



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:54 PM GMT

PDB ID : 3VXU  
Title : The complex between T36-5 TCR and HLA-A24 bound to HIV-1 Nef134-10(2F) peptide  
Authors : Shimizu, A.; Fukai, S.; Yamagata, A.; Iwamoto, A.  
Deposited on : 2012-09-20  
Resolution : 2.70 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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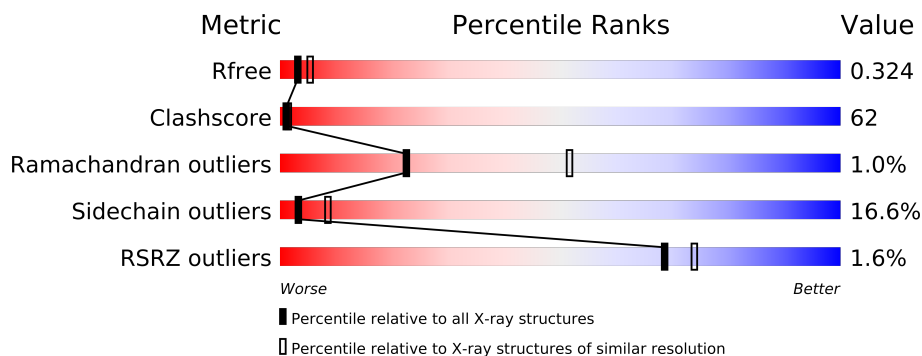
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 66092                       | 1557 (2.70-2.70)                                      |
| Clashscore            | 79885                       | 1939 (2.70-2.70)                                      |
| Ramachandran outliers | 78287                       | 1905 (2.70-2.70)                                      |
| Sidechain outliers    | 78261                       | 1905 (2.70-2.70)                                      |
| RSRZ outliers         | 66119                       | 1559 (2.70-2.70)                                      |

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 275    |                  |
| 1   | F     | 275    |                  |
| 2   | B     | 100    |                  |
| 2   | G     | 100    |                  |
| 3   | C     | 10     |                  |
| 3   | H     | 10     |                  |
| 4   | D     | 205    |                  |
| 4   | I     | 205    |                  |
| 5   | E     | 242    |                  |
| 5   | J     | 242    |                  |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13256 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called HLA class I histocompatibility antigen, A-24 alpha chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 274      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2222  | 1382 | 403 | 427 | 10 |         |         |       |
| 1   | F     | 274      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2222  | 1382 | 403 | 427 | 10 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 0       | MET      | -      | EXPRESSION TAG | UNP P05534 |
| F     | 0       | MET      | -      | EXPRESSION TAG | UNP P05534 |

- Molecule 2 is a protein called Beta-2-microglobulin.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 829   | 528 | 140 | 158 | 3 |         |         |       |
| 2   | G     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 829   | 528 | 140 | 158 | 3 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 0       | MET      | -      | EXPRESSION TAG | UNP P61769 |
| G     | 0       | MET      | -      | EXPRESSION TAG | UNP P61769 |

- Molecule 3 is a protein called 10-mer peptide from Protein Nef.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 3   | C     | 10       | Total | C  | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 91    | 64 | 14 | 12 | 1 |         |         |       |
| 3   | H     | 10       | Total | C  | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 91    | 64 | 14 | 12 | 1 |         |         |       |

- Molecule 4 is a protein called T36-5 TCR alpha chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 199      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1553  | 968 | 257 | 321 | 7 |         |         |       |
| 4   | I     | 199      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1553  | 968 | 257 | 321 | 7 |         |         |       |

- Molecule 5 is a protein called T36-5 TCR beta chain.

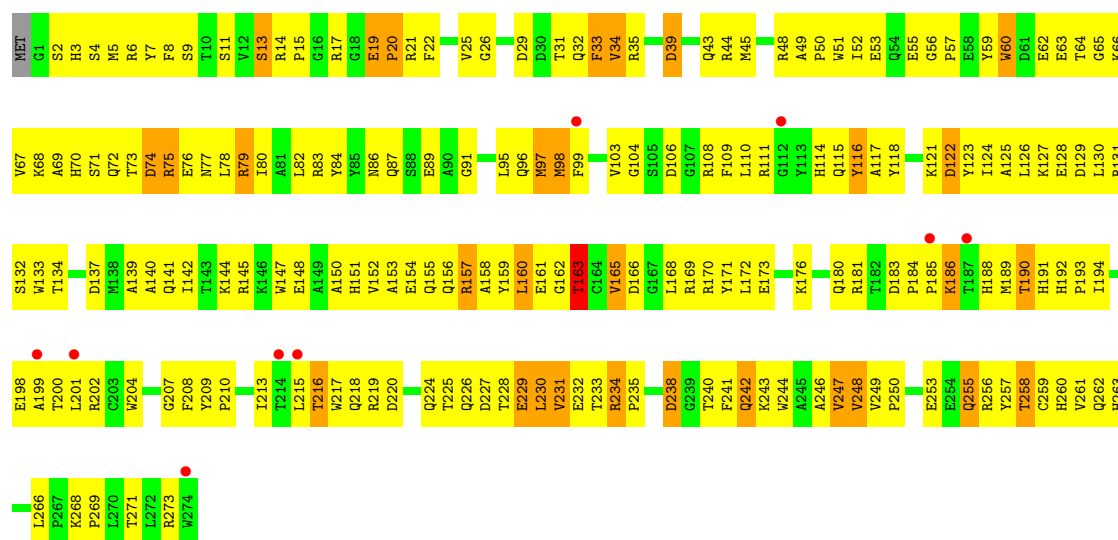
| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | E     | 241      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1933  | 1217 | 336 | 372 | 8 |         |         |       |
| 5   | J     | 241      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1933  | 1217 | 336 | 372 | 8 |         |         |       |

### 3 Residue-property plots

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

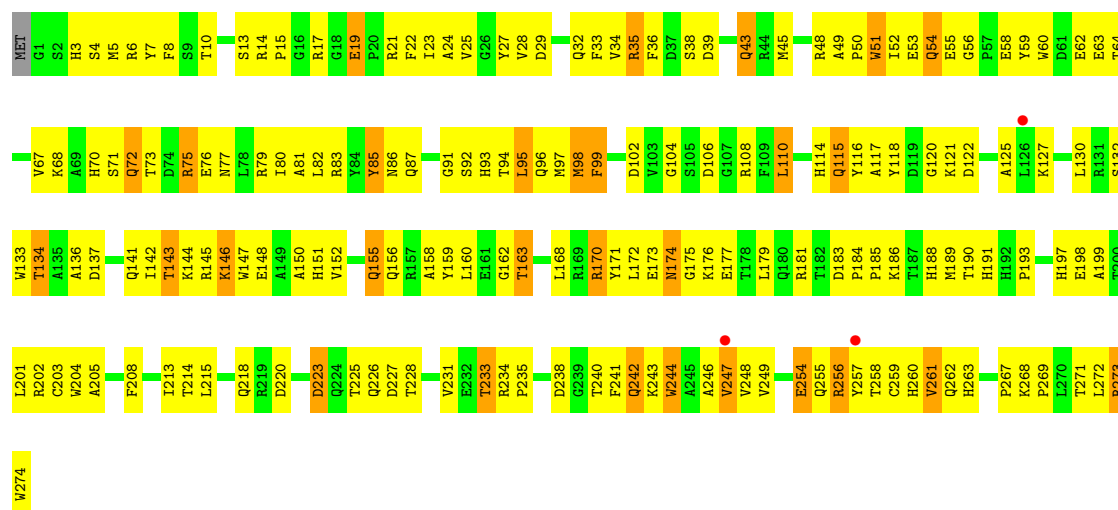
- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain

