | 0.47              |
| 1:B:355:GLU:OE1  | 1:B:359:MET:HB2  | 2.14                     | 0.47              |
| 1:B:242:MET:HE2  | 1:B:266:VAL:HB   | 1.96                     | 0.47              |
| 1:B:343:ARG:HB3  | 1:B:343:ARG:NH1  | 2.30                     | 0.47              |
| 1:A:5:ARG:NH2    | 1:C:203:GLU:HB3  | 2.30                     | 0.47              |
| 1:C:192:ASP:OD1  | 1:C:232:LEU:HD11 | 2.15                     | 0.47              |
| 1:A:174:LEU:O    | 1:A:177:TRP:HB3  | 2.15                     | 0.47              |
| 1:A:179:GLN:HE22 | 1:A:205:LEU:HD23 | 1.80                     | 0.47              |
| 1:A:286:ALA:CA   | 1:A:311:VAL:HG11 | 2.44                     | 0.47              |
| 1:C:29:TYR:HD1   | 1:C:244:TYR:CE2  | 2.33                     | 0.47              |
| 1:C:233:SER:N    | 1:C:276:SER:OG   | 2.47                     | 0.47              |
| 1:A:313:ILE:HG23 | 1:A:317:ASN:ND2  | 2.23                     | 0.47              |
| 1:C:103:ASN:O    | 1:C:106:LEU:HB2  | 2.15                     | 0.47              |
| 1:C:174:LEU:CD1  | 1:C:178:LEU:HD12 | 2.44                     | 0.47              |
| 1:C:10:LEU:HD21  | 1:C:61:ILE:HD12  | 1.97                     | 0.47              |
| 1:A:60:VAL:HG12  | 1:A:61:ILE:N     | 2.26                     | 0.47              |
| 1:B:343:ARG:NH1  | 1:B:383:TYR:HE2  | 2.09                     | 0.47              |
| 1:B:9:THR:OG1    | 1:B:60:VAL:HG13  | 2.15                     | 0.47              |
| 1:C:124:PHE:CZ   | 1:C:190:VAL:HG12 | 2.49                     | 0.47              |
| 1:A:12:PHE:HZ    | 1:A:83:VAL:HG21  | 1.80                     | 0.46              |
| 1:A:223:LEU:CD1  | 1:C:24:GLU:HG3   | 2.27                     | 0.46              |
| 1:A:235:VAL:HG12 | 1:A:236:ALA:N    | 2.30                     | 0.46              |
| 1:B:329:THR:C    | 1:B:331:HIS:H    | 2.18                     | 0.46              |
| 1:B:3:THR:HG23   | 1:B:3:THR:O      | 2.15                     | 0.46              |
| 1:C:127:LEU:HB3  | 1:C:131:SER:OG   | 2.16                     | 0.46              |
| 1:C:141:TYR:HE1  | 1:C:145:GLN:NE2  | 2.13                     | 0.46              |
| 1:C:20:ARG:HB3   | 1:C:20:ARG:NH1   | 2.31                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:299:CYS:HA   | 1:C:338:LYS:HG2  | 1.96                     | 0.46              |
| 1:A:190:VAL:HG23 | 1:A:191:THR:HG23 | 1.97                     | 0.46              |
| 1:B:223:LEU:HD23 | 1:B:223:LEU:N    | 2.29                     | 0.46              |
| 1:C:11:LEU:O     | 1:C:12:PHE:CD1   | 2.68                     | 0.46              |
| 1:C:283:THR:O    | 1:C:285:PRO:CD   | 2.56                     | 0.46              |
| 1:C:291:MET:HA   | 1:C:294:ILE:HD12 | 1.97                     | 0.46              |
| 1:A:159:GLY:HA3  | 1:A:194:ARG:NH2  | 2.29                     | 0.46              |
| 1:A:313:ILE:CB   | 1:A:318:LEU:HD23 | 2.42                     | 0.46              |
| 1:B:332:ALA:O    | 1:B:336:ALA:HB3  | 2.15                     | 0.46              |
| 1:C:102:ASP:HB2  | 1:C:265:LEU:HB3  | 1.96                     | 0.46              |
| 1:C:86:SER:N     | 1:C:103:ASN:ND2  | 2.63                     | 0.46              |
| 1:A:209:VAL:HG13 | 1:A:213:LEU:O    | 2.16                     | 0.46              |
| 1:A:98:TYR:CE2   | 1:A:100:ALA:HB2  | 2.50                     | 0.46              |
| 1:B:378:THR:HB   | 1:B:379:THR:H    | 1.45                     | 0.46              |
| 1:C:221:GLU:O    | 1:C:225:ARG:HG2  | 2.15                     | 0.46              |
| 1:C:298:ALA:HB3  | 1:C:341:LYS:HZ2  | 1.80                     | 0.46              |
| 1:B:274:ARG:HG3  | 1:B:274:ARG:HH11 | 1.81                     | 0.46              |
| 1:C:150:GLU:CG   | 1:C:151:LYS:N    | 2.78                     | 0.46              |
| 1:C:209:VAL:HA   | 1:C:210:PRO:HA   | 1.75                     | 0.46              |
| 1:C:311:VAL:HG21 | 1:C:318:LEU:HD11 | 1.97                     | 0.46              |
| 1:A:192:ASP:O    | 1:A:196:ARG:HG2  | 2.15                     | 0.46              |
| 1:A:341:LYS:O    | 1:A:345:LEU:HG   | 2.16                     | 0.46              |
| 1:B:168:GLN:NE2  | 1:B:172:ASN:OD1  | 2.44                     | 0.46              |
| 1:B:26:VAL:O     | 1:B:29:TYR:N     | 2.49                     | 0.46              |
| 1:B:61:ILE:HD13  | 1:B:81:VAL:O     | 2.15                     | 0.46              |
| 1:C:21:GLN:HB3   | 1:C:239:ALA:CB   | 2.44                     | 0.46              |
| 1:C:333:MET:O    | 1:C:337:GLU:HB2  | 2.16                     | 0.46              |
| 1:A:240:ARG:HD3  | 1:C:350:THR:HB   | 1.97                     | 0.46              |
| 1:A:357:SER:O    | 1:A:362:TYR:HB2  | 2.16                     | 0.46              |
| 1:B:121:ARG:NH1  | 1:B:121:ARG:HG3  | 2.31                     | 0.46              |
| 1:B:13:ASN:C     | 1:B:15:ASN:H     | 2.19                     | 0.46              |
| 1:B:201:VAL:HG13 | 1:B:205:LEU:HD13 | 1.96                     | 0.46              |
| 1:B:300:LYS:O    | 1:B:301:GLY:O    | 2.33                     | 0.46              |
| 1:C:318:LEU:C    | 1:C:318:LEU:HD23 | 2.35                     | 0.46              |
| 1:A:7:ARG:NH1    | 1:A:7:ARG:CB     | 2.79                     | 0.46              |
| 1:C:125:TYR:OH   | 1:C:194:ARG:NH1  | 2.49                     | 0.46              |
| 1:C:128:PRO:HA   | 1:C:158:GLN:HB3  | 1.96                     | 0.46              |
| 1:C:39:ILE:N     | 1:C:39:ILE:HD12  | 2.30                     | 0.46              |
| 1:C:9:THR:OG1    | 1:C:60:VAL:HG22  | 2.15                     | 0.46              |
| 1:B:303:LYS:H    | 1:B:306:GLN:CB   | 2.25                     | 0.46              |