Chain A: 



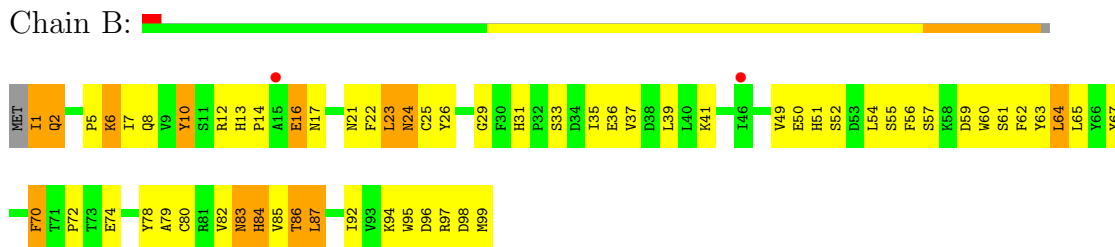
- Molecule 1: HLA class I histocompatibility antigen, A-24 alpha chain

Chain F: 



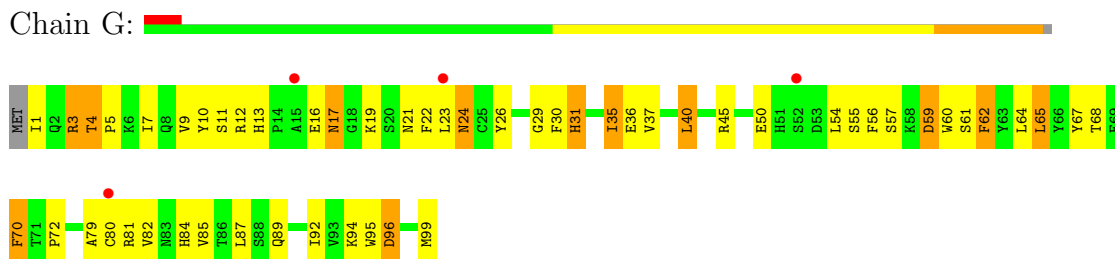
- Molecule 2: Beta-2-microglobulin

Chain B:



- Molecule 2: Beta-2-microglobulin

Chain G:



- Molecule 3: 10-mer peptide from Protein Nef

Chain C:



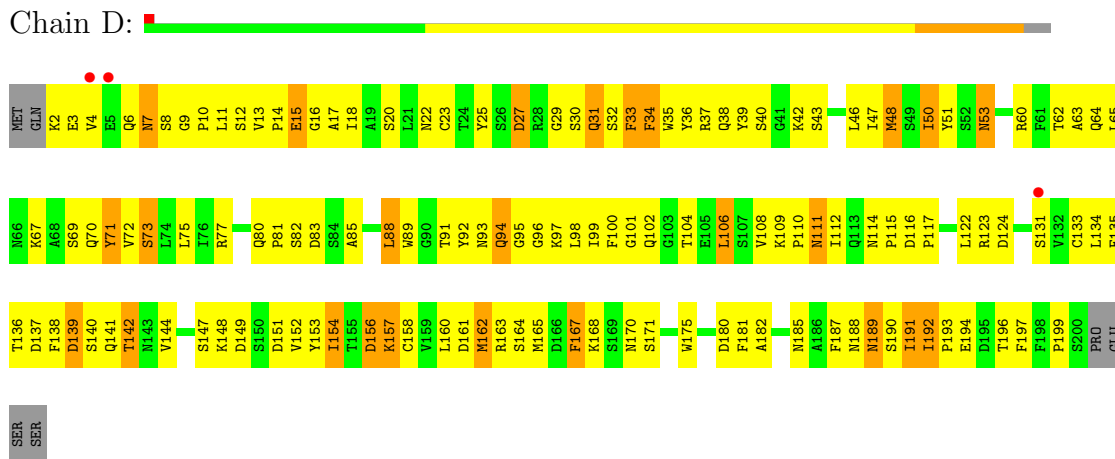
- Molecule 3: 10-mer peptide from Protein Nef

Chain H:



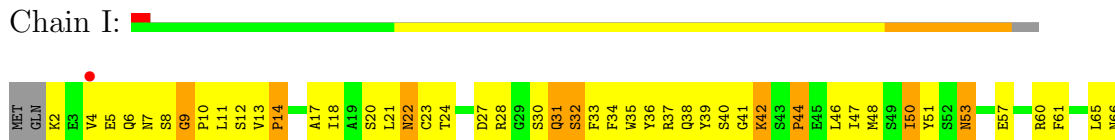
- Molecule 4: T36-5 TCR alpha chain

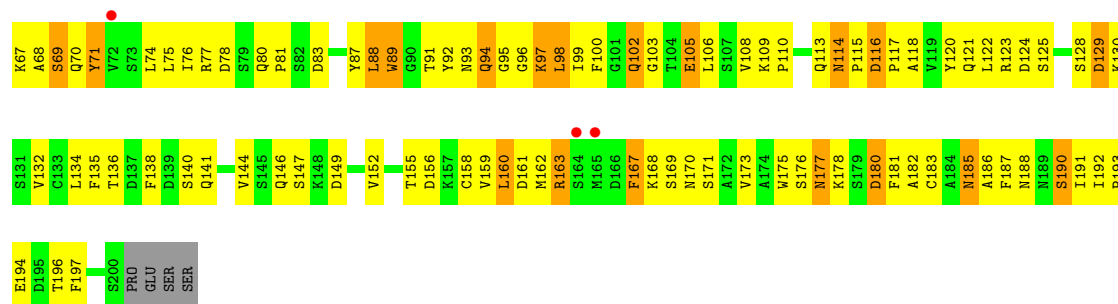
Chain D:



- Molecule 4: T36-5 TCR alpha chain

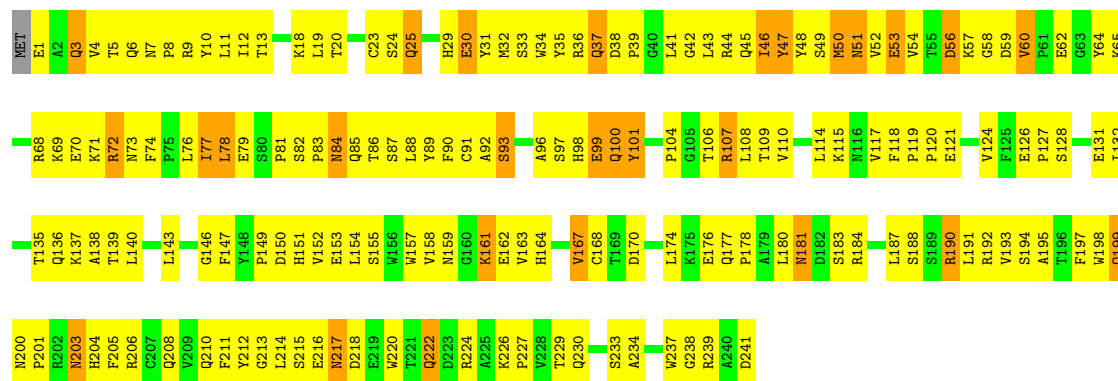
Chain I:





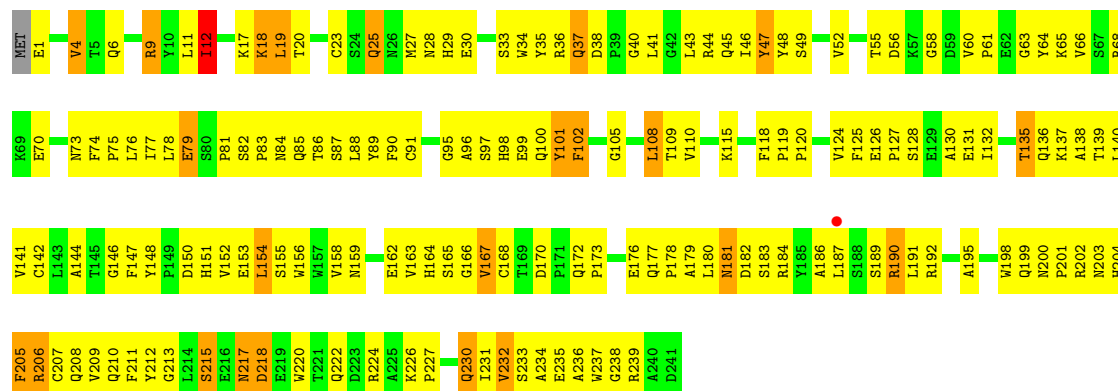
• Molecule 5: T36-5 TCR beta chain

Chain E:



• Molecule 5: T36-5 TCR beta chain

Chain J:



## 4 Data and refinement statistics

| Property  | Value  | Source           |
|---|--|------------------|
| Space group   | P 32   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 73.16Å 73.16Å 415.66Å<br>90.00° 90.00° 120.00°   | Depositor        |
| Resolution (Å)  | 32.35 – 2.70<br>32.35 – 2.60   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 92.2 (32.35-2.70)<br>95.9 (32.35-2.60)   | Depositor<br>EDS |
| $R_{merge}$   | (Not available)  | Depositor        |
| $R_{sym}$   | 0.08   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.36 (at 2.61Å)  | Xtriage          |
| Refinement program  | CNS 1.3  | Depositor        |
| R, $R_{free}$   | 0.272 , 0.323<br>0.274 , 0.324   | Depositor<br>DCC |
| $R_{free}$ test set   | 3510 reflections (5.03%)   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 38.6   | Xtriage          |
| Anisotropy  | 0.111  | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.21 , -20.0   | EDS              |
| Estimated twinning fraction   | 0.500 for h,k,l<br>0.500 for h,-h-k,-l<br>0.069 for -h,-k,l<br>0.499 for h,-h-k,-l<br>0.069 for -k,-h,-l | Xtriage          |
| Reported twinning fraction  | 0.500 for h,k,l<br>0.500 for h,-h-k,-l   | Depositor        |
| L-test for twinning   | $\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$  | Xtriage          |
| Outliers  | 0 of 73574 reflections   | Xtriage          |
| $F_o, F_c$ correlation  | 0.88   | EDS              |
| Total number of atoms   | 13256  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 67.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | A     | 0.53         | 0/2282  | 0.70        | 0/3092         |
| 1   | F     | 0.55         | 0/2282  | 0.74        | 1/3092 (0.0%)  |
| 2   | B     | 0.54         | 0/852   | 0.71        | 0/1152         |
| 2   | G     | 0.60         | 0/852   | 0.71        | 0/1152         |
| 3   | C     | 0.65         | 0/96    | 0.83        | 0/128          |
| 3   | H     | 0.65         | 0/96    | 0.71        | 0/128          |
| 4   | D     | 0.58         | 0/1587  | 0.80        | 0/2149         |
| 4   | I     | 0.59         | 0/1587  | 0.80        | 0/2149         |
| 5   | E     | 0.54         | 0/1986  | 0.71        | 0/2705         |
| 5   | J     | 0.52         | 0/1986  | 0.74        | 1/2705 (0.0%)  |
| All | All   | 0.55         | 0/13606 | 0.74        | 2/18452 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 5   | J     | 0                   | 2                   |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | J     | 12  | ILE  | CB-CA-C  | -5.57 | 100.45      | 111.60   |
| 1   | F     | 95  | LEU  | CA-CB-CG | -5.03 | 103.74      | 115.30   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 5   | J     | 101 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 5   | J     | 47  | TYR  | Sidechain |

## 5.2 Close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2222  | 0        | 2082     | 315     | 0            |
| 1   | F     | 2222  | 0        | 2082     | 278     | 0            |
| 2   | B     | 829   | 0        | 794      | 92      | 0            |
| 2   | G     | 829   | 0        | 794      | 92      | 0            |
| 3   | C     | 91    | 0        | 85       | 24      | 0            |
| 3   | H     | 91    | 0        | 85       | 31      | 0            |
| 4   | D     | 1553  | 0        | 1461     | 212     | 0            |
| 4   | I     | 1553  | 0        | 1461     | 233     | 0            |
| 5   | E     | 1933  | 0        | 1845     | 267     | 0            |
| 5   | J     | 1933  | 0        | 1845     | 282     | 0            |
| All | All   | 13256 | 0        | 12534    | 1612    | 0            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 62.