| 1:A:34:GLN:NE2   | 1:C:229:ARG:CD   | 2.75                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:96:VAL:HG22  | 1:C:97:HIS:N     | 2.30                     | 0.46              |
| 1:A:114:LEU:HD13 | 1:A:186:GLY:HA3  | 1.97                     | 0.45              |
| 1:A:244:TYR:C    | 1:A:244:TYR:CD1  | 2.89                     | 0.45              |
| 1:A:330:ILE:CG2  | 1:A:331:HIS:N    | 2.79                     | 0.45              |
| 1:C:13:ASN:HB3   | 1:C:15:ASN:OD1   | 2.16                     | 0.45              |
| 1:A:216:ILE:HD12 | 1:A:233:SER:C    | 2.36                     | 0.45              |
| 1:A:239:ALA:HA   | 1:A:242:MET:HE3  | 1.97                     | 0.45              |
| 1:A:45:PHE:O     | 1:A:46:ARG:HG3   | 2.16                     | 0.45              |
| 1:B:189:ALA:HB1  | 1:B:194:ARG:HB2  | 1.97                     | 0.45              |
| 1:C:376:TYR:C    | 1:C:378:THR:N    | 2.69                     | 0.45              |
| 1:B:165:GLU:N    | 1:B:165:GLU:OE1  | 2.46                     | 0.45              |
| 1:B:178:LEU:HA   | 1:B:181:LEU:HD12 | 1.98                     | 0.45              |
| 1:C:114:LEU:C    | 1:C:116:GLU:H    | 2.20                     | 0.45              |
| 1:C:208:PRO:HB2  | 1:C:212:LYS:HB2  | 1.97                     | 0.45              |
| 1:A:34:GLN:CG    | 1:C:300:LYS:HZ2  | 2.29                     | 0.45              |
| 1:A:65:ASP:OD2   | 1:A:84:GLY:HA2   | 2.16                     | 0.45              |
| 1:B:127:LEU:HD13 | 1:B:190:VAL:HG21 | 1.97                     | 0.45              |
| 1:B:56:LEU:HD23  | 1:B:78:VAL:HG21  | 1.98                     | 0.45              |
| 1:C:12:PHE:HB3   | 1:C:19:ASP:HB3   | 1.98                     | 0.45              |
| 1:C:161:GLU:HB3  | 1:C:164:PRO:CA   | 2.46                     | 0.45              |
| 1:C:184:GLN:HE21 | 1:C:279:TYR:HE1  | 1.58                     | 0.45              |
| 1:A:297:HIS:O    | 1:A:300:LYS:HB2  | 2.17                     | 0.45              |
| 1:A:64:PHE:CE2   | 1:A:70:GLU:HA    | 2.51                     | 0.45              |
| 1:A:6:HIS:CE1    | 1:A:254:LEU:HD13 | 2.51                     | 0.45              |
| 1:A:70:GLU:CD    | 1:A:94:PRO:HB3   | 2.37                     | 0.45              |
| 1:C:263:ARG:HG2  | 1:C:263:ARG:NH1  | 2.30                     | 0.45              |
| 1:A:128:PRO:C    | 1:A:130:SER:N    | 2.70                     | 0.45              |
| 1:A:207:ILE:HG23 | 1:A:212:LYS:CD   | 2.31                     | 0.45              |
| 1:B:345:LEU:CB   | 1:B:356:ILE:HD12 | 2.44                     | 0.45              |
| 1:B:60:VAL:HG23  | 1:B:80:ILE:HG12  | 1.98                     | 0.45              |
| 1:B:64:PHE:CE2   | 1:B:96:VAL:HG11  | 2.51                     | 0.45              |
| 1:C:18:TYR:O     | 1:C:19:ASP:C     | 2.53                     | 0.45              |
| 1:C:97:HIS:HD2   | 1:C:262:GLN:HG2  | 1.82                     | 0.45              |
| 1:B:184:GLN:O    | 1:B:184:GLN:HG3  | 2.17                     | 0.45              |
| 1:C:344:SER:C    | 1:C:346:LEU:H    | 2.19                     | 0.45              |
| 1:A:190:VAL:CG2  | 1:A:191:THR:N    | 2.78                     | 0.45              |
| 1:A:251:HIS:HA   | 1:A:254:LEU:HD12 | 1.98                     | 0.45              |
| 1:A:282:LEU:HD23 | 1:A:326:VAL:HG23 | 1.97                     | 0.45              |
| 1:A:345:LEU:HB3  | 1:A:356:ILE:HD12 | 1.98                     | 0.45              |
| 1:A:352:SER:O    | 1:A:356:ILE:HG12 | 2.17                     | 0.45              |
| 1:A:386:VAL:CG1  | 1:A:387:ASN:OD1  | 2.60                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:107:VAL:CG2  | 1:C:139:ARG:HG2  | 2.41                     | 0.45              |
| 1:C:216:ILE:HG13 | 1:C:233:SER:O    | 2.16                     | 0.45              |
| 1:C:258:GLU:OE1  | 1:C:258:GLU:HA   | 2.17                     | 0.45              |
| 1:A:184:GLN:N    | 1:A:212:LYS:O    | 2.44                     | 0.45              |
| 1:B:284:ASP:HA   | 1:B:285:PRO:HD3  | 1.81                     | 0.45              |
| 1:A:121:ARG:NH1  | 1:A:121:ARG:HG3  | 2.30                     | 0.45              |
| 1:A:178:LEU:HD22 | 1:A:201:VAL:CG1  | 2.47                     | 0.45              |
| 1:A:383:TYR:O    | 1:A:386:VAL:HB   | 2.17                     | 0.45              |
| 1:B:12:PHE:CE1   | 1:B:62:ALA:C     | 2.91                     | 0.45              |
| 1:B:305:ASP:C    | 1:B:307:VAL:N    | 2.69                     | 0.45              |
| 1:C:64:PHE:CB    | 1:C:98:TYR:HE1   | 2.28                     | 0.45              |
| 1:C:79:PRO:HB3   | 1:C:253:LEU:CD1  | 2.46                     | 0.45              |
| 1:A:232:LEU:C    | 1:A:232:LEU:HD23 | 2.37                     | 0.44              |
| 1:A:347:ILE:HD11 | 1:A:383:TYR:OH   | 2.17                     | 0.44              |
| 1:A:4:LYS:CA     | 1:A:4:LYS:HZ2    | 2.30                     | 0.44              |
| 1:B:165:GLU:CD   | 1:B:165:GLU:H    | 2.21                     | 0.44              |
| 1:A:41:ILE:CG2   | 1:A:41:ILE:O     | 2.61                     | 0.44              |
| 1:A:43:GLU:HG2   | 1:A:46:ARG:HG3   | 1.98                     | 0.44              |
| 1:B:127:LEU:HB3  | 1:B:131:SER:OG   | 2.17                     | 0.44              |
| 1:B:160:LEU:CD1  | 1:B:170:ALA:HA   | 2.47                     | 0.44              |
| 1:C:275:ARG:O    | 1:C:277:THR:N    | 2.50                     | 0.44              |
| 1:C:279:TYR:OH   | 1:C:281:SER:HA   | 2.18                     | 0.44              |
| 1:A:185:THR:CG2  | 1:A:186:GLY:N    | 2.78                     | 0.44              |
| 1:B:135:TRP:HB2  | 1:B:139:ARG:HE   | 1.82                     | 0.44              |
| 1:B:291:MET:HE3  | 1:B:295:ARG:NH2  | 2.32                     | 0.44              |
| 1:B:311:VAL:HG11 | 1:B:318:LEU:HG   | 1.98                     | 0.44              |
| 1:C:115:LYS:O    | 1:C:115:LYS:HG3  | 2.18                     | 0.44              |
| 1:C:181:LEU:HA   | 1:C:182:PRO:HD3  | 1.83                     | 0.44              |
| 1:C:369:TYR:HE1  | 1:C:379:THR:CG2  | 2.30                     | 0.44              |
| 1:C:43:GLU:O     | 1:C:45:PHE:N     | 2.50                     | 0.44              |
| 1:A:157:TYR:OH   | 1:A:174:LEU:HA   | 2.17                     | 0.44              |
| 1:A:286:ALA:C    | 1:A:311:VAL:HG11 | 2.38                     | 0.44              |
| 1:B:4:LYS:HE2    | 1:B:4:LYS:HA     | 2.00                     | 0.44              |
| 1:B:67:LYS:HG3   | 1:B:134:ARG:NH2  | 2.32                     | 0.44              |
| 1:A:152:TYR:O    | 1:A:153:ARG:O    | 2.35                     | 0.44              |
| 1:A:287:VAL:HG22 | 1:A:322:PHE:HA   | 1.99                     | 0.44              |
| 1:A:303:LYS:HG2  | 1:A:306:GLN:HE21 | 1.81                     | 0.44              |
| 1:B:354:ASN:HA   | 1:B:365:LEU:CD1  | 2.34                     | 0.44              |
| 1:C:235:VAL:HA   | 1:C:271:VAL:CG1  | 2.42                     | 0.44              |
| 1:C:305:ASP:C    | 1:C:307:VAL:H    | 2.20                     | 0.44              |
| 1:C:386:VAL:O    | 1:C:386:VAL:HG12 | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:175:ALA:O    | 1:A:178:LEU:N    | 2.50                     | 0.44              |
| 1:A:236:ALA:HB2  | 1:A:272:ILE:HD11 | 1.99                     | 0.44              |
| 1:A:211:GLU:OE1  | 1:A:295:ARG:NH1  | 2.51                     | 0.44              |
| 1:B:25:GLY:HA2   | 1:B:240:ARG:HG3  | 1.99                     | 0.44              |
| 1:A:61:ILE:CD1   | 1:A:250:LEU:HD22 | 2.47                     | 0.44              |
| 1:A:278:ASP:OD1  | 1:A:280:ARG:NH2  | 2.50                     | 0.44              |
| 1:A:34:GLN:HE21  | 1:A:34:GLN:HB3   | 1.54                     | 0.44              |
| 1:B:134:ARG:HG3  | 1:B:134:ARG:NH1  | 2.33                     | 0.44              |
| 1:B:242:MET:CE   | 1:B:266:VAL:HB   | 2.47                     | 0.44              |
| 1:B:327:GLY:O    | 1:B:328:GLU:CD   | 2.56                     | 0.44              |
| 1:C:20:ARG:CB    | 1:C:20:ARG:NH1   | 2.80                     | 0.44              |
| 1:C:291:MET:HA   | 1:C:294:ILE:HB   | 1.98                     | 0.44              |
| 1:C:64:PHE:CE2   | 1:C:70:GLU:HG2   | 2.53                     | 0.44              |
| 1:A:160:LEU:HD13 | 1:A:164:PRO:CG   | 2.42                     | 0.44              |
| 1:A:328:GLU:C    | 1:A:332:ALA:HB3  | 2.38                     | 0.44              |
| 1:A:8:ILE:O      | 1:A:39:ILE:HA    | 2.17                     | 0.44              |
| 1:B:133:LYS:HB3  | 1:B:135:TRP:NE1  | 2.33                     | 0.44              |
| 1:B:142:ALA:O    | 1:B:143:PHE:C    | 2.54                     | 0.44              |
| 1:B:191:THR:HB   | 1:B:194:ARG:HG2  | 2.00                     | 0.44              |
| 1:C:107:VAL:HG22 | 1:C:139:ARG:CG   | 2.42                     | 0.44              |
| 1:C:127:LEU:HD13 | 1:C:194:ARG:NE   | 2.33                     | 0.44              |
| 1:C:192:ASP:HB2  | 1:C:219:ASP:HB3  | 1.94                     | 0.44              |
| 1:C:208:PRO:HG3  | 1:C:289:GLN:OE1  | 2.18                     | 0.44              |
| 1:A:220:ASN:O    | 1:A:221:GLU:C    | 2.56                     | 0.44              |
| 1:A:308:LEU:HB3  | 1:A:313:ILE:O    | 2.18                     | 0.44              |
| 1:C:179:GLN:OE1  | 1:C:207:ILE:HD11 | 2.18                     | 0.44              |
| 1:C:372:PHE:CD2  | 1:C:372:PHE:O    | 2.70                     | 0.44              |
| 1:A:127:LEU:HD11 | 1:A:194:ARG:CZ   | 2.48                     | 0.43              |
| 1:A:180:THR:O    | 1:A:180:THR:HG22 | 2.18                     | 0.43              |
| 1:A:113:HIS:HE1  | 1:A:273:GLU:OE1  | 2.00                     | 0.43              |
| 1:C:159:GLY:HA3  | 1:C:194:ARG:HH12 | 1.83                     | 0.43              |
| 1:A:300:LYS:HE2  | 1:C:2:PHE:CZ     | 2.50                     | 0.43              |
| 1:A:249:LEU:HD23 | 1:A:249:LEU:O    | 2.18                     | 0.43              |
| 1:A:232:LEU:HA   | 1:A:276:SER:HB3  | 1.99                     | 0.43              |
| 1:A:313:ILE:HG21 | 1:A:317:ASN:O    | 2.18                     | 0.43              |
| 1:B:179:GLN:NE2  | 1:B:207:ILE:HD11 | 2.32                     | 0.43              |
| 1:B:228:SER:OG   | 1:B:229:ARG:N    | 2.51                     | 0.43              |
| 1:B:313:ILE:HG22 | 1:B:314:SER:N    | 2.33                     | 0.43              |
| 1:B:345:LEU:C    | 1:B:349:THR:HG23 | 2.37                     | 0.43              |
| 1:C:222:GLU:OE1  | 1:C:225:ARG:HG3  | 2.18                     | 0.43              |
| 1:B:217:GLY:O    | 1:B:234:SER:HA   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:66:ASP:O     | 1:B:69:ILE:HB    | 2.18                     | 0.43              |
| 1:C:249:LEU:HD23 | 1:C:249:LEU:HA   | 1.88                     | 0.43              |
| 1:C:293:TYR:CE2  | 1:C:302:ILE:HG13 | 2.47                     | 0.43              |
| 1:C:372:PHE:CD1  | 1:C:380:PRO:HG3  | 2.53                     | 0.43              |
| 1:A:147:VAL:HG13 | 1:A:148:ALA:N    | 2.33                     | 0.43              |
| 1:A:293:TYR:O    | 1:A:294:ILE:C    | 2.56                     | 0.43              |
| 1:B:254:LEU:HD23 | 1:B:254:LEU:HA   | 1.89                     | 0.43              |
| 1:B:343:ARG:CZ   | 1:B:343:ARG:CB   | 2.96                     | 0.43              |
| 1:C:112:LEU:HB3  | 1:C:116:GLU:OE2  | 2.17                     | 0.43              |
| 1:C:208:PRO:HA   | 1:C:292:HIS:CE1  | 2.53                     | 0.43              |
| 1:C:295:ARG:HG2  | 1:C:295:ARG:O    | 2.18                     | 0.43              |