All (1612) close contacts within the same asymmetric unit are listed below.

| Atom-1          | Atom-2           | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:69:ALA:HA   | 5:E:51:ASN:HB2   | 1.20        | 1.19     |
| 5:J:177:GLN:HB3 | 5:J:180:LEU:HD13 | 1.19        | 1.19     |
| 5:J:35:TYR:HB3  | 5:J:43:LEU:HD11  | 1.24        | 1.16     |
| 1:A:4:SER:HB2   | 1:A:6:ARG:HH12   | 1.08        | 1.14     |
| 4:D:114:ASN:HA  | 1:F:108:ARG:HH22 | 0.98        | 1.11     |
| 4:D:114:ASN:HA  | 1:F:108:ARG:NH2  | 1.66        | 1.10     |
| 4:D:3:GLU:HG3   | 4:D:4:VAL:H      | 1.09        | 1.10     |
| 1:A:68:LYS:HZ1  | 5:E:53:GLU:HB3   | 1.07        | 1.09     |
| 5:E:107:ARG:HB3 | 5:E:107:ARG:HH11 | 1.16        | 1.08     |
| 4:D:114:ASN:CA  | 1:F:108:ARG:HH22 | 1.68        | 1.05     |
| 1:F:45:MET:H    | 1:F:64:THR:HG22  | 1.22        | 1.04     |
| 5:J:181:ASN:ND2 | 5:J:181:ASN:H    | 1.52        | 1.03     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:4:SER:HB2    | 1:A:6:ARG:NH1    | 1.72        | 1.03     |
| 4:I:94:GLN:HB3   | 4:I:97:LYS:HD3   | 1.42        | 1.02     |
| 5:J:206:ARG:HH22 | 5:J:208:GLN:HB2  | 1.24        | 1.02     |
| 4:D:18:ILE:HG12  | 4:D:77:ARG:HA    | 1.42        | 1.01     |
| 4:I:66:ASN:HB3   | 4:I:71:TYR:CE2   | 1.97        | 1.00     |
| 5:J:52:VAL:HA    | 5:J:68:ARG:HG3   | 1.44        | 0.99     |
| 1:A:69:ALA:CA    | 5:E:51:ASN:HB2   | 1.93        | 0.99     |
| 1:F:23:ILE:HD13  | 2:G:54:LEU:HB3   | 1.42        | 0.99     |
| 4:I:161:ASP:HB2  | 4:I:168:LYS:HE2  | 1.40        | 0.99     |
| 5:E:86:THR:HG23  | 5:E:109:THR:HA   | 1.41        | 0.98     |
| 1:F:10:THR:HB    | 1:F:23:ILE:HG22  | 1.44        | 0.98     |
| 1:A:144:LYS:O    | 1:A:148:GLU:HG3  | 1.62        | 0.98     |
| 5:E:92:ALA:HB1   | 5:E:100:GLN:HG2  | 1.44        | 0.98     |
| 1:A:115:GLN:HG2  | 1:A:125:ALA:HB1  | 1.42        | 0.98     |
| 1:F:159:TYR:HD2  | 1:F:160:LEU:HD23 | 1.26        | 0.97     |
| 1:A:69:ALA:HA    | 5:E:51:ASN:CB    | 1.95        | 0.97     |
| 5:J:181:ASN:H    | 5:J:181:ASN:HD22 | 1.07        | 0.96     |
| 1:F:49:ALA:O     | 1:F:52:ILE:HG22  | 1.64        | 0.96     |
| 1:A:200:THR:HG21 | 1:A:202:ARG:HH12 | 1.27        | 0.96     |
| 1:F:33:PHE:HD2   | 1:F:34:VAL:HG13  | 1.31        | 0.95     |
| 4:D:14:PRO:HB2   | 4:I:71:TYR:CZ    | 2.01        | 0.95     |
| 4:I:167:PHE:HZ   | 5:J:192:ARG:HH11 | 1.03        | 0.95     |
| 1:F:156:GLN:HA   | 1:F:156:GLN:NE2  | 1.81        | 0.95     |
| 4:I:185:ASN:HA   | 4:I:188:ASN:ND2  | 1.81        | 0.95     |
| 5:E:177:GLN:HB3  | 5:E:180:LEU:HD13 | 1.45        | 0.95     |
| 1:A:243:LYS:HD3  | 1:A:244:TRP:N    | 1.82        | 0.94     |
| 1:A:76:GLU:HA    | 1:A:79:ARG:HD3   | 1.49        | 0.94     |
| 5:J:36:ARG:HH12  | 5:J:85:GLN:HA    | 1.32        | 0.93     |
| 1:A:216:THR:HG23 | 1:A:260:HIS:HB2  | 1.51        | 0.93     |
| 4:I:10:PRO:HB3   | 4:I:105:GLU:HG2  | 1.47        | 0.93     |
| 1:A:45:MET:HG3   | 1:A:67:VAL:HG11  | 1.47        | 0.93     |
| 4:D:3:GLU:HG3    | 4:D:4:VAL:N      | 1.82        | 0.92     |
| 5:J:154:LEU:HD21 | 5:J:207:CYS:SG   | 2.10        | 0.92     |
| 4:I:161:ASP:HB2  | 4:I:168:LYS:CE   | 1.99        | 0.91     |
| 1:A:156:GLN:O    | 1:A:160:LEU:HG   | 1.69        | 0.91     |
| 1:F:234:ARG:HG3  | 1:F:242:GLN:HG3  | 1.53        | 0.91     |
| 2:G:12:ARG:HG2   | 2:G:21:ASN:HD21  | 1.36        | 0.90     |
| 1:F:156:GLN:HA   | 1:F:156:GLN:HE21 | 1.35        | 0.90     |
| 2:G:24:ASN:HD22  | 2:G:24:ASN:H     | 1.18        | 0.89     |
| 5:J:230:GLN:HE22 | 5:J:232:VAL:HG13 | 1.38        | 0.89     |
| 2:G:37:VAL:HG22  | 2:G:82:VAL:HG22  | 1.53        | 0.89     |
| 1:A:62:GLU:OE1   | 4:D:95:GLY:HA3   | 1.72        | 0.89     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:35:ARG:HH12  | 1:A:48:ARG:NE    | 1.70        | 0.89     |
| 5:J:206:ARG:NH1  | 5:J:233:SER:HB3  | 1.87        | 0.88     |
| 4:I:66:ASN:HB3   | 4:I:71:TYR:HE2   | 1.36        | 0.88     |
| 5:E:212:TYR:HA   | 5:E:229:THR:HG23 | 1.56        | 0.88     |
| 1:F:156:GLN:O    | 1:F:160:LEU:HG   | 1.74        | 0.88     |