| 1:A:291:MET:C    | 1:A:293:TYR:N    | 2.72                     | 0.43              |
| 1:A:313:ILE:O    | 1:A:318:LEU:HB2  | 2.17                     | 0.43              |
| 1:B:125:TYR:HE1  | 1:B:159:GLY:CA   | 2.30                     | 0.43              |
| 1:B:33:SER:C     | 1:B:35:SER:N     | 2.72                     | 0.43              |
| 1:C:147:VAL:HG21 | 1:C:154:GLY:N    | 2.33                     | 0.43              |
| 1:C:308:LEU:HD13 | 1:C:315:ARG:CB   | 2.46                     | 0.43              |
| 1:A:370:SER:HA   | 1:A:373:LYS:NZ   | 2.33                     | 0.43              |
| 1:B:121:ARG:HH12 | 1:B:184:GLN:HG3  | 1.83                     | 0.43              |
| 1:B:56:LEU:HD11  | 1:B:60:VAL:HG11  | 2.00                     | 0.43              |
| 1:C:226:TYR:O    | 1:C:228:SER:N    | 2.52                     | 0.43              |
| 1:C:98:TYR:N     | 1:C:262:GLN:O    | 2.47                     | 0.43              |
| 1:C:229:ARG:NH2  | 1:C:296:ASN:OD1  | 2.52                     | 0.43              |
| 1:C:293:TYR:CZ   | 1:C:297:HIS:HB2  | 2.53                     | 0.43              |
| 1:A:379:THR:HB   | 1:A:380:PRO:CD   | 2.48                     | 0.43              |
| 1:A:7:ARG:HB2    | 1:A:7:ARG:HH11   | 1.84                     | 0.43              |
| 1:B:345:LEU:HD12 | 1:B:356:ILE:HG23 | 2.00                     | 0.43              |
| 1:C:228:SER:O    | 1:C:230:VAL:N    | 2.52                     | 0.43              |
| 1:C:305:ASP:O    | 1:C:305:ASP:OD1  | 2.36                     | 0.43              |
| 1:A:79:PRO:CB    | 1:A:253:LEU:HD22 | 2.49                     | 0.43              |
| 1:A:231:ALA:O    | 1:A:276:SER:HB3  | 2.18                     | 0.43              |
| 1:C:299:CYS:H    | 1:C:341:LYS:HZ2  | 1.67                     | 0.43              |
| 1:C:328:GLU:OE2  | 1:C:333:MET:HG2  | 2.19                     | 0.43              |
| 1:A:175:ALA:O    | 1:A:176:ASP:C    | 2.58                     | 0.43              |
| 1:B:1:MET:HA     | 1:B:1:MET:HE3    | 2.01                     | 0.43              |
| 1:B:317:ASN:HB3  | 1:B:321:ARG:CD   | 2.45                     | 0.43              |
| 1:A:14:ALA:HB3   | 1:C:15:ASN:O     | 2.19                     | 0.43              |
| 1:C:159:GLY:CA   | 1:C:194:ARG:HH22 | 2.31                     | 0.43              |
| 1:C:288:ILE:HG22 | 1:C:289:GLN:N    | 2.33                     | 0.43              |
| 1:C:304:VAL:O    | 1:C:315:ARG:NH2  | 2.52                     | 0.43              |
| 1:C:370:SER:C    | 1:C:372:PHE:H    | 2.21                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:166:ASN:HB2  | 1:A:169:HIS:HB2  | 2.00                     | 0.43              |
| 1:A:20:ARG:HE    | 1:A:20:ARG:HB3   | 1.63                     | 0.43              |
| 1:B:60:VAL:HG23  | 1:B:80:ILE:HG23  | 2.01                     | 0.43              |
| 1:C:133:LYS:HE3  | 1:C:133:LYS:N    | 2.34                     | 0.43              |
| 1:C:20:ARG:CZ    | 1:C:20:ARG:HB3   | 2.48                     | 0.43              |
| 1:C:278:ASP:CA   | 1:C:280:ARG:NH2  | 2.82                     | 0.43              |
| 1:C:303:LYS:C    | 1:C:305:ASP:H    | 2.23                     | 0.43              |
| 1:A:12:PHE:HD2   | 1:A:23:VAL:CG2   | 2.31                     | 0.42              |
| 1:A:233:SER:OG   | 1:A:273:GLU:HA   | 2.19                     | 0.42              |
| 1:B:199:LEU:HD23 | 1:B:199:LEU:HA   | 1.84                     | 0.42              |
| 1:C:114:LEU:HB2  | 1:C:122:PHE:HE2  | 1.84                     | 0.42              |
| 1:C:225:ARG:NH2  | 1:C:272:ILE:HD12 | 2.34                     | 0.42              |
| 1:C:248:LYS:O    | 1:C:252:ARG:HG3  | 2.19                     | 0.42              |
| 1:A:218:ILE:O    | 1:A:220:ASN:N    | 2.52                     | 0.42              |
| 1:A:219:ASP:C    | 1:A:221:GLU:H    | 2.23                     | 0.42              |
| 1:A:101:THR:HG21 | 1:A:237:GLN:OE1  | 2.18                     | 0.42              |
| 1:A:79:PRO:HB3   | 1:A:253:LEU:HD13 | 2.00                     | 0.42              |
| 1:B:378:THR:HG22 | 1:B:382:GLU:OE1  | 2.20                     | 0.42              |
| 1:B:56:LEU:HD21  | 1:B:60:VAL:HG22  | 2.00                     | 0.42              |
| 1:C:14:ALA:O     | 1:C:20:ARG:CD    | 2.63                     | 0.42              |
| 1:C:305:ASP:C    | 1:C:307:VAL:N    | 2.71                     | 0.42              |
| 1:B:185:THR:HB   | 1:B:213:LEU:CD2  | 2.47                     | 0.42              |
| 1:B:272:ILE:CG2  | 1:B:274:ARG:NE   | 2.82                     | 0.42              |
| 1:C:144:ARG:HG3  | 1:C:144:ARG:HH11 | 1.85                     | 0.42              |
| 1:C:25:GLY:O     | 1:C:28:GLU:HB2   | 2.19                     | 0.42              |
| 1:B:143:PHE:CZ   | 1:B:147:VAL:HG11 | 2.54                     | 0.42              |
| 1:C:346:LEU:HB2  | 1:C:347:ILE:HD12 | 2.01                     | 0.42              |
| 1:C:159:GLY:HA3  | 1:C:194:ARG:CZ   | 2.50                     | 0.42              |
| 1:C:354:ASN:HD22 | 1:C:354:ASN:HA   | 1.61                     | 0.42              |
| 1:A:220:ASN:HB2  | 1:A:235:VAL:O    | 2.19                     | 0.42              |
| 1:A:365:LEU:O    | 1:A:368:PHE:HB3  | 2.18                     | 0.42              |
| 1:A:173:ARG:HE   | 1:A:173:ARG:HA   | 1.85                     | 0.42              |
| 1:A:233:SER:HA   | 1:A:274:ARG:CG   | 2.50                     | 0.42              |
| 1:B:274:ARG:HG3  | 1:B:274:ARG:NH1  | 2.35                     | 0.42              |
| 1:B:99:ILE:HD13  | 1:B:264:ILE:CG2  | 2.50                     | 0.42              |
| 1:C:140:GLU:O    | 1:C:143:PHE:HB3  | 2.20                     | 0.42              |
| 1:C:18:TYR:O     | 1:C:21:GLN:N     | 2.53                     | 0.42              |
| 1:C:360:CYS:HB3  | 1:C:362:TYR:CE2  | 2.55                     | 0.42              |