| 1:A:213:ILE:HG13 | 1:A:262:GLN:O    | 1.74        | 0.87     |
| 1:F:70:HIS:HD1   | 3:H:2:PHE:HZ     | 1.23        | 0.87     |
| 5:J:180:LEU:N    | 5:J:180:LEU:HD12 | 1.89        | 0.87     |
| 4:I:159:VAL:HG12 | 4:I:168:LYS:NZ   | 1.88        | 0.87     |
| 1:F:234:ARG:CG   | 1:F:242:GLN:HG3  | 2.04        | 0.87     |
| 1:F:233:THR:HG23 | 1:F:243:LYS:HB2  | 1.57        | 0.86     |
| 1:A:185:PRO:HB3  | 1:A:208:PHE:HB3  | 1.55        | 0.86     |
| 5:J:66:VAL:HG12  | 5:J:75:PRO:O     | 1.75        | 0.86     |
| 2:G:12:ARG:HD2   | 2:G:22:PHE:HB2   | 1.58        | 0.86     |
| 1:F:106:ASP:OD2  | 1:F:108:ARG:HB2  | 1.75        | 0.86     |
| 5:E:64:TYR:O     | 5:E:65:LYS:HD2   | 1.75        | 0.86     |
| 1:A:145:ARG:HA   | 1:A:148:GLU:OE2  | 1.77        | 0.85     |
| 4:I:159:VAL:HG12 | 4:I:168:LYS:HZ2  | 1.42        | 0.85     |
| 4:D:97:LYS:HB2   | 5:E:45:GLN:OE1   | 1.77        | 0.85     |
| 1:A:249:VAL:HG13 | 1:A:257:TYR:HE2  | 1.41        | 0.85     |
| 4:I:88:LEU:N     | 4:I:88:LEU:HD23  | 1.91        | 0.85     |
| 1:A:25:VAL:HB    | 1:A:32:GLN:HE22  | 1.41        | 0.85     |
| 5:J:173:PRO:HA   | 5:J:187:LEU:HD13 | 1.59        | 0.85     |
| 5:J:159:ASN:HD21 | 5:J:204:HIS:H    | 1.22        | 0.84     |
| 5:J:35:TYR:CB    | 5:J:43:LEU:HD11  | 2.07        | 0.84     |
| 1:A:63:GLU:OE1   | 3:C:1:ARG:HG3    | 1.76        | 0.84     |
| 5:E:107:ARG:HB3  | 5:E:107:ARG:NH1  | 1.92        | 0.84     |
| 5:E:19:LEU:HD12  | 5:E:78:LEU:HD13  | 1.59        | 0.84     |
| 5:E:46:ILE:N     | 5:E:46:ILE:HD12  | 1.90        | 0.84     |
| 5:J:142:CYS:HB2  | 5:J:156:TRP:CH2  | 2.13        | 0.83     |
| 1:F:19:GLU:HG3   | 1:F:75:ARG:HE    | 1.42        | 0.83     |
| 5:J:36:ARG:NH1   | 5:J:85:GLN:HA    | 1.92        | 0.83     |
| 5:E:135:THR:HG22 | 5:E:137:LYS:HG3  | 1.59        | 0.83     |
| 1:A:69:ALA:HB2   | 5:E:50:MET:HB2   | 1.61        | 0.83     |
| 1:F:268:LYS:HD2  | 1:F:269:PRO:HD2  | 1.61        | 0.83     |
| 1:A:68:LYS:NZ    | 5:E:53:GLU:HB3   | 1.92        | 0.82     |
| 5:E:36:ARG:HH21  | 5:E:87:SER:HB2   | 1.43        | 0.82     |
| 5:J:159:ASN:ND2  | 5:J:204:HIS:H    | 1.77        | 0.82     |
| 1:F:45:MET:H     | 1:F:64:THR:CG2   | 1.92        | 0.82     |
| 4:I:120:TYR:CE1  | 5:J:131:GLU:HA   | 2.14        | 0.81     |
| 1:A:4:SER:CB     | 1:A:6:ARG:HH12   | 1.89        | 0.81     |
| 4:D:114:ASN:HB3  | 1:F:108:ARG:HH12 | 1.45        | 0.81     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:E:88:LEU:HD13  | 5:E:107:ARG:HG2  | 1.62        | 0.81     |
| 4:I:158:CYS:HB3  | 5:J:190:ARG:NH1  | 1.95        | 0.81     |
| 2:G:24:ASN:N     | 2:G:24:ASN:HD22  | 1.72        | 0.81     |
| 2:G:56:PHE:HB2   | 2:G:61:SER:O     | 1.81        | 0.81     |
| 1:A:215:LEU:HD12 | 1:A:243:LYS:HD2  | 1.62        | 0.81     |
| 2:G:24:ASN:N     | 2:G:24:ASN:ND2   | 2.25        | 0.81     |
| 4:I:61:PHE:C     | 4:I:77:ARG:HH22  | 1.83        | 0.81     |
| 1:A:152:VAL:HG12 | 1:A:156:GLN:HE21 | 1.45        | 0.81     |
| 4:D:3:GLU:CG     | 4:D:4:VAL:H      | 1.90        | 0.81     |
| 4:I:144:VAL:HG21 | 4:I:156:ASP:HA   | 1.63        | 0.81     |
| 2:B:51:HIS:HD2   | 2:B:64:LEU:HD21  | 1.45        | 0.81     |
| 1:A:249:VAL:HG13 | 1:A:257:TYR:CE2  | 2.15        | 0.81     |
| 4:I:78:ASP:OD1   | 4:I:78:ASP:O     | 1.99        | 0.81     |
| 5:E:190:ARG:N    | 5:E:190:ARG:HD2  | 1.95        | 0.80     |
| 5:E:137:LYS:HB2  | 5:E:192:ARG:CZ   | 2.11        | 0.80     |
| 1:A:165:VAL:O    | 1:A:169:ARG:HG3  | 1.81        | 0.80     |
| 5:J:38:ASP:H     | 5:J:44:ARG:NH2   | 1.79        | 0.80     |
| 4:I:160:LEU:HD11 | 4:I:167:PHE:HE2  | 1.46        | 0.80     |
| 5:E:19:LEU:CD1   | 5:E:78:LEU:HD13  | 2.11        | 0.80     |
| 1:A:200:THR:HG21 | 1:A:202:ARG:NH1  | 1.97        | 0.80     |
| 5:J:177:GLN:HB3  | 5:J:180:LEU:CD1  | 2.09        | 0.80     |
| 1:F:75:ARG:HG2   | 1:F:75:ARG:HH11  | 1.46        | 0.80     |
| 1:F:259:CYS:SG   | 1:F:272:LEU:HD13 | 2.22        | 0.80     |
| 1:F:202:ARG:NH1  | 1:F:246:ALA:HB2  | 1.95        | 0.80     |
| 1:F:115:GLN:HG3  | 2:G:60:TRP:CH2   | 2.16        | 0.79     |