| 1:A:351:LEU:N    | 1:A:384:ARG:HH22 | 2.15                     | 0.42              |
| 1:B:327:GLY:O    | 1:B:328:GLU:OE2  | 2.37                     | 0.42              |
| 1:C:86:SER:H     | 1:C:103:ASN:ND2  | 2.18                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:182:PRO:HA   | 1:A:183:PRO:HD3  | 1.91                     | 0.42              |
| 1:B:104:TYR:HE2  | 1:B:108:GLU:OE1  | 2.02                     | 0.42              |
| 1:B:101:THR:HB   | 1:B:242:MET:HE1  | 2.01                     | 0.42              |
| 1:B:28:GLU:OE1   | 1:B:240:ARG:HD3  | 2.20                     | 0.42              |
| 1:A:189:ALA:CB   | 1:A:195:ALA:HB2  | 2.46                     | 0.42              |
| 1:A:304:VAL:O    | 1:A:307:VAL:HB   | 2.20                     | 0.42              |
| 1:A:347:ILE:HA   | 1:A:388:SER:HA   | 2.01                     | 0.42              |
| 1:B:216:ILE:HD12 | 1:B:233:SER:HB2  | 2.02                     | 0.42              |
| 1:C:373:LYS:HA   | 1:C:376:TYR:O    | 2.20                     | 0.42              |
| 1:A:302:ILE:O    | 1:A:334:ILE:HD12 | 2.20                     | 0.41              |
| 1:B:284:ASP:CB   | 1:B:325:GLU:OE1  | 2.65                     | 0.41              |
| 1:C:373:LYS:HE2  | 1:C:373:LYS:HB2  | 1.83                     | 0.41              |
| 1:C:7:ARG:CB     | 1:C:7:ARG:HH11   | 2.33                     | 0.41              |
| 1:A:102:ASP:HB3  | 1:A:105:ALA:HB3  | 2.02                     | 0.41              |
| 1:B:121:ARG:CG   | 1:B:121:ARG:HH11 | 2.33                     | 0.41              |
| 1:B:155:VAL:HG12 | 1:B:156:VAL:H    | 1.85                     | 0.41              |
| 1:B:89:LEU:HB2   | 1:B:92:SER:HB2   | 2.01                     | 0.41              |
| 1:C:11:LEU:HB2   | 1:C:62:ALA:CB    | 2.51                     | 0.41              |
| 1:A:234:SER:OG   | 1:A:235:VAL:N    | 2.54                     | 0.41              |
| 1:A:84:GLY:O     | 1:A:100:ALA:HB1  | 2.20                     | 0.41              |
| 1:B:124:PHE:CD1  | 1:B:143:PHE:HB2  | 2.55                     | 0.41              |
| 1:B:192:ASP:OD1  | 1:B:218:ILE:N    | 2.53                     | 0.41              |
| 1:B:305:ASP:C    | 1:B:307:VAL:H    | 2.23                     | 0.41              |
| 1:B:55:TRP:C     | 1:B:56:LEU:O     | 2.59                     | 0.41              |
| 1:C:144:ARG:HG3  | 1:C:144:ARG:NH1  | 2.34                     | 0.41              |
| 1:C:259:MET:HG2  | 1:C:262:GLN:HE21 | 1.85                     | 0.41              |
| 1:C:291:MET:HA   | 1:C:294:ILE:CG1  | 2.51                     | 0.41              |
| 1:A:118:GLY:O    | 1:A:119:VAL:O    | 2.39                     | 0.41              |
| 1:A:122:PHE:N    | 1:A:122:PHE:CD1  | 2.88                     | 0.41              |
| 1:A:203:GLU:HB3  | 1:C:5:ARG:NH1    | 2.34                     | 0.41              |
| 1:C:184:GLN:HA   | 1:C:212:LYS:O    | 2.19                     | 0.41              |
| 1:C:2:PHE:O      | 1:C:2:PHE:HD1    | 2.02                     | 0.41              |
| 1:A:121:ARG:O    | 1:A:185:THR:HG23 | 2.21                     | 0.41              |
| 1:A:174:LEU:HD12 | 1:A:175:ALA:N    | 2.35                     | 0.41              |
| 1:A:187:ILE:HD11 | 1:A:213:LEU:HD13 | 2.01                     | 0.41              |
| 1:B:218:ILE:HG13 | 1:B:235:VAL:CG2  | 2.51                     | 0.41              |
| 1:B:311:VAL:CG1  | 1:B:312:GLY:N    | 2.82                     | 0.41              |
| 1:B:84:GLY:HA3   | 1:B:98:TYR:OH    | 2.20                     | 0.41              |
| 1:C:164:PRO:HG2  | 1:C:167:TRP:HA   | 2.02                     | 0.41              |
| 1:C:46:ARG:NH1   | 1:C:46:ARG:HG2   | 2.35                     | 0.41              |
| 1:A:347:ILE:HG23 | 1:A:389:GLU:N    | 2.22                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:373:LYS:HE2  | 1:A:373:LYS:HB2  | 1.96                     | 0.41              |
| 1:B:178:LEU:O    | 1:B:181:LEU:HB2  | 2.21                     | 0.41              |
| 1:B:204:HIS:CD2  | 1:B:205:LEU:HD12 | 2.55                     | 0.41              |
| 1:B:205:LEU:CD1  | 1:B:205:LEU:N    | 2.83                     | 0.41              |
| 1:B:254:LEU:C    | 1:B:256:LYS:H    | 2.23                     | 0.41              |
| 1:B:287:VAL:O    | 1:B:288:ILE:C    | 2.59                     | 0.41              |
| 1:C:222:GLU:OE1  | 1:C:222:GLU:HA   | 2.21                     | 0.41              |
| 1:C:346:LEU:HD13 | 1:C:384:ARG:HG2  | 2.01                     | 0.41              |
| 1:C:351:LEU:HD22 | 1:C:352:SER:H    | 1.85                     | 0.41              |
| 1:A:198:ILE:HG21 | 1:A:215:VAL:CG1  | 2.51                     | 0.41              |
| 1:A:211:GLU:HG2  | 1:A:292:HIS:HB2  | 2.01                     | 0.41              |
| 1:B:308:LEU:HD22 | 1:B:315:ARG:HA   | 2.02                     | 0.41              |
| 1:B:313:ILE:HG22 | 1:B:314:SER:O    | 2.21                     | 0.41              |
| 1:C:127:LEU:HD22 | 1:C:190:VAL:HG21 | 2.02                     | 0.41              |
| 1:C:22:VAL:O     | 1:C:25:GLY:N     | 2.54                     | 0.41              |
| 1:C:249:LEU:HD11 | 1:C:262:GLN:HG3  | 2.02                     | 0.41              |
| 1:C:311:VAL:HB   | 1:C:318:LEU:CD1  | 2.38                     | 0.41              |
| 1:C:284:ASP:HB3  | 1:C:325:GLU:OE2  | 2.20                     | 0.41              |
| 1:C:86:SER:C     | 1:C:87:TYR:HD1   | 2.23                     | 0.41              |
| 1:B:152:TYR:N    | 1:B:152:TYR:CD1  | 2.89                     | 0.41              |
| 1:B:164:PRO:HB2  | 1:B:170:ALA:HB2  | 2.01                     | 0.41              |
| 1:C:159:GLY:HA3  | 1:C:194:ARG:NH2  | 2.35                     | 0.41              |
| 1:C:233:SER:CB   | 1:C:276:SER:OG   | 2.68                     | 0.41              |
| 1:C:275:ARG:HH22 | 1:C:296:ASN:ND2  | 2.17                     | 0.41              |
| 1:C:23:VAL:HG11  | 1:C:41:ILE:HD13  | 2.02                     | 0.41              |
| 1:A:206:HIS:O    | 1:A:208:PRO:HD3  | 2.21                     | 0.41              |
| 1:A:244:TYR:HD1  | 1:A:245:GLN:NE2  | 2.16                     | 0.41              |
| 1:B:174:LEU:O    | 1:B:175:ALA:C    | 2.58                     | 0.41              |
| 1:B:188:ILE:HG12 | 1:B:216:ILE:HG21 | 2.03                     | 0.41              |
| 1:B:191:THR:HG22 | 1:B:192:ASP:N    | 2.35                     | 0.41              |
| 1:B:106:LEU:HB3  | 1:B:218:ILE:HD11 | 2.02                     | 0.41              |
| 1:C:141:TYR:CD1  | 1:C:141:TYR:C    | 2.95                     | 0.41              |
| 1:C:185:THR:HG22 | 1:C:186:GLY:N    | 2.36                     | 0.41              |
| 1:C:356:ILE:N    | 1:C:356:ILE:HD13 | 2.36                     | 0.41              |
| 1:C:4:LYS:HZ2    | 1:C:4:LYS:HA     | 1.86                     | 0.41              |
| 1:C:84:GLY:O     | 1:C:100:ALA:HA   | 2.21                     | 0.41              |
| 1:B:216:ILE:CD1  | 1:B:277:THR:HG21 | 2.51                     | 0.41              |
| 1:B:29:TYR:CE1   | 1:B:248:LYS:HA   | 2.55                     | 0.41              |
| 1:C:278:ASP:O    | 1:C:280:ARG:CZ   | 2.69                     | 0.41              |
| 1:C:75:ASP:O     | 1:C:75:ASP:CG    | 2.59                     | 0.41              |
| 1:A:99:ILE:HG23  | 1:A:264:ILE:HG13 | 2.02                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:292:HIS:C    | 1:B:294:ILE:N    | 2.75                     | 0.40              |
| 1:B:308:LEU:HD13 | 1:B:315:ARG:CB   | 2.51                     | 0.40              |
| 1:B:331:HIS:C    | 1:B:333:MET:N    | 2.73                     | 0.40              |
| 1:B:369:TYR:CE2  | 1:B:373:LYS:HD2  | 2.56                     | 0.40              |
| 1:C:230:VAL:O    | 1:C:231:ALA:C    | 2.59                     | 0.40              |
| 1:C:308:LEU:CD1  | 1:C:315:ARG:HB2  | 2.49                     | 0.40              |
| 1:C:58:ASP:O     | 1:C:78:VAL:HB    | 2.21                     | 0.40              |
| 1:A:114:LEU:HB2  | 1:A:122:PHE:HE2  | 1.86                     | 0.40              |
| 1:A:157:TYR:CE1  | 1:A:177:TRP:HB2  | 2.56                     | 0.40              |
| 1:A:131:SER:O    | 1:A:132:GLY:C    | 2.59                     | 0.40              |
| 1:A:216:ILE:HD11 | 1:A:234:SER:HA   | 2.03                     | 0.40              |
| 1:A:65:ASP:OD1   | 1:A:85:GLY:N     | 2.52                     | 0.40              |
| 1:B:144:ARG:HG3  | 1:B:144:ARG:NH1  | 2.31                     | 0.40              |
| 1:B:41:ILE:O     | 1:B:41:ILE:HG22  | 2.21                     | 0.40              |
| 1:A:147:VAL:C    | 1:A:149:GLU:H    | 2.24                     | 0.40              |
| 1:A:185:THR:O    | 1:A:214:CYS:HB2  | 2.22                     | 0.40              |
| 1:A:24:GLU:HB3   | 1:A:240:ARG:HH12 | 1.86                     | 0.40              |
| 1:A:297:HIS:NE2  | 1:C:1:MET:SD     | 2.94                     | 0.40              |
| 1:B:291:MET:CE   | 1:B:295:ARG:NH2  | 2.84                     | 0.40              |
| 1:C:180:THR:HG22 | 1:C:180:THR:O    | 2.22                     | 0.40              |
| 1:C:209:VAL:HG12 | 1:C:213:LEU:O    | 2.22                     | 0.40              |
| 1:C:272:ILE:HB   | 1:C:274:ARG:NH1  | 2.37                     | 0.40              |
| 1:A:125:TYR:CD2  | 1:A:198:ILE:HD11 | 2.57                     | 0.40              |
| 1:A:188:ILE:HA   | 1:A:216:ILE:HG23 | 2.02                     | 0.40              |
| 1:A:352:SER:OG   | 1:A:355:GLU:HB3  | 2.20                     | 0.40              |
| 1:B:135:TRP:O    | 1:B:139:ARG:HD2  | 2.21                     | 0.40              |
| 1:B:181:LEU:HA   | 1:B:182:PRO:HD3  | 1.92                     | 0.40              |
| 1:B:222:GLU:O    | 1:B:225:ARG:HB2  | 2.21                     | 0.40              |
| 1:B:216:ILE:HD13 | 1:B:277:THR:HG21 | 2.03                     | 0.40              |
| 1:B:74:ALA:C     | 1:B:75:ASP:OD1   | 2.59                     | 0.40              |
| 1:C:86:SER:O     | 1:C:87:TYR:CD1   | 2.75                     | 0.40              |

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

| Atom-1         | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 1:C:320:LYS:NZ | 1:C:320:LYS:NZ[6_554] | 1.76                     | 0.44              |

## 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     | 374/392 (95%)   | 272 (73%) | 64 (17%)  | 38 (10%) | 0           | 7  |
| 1   | B     | 374/392 (95%)   | 277 (74%) | 74 (20%)  | 23 (6%)  | 1           | 16 |
| 1   | C     | 374/392 (95%)   | 292 (78%) | 57 (15%)  | 25 (7%)  | 1           | 14 |
| All | All   | 1122/1176 (95%) | 841 (75%) | 195 (17%) | 86 (8%)  | 1           | 11 |

All (86) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 96  | VAL  |
| 1   | A     | 119 | VAL  |
| 1   | A     | 153 | ARG  |
| 1   | A     | 159 | GLY  |
| 1   | A     | 225 | ARG  |
| 1   | A     | 269 | VAL  |
| 1   | A     | 278 | ASP  |
| 1   | A     | 386 | VAL  |
| 1   | B     | 56  | LEU  |
| 1   | B     | 132 | GLY  |
| 1   | B     | 276 | SER  |
| 1   | C     | 56  | LEU  |
| 1   | C     | 227 | LEU  |
| 1   | A     | 2   | PHE  |
| 1   | A     | 7   | ARG  |
| 1   | A     | 56  | LEU  |
| 1   | A     | 219 | ASP  |
| 1   | A     | 237 | GLN  |
| 1   | A     | 276 | SER  |
| 1   | A     | 298 | ALA  |
| 1   | A     | 299 | CYS  |
| 1   | A     | 327 | GLY  |
| 1   | A     | 328 | GLU  |
| 1   | B     | 14  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 96  | VAL  |
| 1   | B     | 119 | VAL  |
| 1   | B     | 159 | GLY  |
| 1   | B     | 293 | TYR  |
| 1   | B     | 301 | GLY  |