| 5:E:170:ASP:HB2  | 5:E:187:LEU:HD11 | 1.62        | 0.79     |
| 2:G:13:HIS:HB2   | 2:G:21:ASN:ND2   | 1.97        | 0.79     |
| 5:E:199:GLN:O    | 5:E:201:PRO:HD3  | 1.82        | 0.79     |
| 5:E:83:PRO:HA    | 5:E:110:VAL:HB   | 1.63        | 0.79     |
| 1:A:141:GLN:O    | 1:A:145:ARG:HG3  | 1.82        | 0.79     |
| 4:I:155:THR:HG22 | 4:I:173:VAL:H    | 1.46        | 0.79     |
| 2:G:12:ARG:HG2   | 2:G:21:ASN:ND2   | 1.97        | 0.79     |
| 1:A:152:VAL:CG1  | 1:A:156:GLN:HE21 | 1.96        | 0.78     |
| 1:F:75:ARG:HG2   | 1:F:75:ARG:NH1   | 1.99        | 0.78     |
| 1:A:19:GLU:OE2   | 1:A:19:GLU:HA    | 1.82        | 0.78     |
| 1:F:58:GLU:O     | 1:F:62:GLU:HG3   | 1.84        | 0.78     |
| 1:A:57:PRO:HA    | 1:A:60:TRP:HD1   | 1.48        | 0.78     |
| 2:B:21:ASN:CG    | 2:B:22:PHE:H     | 1.88        | 0.77     |
| 4:D:31:GLN:HB3   | 4:D:67:LYS:NZ    | 2.00        | 0.77     |
| 5:J:12:ILE:HD12  | 5:J:12:ILE:H     | 1.49        | 0.77     |
| 2:B:56:PHE:HB3   | 2:B:62:PHE:CD2   | 2.18        | 0.77     |
| 4:D:153:TYR:HB2  | 4:D:175:TRP:CZ2  | 2.20        | 0.77     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:I:66:ASN:CB    | 4:I:71:TYR:HE2   | 1.96        | 0.77     |
| 5:J:86:THR:HG23  | 5:J:109:THR:HA   | 1.65        | 0.77     |
| 4:D:31:GLN:HA    | 4:D:67:LYS:HE2   | 1.65        | 0.77     |
| 5:E:52:VAL:HA    | 5:E:68:ARG:CG    | 2.14        | 0.77     |
| 5:E:159:ASN:HD21 | 5:E:204:HIS:H    | 1.33        | 0.77     |
| 5:J:154:LEU:HD23 | 5:J:208:GLN:O    | 1.86        | 0.76     |
| 1:A:26:GLY:HA3   | 1:A:33:PHE:CE1   | 2.20        | 0.76     |
| 4:I:123:ARG:HB3  | 5:J:126:GLU:HB2  | 1.68        | 0.76     |
| 5:J:181:ASN:N    | 5:J:181:ASN:HD22 | 1.83        | 0.76     |
| 2:B:56:PHE:HB2   | 2:B:61:SER:O     | 1.84        | 0.76     |
| 4:I:47:ILE:HD12  | 4:I:48:MET:N     | 2.00        | 0.76     |
| 5:E:154:LEU:HD23 | 5:E:155:SER:N    | 2.00        | 0.76     |
| 4:I:159:VAL:HG22 | 4:I:170:ASN:OD1  | 1.86        | 0.76     |
| 1:A:243:LYS:HD3  | 1:A:244:TRP:H    | 1.50        | 0.76     |
| 5:J:64:TYR:O     | 5:J:65:LYS:HD2   | 1.85        | 0.76     |
| 1:F:45:MET:N     | 1:F:64:THR:HG22  | 1.98        | 0.76     |
| 4:I:120:TYR:CZ   | 5:J:131:GLU:HA   | 2.20        | 0.76     |
| 1:F:25:VAL:HB    | 1:F:32:GLN:NE2   | 2.00        | 0.76     |
| 4:I:46:LEU:HD22  | 5:J:99:GLU:HB3   | 1.67        | 0.75     |
| 1:F:8:PHE:HD2    | 1:F:25:VAL:HG23  | 1.50        | 0.75     |
| 1:F:45:MET:HG3   | 1:F:60:TRP:HZ3   | 1.49        | 0.75     |
| 1:A:33:PHE:CD1   | 1:A:34:VAL:N     | 2.55        | 0.75     |
| 4:I:122:LEU:HB3  | 5:J:125:PHE:HB3  | 1.68        | 0.75     |
| 1:A:108:ARG:NH2  | 4:I:114:ASN:HB2  | 2.01        | 0.75     |
| 1:A:35:ARG:NH1   | 1:A:48:ARG:NE    | 2.34        | 0.75     |
| 5:E:159:ASN:ND2  | 5:E:204:HIS:H    | 1.84        | 0.75     |
| 3:C:7:GLY:H      | 5:E:30:GLU:HG3   | 1.51        | 0.75     |
| 5:J:63:GLY:O     | 5:J:78:LEU:HD12  | 1.87        | 0.75     |
| 5:E:52:VAL:HA    | 5:E:68:ARG:HG2   | 1.69        | 0.74     |
| 2:B:10:TYR:O     | 2:B:24:ASN:ND2   | 2.20        | 0.74     |
| 1:A:215:LEU:CD1  | 1:A:243:LYS:HD2  | 2.18        | 0.74     |
| 4:D:71:TYR:HD2   | 4:D:71:TYR:O     | 1.70        | 0.74     |
| 5:J:85:GLN:O     | 5:J:108:LEU:HD11 | 1.87        | 0.74     |
| 1:F:59:TYR:O     | 1:F:63:GLU:HG2   | 1.87        | 0.74     |
| 4:D:29:GLY:O     | 4:D:31:GLN:HG3   | 1.87        | 0.74     |
| 5:J:35:TYR:HB3   | 5:J:43:LEU:CD1   | 2.14        | 0.74     |
| 1:A:115:GLN:HG2  | 1:A:125:ALA:CB   | 2.18        | 0.74     |
| 5:J:181:ASN:ND2  | 5:J:181:ASN:N    | 2.33        | 0.74     |
| 5:E:100:GLN:C    | 5:E:101:TYR:HD2  | 1.92        | 0.73     |
| 1:A:45:MET:CG    | 1:A:67:VAL:HG11  | 2.17        | 0.73     |
| 1:A:80:ILE:HG23  | 1:A:83:ARG:NH2   | 2.02        | 0.73     |
| 4:D:50:ILE:HD11  | 4:D:65:LEU:HB3   | 1.71        | 0.73     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:258:THR:HB   | 1:A:260:HIS:CE1  | 2.22        | 0.73     |
| 1:F:22:PHE:CD2   | 1:F:71:SER:HB3   | 2.22        | 0.73     |
| 1:F:156:GLN:HE21 | 1:F:156:GLN:CA   | 2.01        | 0.73     |