| 1   | B     | 363 | PRO  |
| 1   | C     | 132 | GLY  |
| 1   | C     | 159 | GLY  |
| 1   | C     | 167 | TRP  |
| 1   | C     | 229 | ARG  |
| 1   | C     | 256 | LYS  |
| 1   | C     | 269 | VAL  |
| 1   | C     | 276 | SER  |
| 1   | C     | 325 | GLU  |
| 1   | C     | 370 | SER  |
| 1   | C     | 377 | ASP  |
| 1   | A     | 118 | GLY  |
| 1   | A     | 220 | ASN  |
| 1   | A     | 281 | SER  |
| 1   | A     | 288 | ILE  |
| 1   | A     | 329 | THR  |
| 1   | B     | 86  | SER  |
| 1   | B     | 237 | GLN  |
| 1   | B     | 357 | SER  |
| 1   | C     | 190 | VAL  |
| 1   | C     | 225 | ARG  |
| 1   | C     | 226 | TYR  |
| 1   | A     | 86  | SER  |
| 1   | A     | 148 | ALA  |
| 1   | A     | 211 | GLU  |
| 1   | A     | 224 | THR  |
| 1   | A     | 301 | GLY  |
| 1   | A     | 308 | LEU  |
| 1   | A     | 361 | GLY  |
| 1   | B     | 78  | VAL  |
| 1   | B     | 102 | ASP  |
| 1   | C     | 131 | SER  |
| 1   | C     | 160 | LEU  |
| 1   | C     | 304 | VAL  |
| 1   | C     | 311 | VAL  |
| 1   | C     | 312 | GLY  |
| 1   | C     | 371 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 228 | SER  |
| 1   | A     | 261 | LEU  |
| 1   | A     | 314 | SER  |
| 1   | A     | 349 | THR  |
| 1   | A     | 388 | SER  |
| 1   | B     | 256 | LYS  |
| 1   | B     | 278 | ASP  |
| 1   | B     | 359 | MET  |
| 1   | B     | 370 | SER  |
| 1   | C     | 285 | PRO  |
| 1   | A     | 208 | PRO  |
| 1   | B     | 179 | GLN  |
| 1   | B     | 322 | PHE  |
| 1   | C     | 128 | PRO  |
| 1   | C     | 278 | ASP  |
| 1   | A     | 363 | PRO  |
| 1   | B     | 334 | ILE  |
| 1   | B     | 362 | TYR  |
| 1   | C     | 284 | ASP  |
| 1   | A     | 271 | VAL  |

### 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     | 326/338 (96%)  | 260 (80%) | 66 (20%)  | 1           | 6  |
| 1   | B     | 326/338 (96%)  | 267 (82%) | 59 (18%)  | 2           | 9  |
| 1   | C     | 326/338 (96%)  | 273 (84%) | 53 (16%)  | 2           | 14 |
| All | All   | 978/1014 (96%) | 800 (82%) | 178 (18%) | 2           | 9  |

All (178) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | MET  |
| 1   | A     | 4   | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 9   | THR  |
| 1   | A     | 19  | ASP  |
| 1   | A     | 20  | ARG  |
| 1   | A     | 30  | LEU  |
| 1   | A     | 34  | GLN  |
| 1   | A     | 35  | SER  |
| 1   | A     | 38  | ASP  |
| 1   | A     | 40  | PHE  |
| 1   | A     | 43  | GLU  |
| 1   | A     | 55  | TRP  |
| 1   | A     | 58  | ASP  |
| 1   | A     | 66  | ASP  |
| 1   | A     | 75  | ASP  |
| 1   | A     | 86  | SER  |
| 1   | A     | 91  | GLU  |
| 1   | A     | 117 | LYS  |
| 1   | A     | 120 | ASN  |
| 1   | A     | 134 | ARG  |
| 1   | A     | 145 | GLN  |
| 1   | A     | 152 | TYR  |
| 1   | A     | 153 | ARG  |
| 1   | A     | 160 | LEU  |
| 1   | A     | 165 | GLU  |
| 1   | A     | 167 | TRP  |
| 1   | A     | 179 | GLN  |
| 1   | A     | 192 | ASP  |
| 1   | A     | 197 | HIS  |
| 1   | A     | 201 | VAL  |
| 1   | A     | 208 | PRO  |
| 1   | A     | 211 | GLU  |
| 1   | A     | 215 | VAL  |
| 1   | A     | 221 | GLU  |
| 1   | A     | 222 | GLU  |
| 1   | A     | 224 | THR  |
| 1   | A     | 226 | TYR  |
| 1   | A     | 227 | LEU  |
| 1   | A     | 229 | ARG  |
| 1   | A     | 230 | VAL  |
| 1   | A     | 241 | GLN  |
| 1   | A     | 252 | ARG  |
| 1   | A     | 256 | LYS  |
| 1   | A     | 257 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 263 | ARG  |
| 1   | A     | 264 | ILE  |
| 1   | A     | 272 | ILE  |
| 1   | A     | 275 | ARG  |
| 1   | A     | 280 | ARG  |
| 1   | A     | 289 | GLN  |
| 1   | A     | 291 | MET  |
| 1   | A     | 299 | CYS  |
| 1   | A     | 304 | VAL  |
| 1   | A     | 320 | LYS  |
| 1   | A     | 321 | ARG  |
| 1   | A     | 323 | LYS  |
| 1   | A     | 328 | GLU  |
| 1   | A     | 330 | ILE  |
| 1   | A     | 335 | HIS  |
| 1   | A     | 348 | SER  |
| 1   | A     | 349 | THR  |
| 1   | A     | 352 | SER  |
| 1   | A     | 355 | GLU  |
| 1   | A     | 369 | TYR  |
| 1   | A     | 373 | LYS  |
| 1   | A     | 385 | ASP  |
| 1   | B     | 1   | MET  |
| 1   | B     | 4   | LYS  |
| 1   | B     | 6   | HIS  |
| 1   | B     | 9   | THR  |
| 1   | B     | 13  | ASN  |
| 1   | B     | 23  | VAL  |
| 1   | B     | 28  | GLU  |
| 1   | B     | 42  | GLU  |
| 1   | B     | 58  | ASP  |
| 1   | B     | 60  | VAL  |
| 1   | B     | 64  | PHE  |
| 1   | B     | 77  | ASP  |
| 1   | B     | 91  | GLU  |
| 1   | B     | 98  | TYR  |
| 1   | B     | 121 | ARG  |
| 1   | B     | 122 | PHE  |
| 1   | B     | 124 | PHE  |
| 1   | B     | 125 | TYR  |
| 1   | B     | 135 | TRP  |
| 1   | B     | 146 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 153 | ARG  |
| 1   | B     | 165 | GLU  |
| 1   | B     | 167 | TRP  |
| 1   | B     | 171 | GLN  |
| 1   | B     | 173 | ARG  |
| 1   | B     | 176 | ASP  |
| 1   | B     | 178 | LEU  |
| 1   | B     | 179 | GLN  |
| 1   | B     | 180 | THR  |
| 1   | B     | 181 | LEU  |
| 1   | B     | 190 | VAL  |
| 1   | B     | 196 | ARG  |
| 1   | B     | 219 | ASP  |
| 1   | B     | 221 | GLU  |
| 1   | B     | 226 | TYR  |
| 1   | B     | 230 | VAL  |
| 1   | B     | 232 | LEU  |
| 1   | B     | 234 | SER  |
| 1   | B     | 248 | LYS  |
| 1   | B     | 256 | LYS  |
| 1   | B     | 270 | ARG  |
| 1   | B     | 281 | SER  |
| 1   | B     | 291 | MET  |
| 1   | B     | 294 | ILE  |
| 1   | B     | 307 | VAL  |
| 1   | B     | 318 | LEU  |
| 1   | B     | 323 | LYS  |
| 1   | B     | 325 | GLU  |
| 1   | B     | 328 | GLU  |
| 1   | B     | 329 | THR  |
| 1   | B     | 330 | ILE  |
| 1   | B     | 343 | ARG  |
| 1   | B     | 348 | SER  |
| 1   | B     | 349 | THR  |
| 1   | B     | 359 | MET  |
| 1   | B     | 360 | CYS  |
| 1   | B     | 369 | TYR  |
| 1   | B     | 378 | THR  |
| 1   | B     | 389 | GLU  |
| 1   | C     | 4   | LYS  |
| 1   | C     | 19  | ASP  |
| 1   | C     | 30  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 38  | ASP  |
| 1   | C     | 39  | ILE  |
| 1   | C     | 75  | ASP  |
| 1   | C     | 131 | SER  |
| 1   | C     | 133 | LYS  |
| 1   | C     | 141 | TYR  |
| 1   | C     | 144 | ARG  |
| 1   | C     | 152 | TYR  |
| 1   | C     | 160 | LEU  |
| 1   | C     | 165 | GLU  |
| 1   | C     | 166 | ASN  |
| 1   | C     | 167 | TRP  |
| 1   | C     | 172 | ASN  |
| 1   | C     | 174 | LEU  |
| 1   | C     | 192 | ASP  |
| 1   | C     | 202 | CYS  |
| 1   | C     | 209 | VAL  |
| 1   | C     | 219 | ASP  |
| 1   | C     | 224 | THR  |
| 1   | C     | 228 | SER  |
| 1   | C     | 230 | VAL  |
| 1   | C     | 237 | GLN  |
| 1   | C     | 248 | LYS  |
| 1   | C     | 249 | LEU  |
| 1   | C     | 253 | LEU  |
| 1   | C     | 256 | LYS  |
| 1   | C     | 257 | GLU  |
| 1   | C     | 258 | GLU  |
| 1   | C     | 263 | ARG  |
| 1   | C     | 271 | VAL  |
| 1   | C     | 275 | ARG  |
| 1   | C     | 280 | ARG  |
| 1   | C     | 282 | LEU  |
| 1   | C     | 285 | PRO  |
| 1   | C     | 289 | GLN  |
| 1   | C     | 302 | ILE  |
| 1   | C     | 308 | LEU  |
| 1   | C     | 320 | LYS  |
| 1   | C     | 322 | PHE  |
| 1   | C     | 331 | HIS  |
| 1   | C     | 348 | SER  |
| 1   | C     | 349 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 351 | LEU  |
| 1   | C     | 354 | ASN  |
| 1   | C     | 356 | ILE  |
| 1   | C     | 358 | GLN  |
| 1   | C     | 366 | GLN  |
| 1   | C     | 373 | LYS  |
| 1   | C     | 376 | TYR  |
| 1   | C     | 384 | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 34  | GLN  |
| 1   | A     | 113 | HIS  |
| 1   | A     | 179 | GLN  |
| 1   | A     | 245 | GLN  |
| 1   | A     | 289 | GLN  |
| 1   | A     | 292 | HIS  |
| 1   | A     | 306 | GLN  |
| 1   | A     | 317 | ASN  |
| 1   | A     | 354 | ASN  |
| 1   | B     | 13  | ASN  |
| 1   | B     | 15  | ASN  |
| 1   | B     | 88  | HIS  |
| 1   | B     | 97  | HIS  |
| 1   | B     | 113 | HIS  |
| 1   | B     | 168 | GLN  |
| 1   | B     | 171 | GLN  |
| 1   | B     | 172 | ASN  |
| 1   | B     | 179 | GLN  |
| 1   | B     | 184 | GLN  |
| 1   | B     | 200 | GLN  |
| 1   | B     | 204 | HIS  |
| 1   | B     | 245 | GLN  |
| 1   | B     | 292 | HIS  |
| 1   | B     | 297 | HIS  |
| 1   | B     | 331 | HIS  |
| 1   | C     | 21  | GLN  |
| 1   | C     | 97  | HIS  |
| 1   | C     | 113 | HIS  |
| 1   | C     | 145 | GLN  |
| 1   | C     | 172 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 200 | GLN  |
| 1   | C     | 241 | GLN  |
| 1   | C     | 251 | HIS  |
| 1   | C     | 262 | GLN  |
| 1   | C     | 292 | HIS  |
| 1   | C     | 317 | ASN  |
| 1   | C     | 354 | ASN  |
| 1   | C     | 358 | GLN  |
| 1   | C     | 366 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  |       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------|-------|-----------------------|-------|
| 1   | A     | 380/392 (96%)   | 0.33   | 21 (5%)  | 25 24 | 70, 120, 159, 178     | 0     |
| 1   | B     | 380/392 (96%)   | 0.33   | 10 (2%)  | 56 52 | 56, 102, 140, 162     | 0     |
| 1   | C     | 380/392 (96%)   | 0.53   | 38 (10%) | 7 9   | 69, 114, 166, 178     | 0     |
| All | All   | 1140/1176 (96%) | 0.40   | 69 (6%)  | 21 21 | 56, 112, 160, 178     | 0     |

All (69) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 353 | ILE  | 8.9  |
| 1   | A     | 347 | ILE  | 6.0  |
| 1   | A     | 311 | VAL  | 5.6  |
| 1   | C     | 347 | ILE  | 5.5  |
| 1   | C     | 318 | LEU  | 5.0  |
| 1   | C     | 330 | ILE  | 4.6  |
| 1   | A     | 73  | LEU  | 4.4  |
| 1   | C     | 327 | GLY  | 4.3  |
| 1   | C     | 386 | VAL  | 4.2  |
| 1   | C     | 325 | GLU  | 4.1  |
| 1   | C     | 311 | VAL  | 4.1  |
| 1   | B     | 312 | GLY  | 3.9  |
| 1   | C     | 337 | GLU  | 3.8  |
| 1   | C     | 289 | GLN  | 3.7  |
| 1   | A     | 356 | ILE  | 3.7  |
| 1   | A     | 348 | SER  | 3.6  |
| 1   | A     | 42  | GLU  | 3.5  |
| 1   | B     | 73  | LEU  | 3.5  |
| 1   | C     | 335 | HIS  | 3.5  |
| 1   | A     | 309 | ASP  | 3.3  |
| 1   | C     | 346 | LEU  | 3.3  |
| 1   | C     | 374 | LYS  | 3.2  |
| 1   | C     | 354 | ASN  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 375 | ALA  | 3.1  |
| 1   | A     | 69  | ILE  | 3.1  |
| 1   | C     | 329 | THR  | 3.1  |
| 1   | B     | 313 | ILE  | 3.1  |
| 1   | B     | 160 | LEU  | 3.0  |
| 1   | C     | 371 | VAL  | 3.0  |
| 1   | C     | 383 | TYR  | 3.0  |
| 1   | A     | 310 | ALA  | 2.8  |
| 1   | A     | 350 | THR  | 2.8  |
| 1   | C     | 387 | ASN  | 2.7  |
| 1   | C     | 306 | GLN  | 2.6  |
| 1   | A     | 318 | LEU  | 2.6  |
| 1   | B     | 318 | LEU  | 2.6  |
| 1   | C     | 213 | LEU  | 2.5  |
| 1   | A     | 302 | ILE  | 2.5  |
| 1   | C     | 226 | TYR  | 2.5  |
| 1   | C     | 352 | SER  | 2.5  |
| 1   | A     | 334 | ILE  | 2.5  |
| 1   | C     | 73  | LEU  | 2.4  |
| 1   | B     | 273 | GLU  | 2.4  |
| 1   | C     | 312 | GLY  | 2.4  |
| 1   | C     | 336 | ALA  | 2.4  |
| 1   | C     | 302 | ILE  | 2.4  |
| 1   | C     | 307 | VAL  | 2.4  |
| 1   | A     | 111 | PHE  | 2.4  |
| 1   | B     | 298 | ALA  | 2.4  |
| 1   | C     | 381 | LYS  | 2.4  |
| 1   | B     | 3   | THR  | 2.3  |
| 1   | C     | 356 | ILE  | 2.3  |
| 1   | C     | 283 | THR  | 2.3  |
| 1   | A     | 122 | PHE  | 2.3  |
| 1   | A     | 152 | TYR  | 2.2  |
| 1   | C     | 264 | ILE  | 2.2  |
| 1   | C     | 41  | ILE  | 2.2  |
| 1   | A     | 312 | GLY  | 2.2  |
| 1   | C     | 313 | ILE  | 2.2  |
| 1   | A     | 119 | VAL  | 2.2  |
| 1   | B     | 227 | LEU  | 2.1  |
| 1   | B     | 57  | GLY  | 2.1  |
| 1   | A     | 12  | PHE  | 2.1  |
| 1   | C     | 331 | HIS  | 2.1  |
| 1   | A     | 363 | PRO  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 326 | VAL  | 2.1  |
| 1   | C     | 324 | GLU  | 2.0  |
| 1   | A     | 353 | ILE  | 2.0  |
| 1   | C     | 385 | ASP  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.