| 5:E:119:PRO:HD3  | 5:E:227:PRO:HB3  | 1.69        | 0.73     |
| 5:E:161:LYS:HB2  | 5:E:161:LYS:NZ   | 2.04        | 0.73     |
| 4:I:160:LEU:HD12 | 4:I:160:LEU:C    | 2.08        | 0.73     |
| 1:F:121:LYS:HE2  | 2:G:1:ILE:HG12   | 1.70        | 0.73     |
| 5:J:205:PHE:HE2  | 5:J:238:GLY:N    | 1.86        | 0.72     |
| 5:J:9:ARG:HB3    | 5:J:9:ARG:HH11   | 1.53        | 0.72     |
| 1:A:213:ILE:HB   | 1:A:263:HIS:HD2  | 1.54        | 0.72     |
| 2:B:35:ILE:HD12  | 2:B:84:HIS:HD2   | 1.54        | 0.72     |
| 1:A:157:ARG:HA   | 1:A:160:LEU:CD1  | 2.19        | 0.72     |
| 1:A:137:ASP:O    | 1:A:141:GLN:HG3  | 1.90        | 0.72     |
| 5:E:158:VAL:HG23 | 5:E:163:VAL:HG21 | 1.70        | 0.72     |
| 4:I:50:ILE:C     | 4:I:50:ILE:HD12  | 2.10        | 0.72     |
| 1:F:159:TYR:CD2  | 1:F:160:LEU:HD23 | 2.18        | 0.72     |
| 1:F:4:SER:HB2    | 1:F:102:ASP:OD1  | 1.89        | 0.72     |
| 4:D:22:ASN:HD22  | 4:D:71:TYR:HE1   | 1.38        | 0.72     |
| 5:E:19:LEU:HD11  | 5:E:78:LEU:HD22  | 1.71        | 0.71     |
| 5:J:77:ILE:N     | 5:J:77:ILE:HD12  | 2.04        | 0.71     |
| 4:I:160:LEU:HD12 | 4:I:160:LEU:O    | 1.90        | 0.71     |
| 1:A:258:THR:HG22 | 1:A:271:THR:HG23 | 1.70        | 0.71     |
| 1:F:272:LEU:HD12 | 1:F:272:LEU:N    | 2.05        | 0.71     |
| 2:G:84:HIS:ND1   | 2:G:85:VAL:N     | 2.39        | 0.71     |
| 1:F:173:GLU:OE2  | 1:F:176:LYS:NZ   | 2.22        | 0.71     |
| 4:D:94:GLN:CB    | 4:D:97:LYS:HE2   | 2.20        | 0.71     |
| 2:G:31:HIS:HE1   | 2:G:60:TRP:O     | 1.72        | 0.71     |
| 1:A:75:ARG:HD3   | 1:A:79:ARG:HD2   | 1.72        | 0.71     |
| 4:D:122:LEU:HG   | 5:E:126:GLU:O    | 1.90        | 0.71     |
| 5:E:49:SER:OG    | 5:E:68:ARG:HD3   | 1.89        | 0.71     |
| 1:F:51:TRP:CZ2   | 1:F:179:LEU:HD21 | 2.26        | 0.71     |
| 4:I:160:LEU:HD13 | 4:I:162:MET:HE3  | 1.71        | 0.71     |
| 1:A:216:THR:CG2  | 1:A:260:HIS:HB2  | 2.19        | 0.71     |
| 4:I:149:ASP:HB3  | 4:I:152:VAL:CG1  | 2.21        | 0.71     |
| 1:A:63:GLU:OE2   | 1:A:63:GLU:HA    | 1.90        | 0.71     |
| 2:G:81:ARG:HA    | 2:G:92:ILE:HG12  | 1.72        | 0.71     |
| 3:C:4:LEU:HD21   | 4:D:96:GLY:HA2   | 1.72        | 0.70     |
| 1:A:253:GLU:O    | 1:A:257:TYR:CE2  | 2.44        | 0.70     |
| 4:I:18:ILE:HG12  | 4:I:77:ARG:HA    | 1.73        | 0.70     |
| 4:D:64:GLN:OE1   | 4:I:17:ALA:HA    | 1.92        | 0.70     |
| 4:D:62:THR:HG22  | 4:D:75:LEU:HD13  | 1.74        | 0.70     |
| 4:D:167:PHE:HD2  | 4:D:168:LYS:N    | 1.89        | 0.70     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:D:71:TYR:C     | 4:D:71:TYR:CD2   | 2.64        | 0.70     |
| 1:F:51:TRP:CE2   | 1:F:179:LEU:HD11 | 2.27        | 0.70     |
| 1:A:190:THR:HG21 | 2:B:98:ASP:OD1   | 1.92        | 0.70     |
| 1:F:28:VAL:HG23  | 1:F:33:PHE:CD1   | 2.26        | 0.70     |
| 5:E:5:THR:HB     | 5:E:24:SER:OG    | 1.92        | 0.70     |
| 4:I:100:PHE:CE2  | 5:J:43:LEU:HD23  | 2.27        | 0.70     |
| 5:J:200:ASN:HD21 | 5:J:202:ARG:HB3  | 1.55        | 0.70     |
| 5:J:102:PHE:N    | 5:J:102:PHE:CD2  | 2.59        | 0.70     |
| 4:I:178:LYS:HE3  | 4:I:180:ASP:HB2  | 1.72        | 0.70     |
| 4:D:71:TYR:CE2   | 4:D:73:SER:HB3   | 2.27        | 0.70     |
| 1:F:19:GLU:HG3   | 1:F:75:ARG:NE    | 2.07        | 0.70     |
| 1:A:57:PRO:HA    | 1:A:60:TRP:CD1   | 2.26        | 0.70     |
| 5:J:119:PRO:HD3  | 5:J:227:PRO:HB3  | 1.71        | 0.70     |
| 4:D:94:GLN:HB3   | 4:D:97:LYS:NZ    | 2.06        | 0.69     |
| 4:D:185:ASN:HA   | 4:D:188:ASN:ND2  | 2.06        | 0.69     |
| 5:E:77:ILE:N     | 5:E:77:ILE:HD12  | 2.07        | 0.69     |
| 1:F:35:ARG:HH11  | 1:F:35:ARG:HG2   | 1.58        | 0.69     |
| 2:B:29:GLY:HA2   | 2:B:61:SER:HB2   | 1.74        | 0.69     |
| 1:F:185:PRO:HB3  | 1:F:208:PHE:HB3  | 1.74        | 0.69     |
| 3:H:4:LEU:HD22   | 3:H:6:PHE:CE2    | 2.28        | 0.69     |
| 1:A:200:THR:CG2  | 1:A:202:ARG:HH12 | 2.02        | 0.69     |
| 1:A:33:PHE:HD1   | 1:A:34:VAL:H     | 1.40        | 0.69     |
| 5:J:108:LEU:HD12 | 5:J:108:LEU:C    | 2.12        | 0.69     |
| 1:F:28:VAL:HG23  | 1:F:33:PHE:HD1   | 1.57        | 0.69     |
| 3:H:4:LEU:HD22   | 3:H:6:PHE:HE2    | 1.57        | 0.69     |
| 4:I:185:ASN:HA   | 4:I:188:ASN:HD21 | 1.58        | 0.69     |
| 1:A:231:VAL:O    | 1:A:243:LYS:HE3  | 1.92        | 0.69     |
| 1:A:26:GLY:HA3   | 1:A:33:PHE:HE1   | 1.57        | 0.69     |
| 1:F:202:ARG:HD3  | 1:F:244:TRP:CD1  | 2.28        | 0.69     |
| 5:E:132:ILE:HG23 | 5:E:195:ALA:CB   | 2.23        | 0.69     |
| 5:E:132:ILE:HG23 | 5:E:195:ALA:HB1  | 1.74        | 0.69     |
| 1:F:108:ARG:HH11 | 1:F:108:ARG:HG3  | 1.57        | 0.69     |
| 4:I:97:LYS:HE3   | 5:J:48:TYR:HE2   | 1.57        | 0.69     |
| 5:E:118:PHE:HB3  | 5:E:184:ARG:HH21 | 1.57        | 0.69     |
| 4:D:148:LYS:HD3  | 4:D:189:ASN:OD1  | 1.93        | 0.69     |
| 1:A:68:LYS:HZ1   | 5:E:53:GLU:CB    | 1.97        | 0.69     |
| 1:A:209:TYR:HD1  | 1:A:241:PHE:HE1  | 1.41        | 0.69     |
| 5:E:78:LEU:N     | 5:E:78:LEU:HD12  | 2.08        | 0.68     |
| 5:E:37:GLN:CG    | 5:E:43:LEU:HD12  | 2.23        | 0.68     |
| 2:G:7:ILE:N      | 2:G:7:ILE:HD12   | 2.09        | 0.68     |
| 4:I:34:PHE:HZ    | 5:J:98:HIS:HB2   | 1.59        | 0.68     |
| 2:B:23:LEU:HD21  | 2:B:39:LEU:HD22  | 1.74        | 0.68     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:156:GLN:O    | 1:A:160:LEU:CG   | 2.41        | 0.68     |
| 2:B:95:TRP:CZ2   | 2:B:97:ARG:HG2   | 2.29        | 0.68     |
| 2:G:13:HIS:H     | 2:G:21:ASN:HD21  | 1.42        | 0.68     |
| 5:J:127:PRO:HD3  | 5:J:140:LEU:CD2  | 2.23        | 0.68     |
| 1:F:51:TRP:CZ2   | 1:F:179:LEU:HD11 | 2.28        | 0.68     |
| 5:J:18:LYS:HG3   | 5:J:79:GLU:OE1   | 1.94        | 0.68     |
| 4:I:35:TRP:HB3   | 4:I:47:ILE:HD11  | 1.76        | 0.68     |
| 4:D:33:PHE:O     | 4:D:50:ILE:HG23  | 1.93        | 0.68     |
| 2:G:12:ARG:HG3   | 2:G:13:HIS:HD2   | 1.58        | 0.68     |
| 1:A:235:PRO:HG2  | 2:B:65:LEU:HD13  | 1.76        | 0.67     |
| 1:A:75:ARG:NH1   | 1:A:79:ARG:HE    | 1.93        | 0.67     |
| 4:I:46:LEU:HD21  | 5:J:99:GLU:OE2   | 1.95        | 0.67     |
| 2:G:29:GLY:HA2   | 2:G:61:SER:HB2   | 1.75        | 0.67     |
| 1:F:25:VAL:HB    | 1:F:32:GLN:HE21  | 1.57        | 0.67     |
| 1:F:14:ARG:HB3   | 1:F:17:ARG:HB2   | 1.77        | 0.67     |
| 1:F:96:GLN:OE1   | 2:G:60:TRP:HB3   | 1.95        | 0.67     |
| 1:F:19:GLU:CD    | 1:F:75:ARG:HH21  | 1.97        | 0.67     |
| 1:A:49:ALA:O     | 1:A:52:ILE:HG22  | 1.93        | 0.67     |
| 5:J:87:SER:OG    | 5:J:88:LEU:N     | 2.25        | 0.67     |
| 1:F:27:TYR:CZ    | 1:F:32:GLN:HB2   | 2.29        | 0.67     |
| 4:D:144:VAL:HG21 | 4:D:156:ASP:HA   | 1.76        | 0.67     |
| 4:I:20:SER:C     | 4:I:21:LEU:HD23  | 2.15        | 0.67     |
| 4:D:12:SER:HA    | 4:D:109:LYS:HZ3  | 1.60        | 0.67     |
| 5:J:199:GLN:O    | 5:J:201:PRO:HD3  | 1.94        | 0.67     |
| 1:A:69:ALA:O     | 5:E:51:ASN:ND2   | 2.28        | 0.67     |
| 5:J:179:ALA:C    | 5:J:180:LEU:HD12 | 2.15        | 0.67     |
| 4:D:14:PRO:HD2   | 4:I:71:TYR:CE1   | 2.29        | 0.67     |
| 5:E:167:VAL:HG12 | 5:E:191:LEU:HD13 | 1.76        | 0.67     |
| 5:J:12:ILE:HD12  | 5:J:12:ILE:N     | 2.09        | 0.67     |
| 1:F:146:LYS:NZ   | 1:F:146:LYS:HB3  | 2.10        | 0.67     |
| 1:F:127:LYS:HE2  | 1:F:134:THR:HB   | 1.76        | 0.67     |
| 4:I:162:MET:HE3  | 5:J:166:GLY:HA2  | 1.76        | 0.67     |
| 4:D:191:ILE:H    | 4:D:191:ILE:HD12 | 1.60        | 0.67     |
| 1:F:181:ARG:HG2  | 1:F:181:ARG:HH11 | 1.60        | 0.67     |
| 1:A:186:LYS:NZ   | 1:A:186:LYS:HB2  | 2.10        | 0.67     |
| 4:D:91:THR:HG23  | 4:D:91:THR:O     | 1.95        | 0.67     |
| 4:D:112:ILE:HG13 | 4:D:170:ASN:HD21 | 1.58        | 0.67     |
| 1:A:226:GLN:OE1  | 1:A:226:GLN:HA   | 1.95        | 0.67     |
| 1:F:146:LYS:CB   | 1:F:146:LYS:NZ   | 2.58        | 0.66     |
| 4:I:159:VAL:CG1  | 4:I:168:LYS:HZ2  | 2.07        | 0.66     |
| 4:D:89:TRP:HZ3   | 4:D:91:THR:CG2   | 2.09        | 0.66     |
| 4:D:18:ILE:CD1   | 4:D:77:ARG:HG2   | 2.25        | 0.66     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:F:234:ARG:HE   | 1:F:242:GLN:CD   | 1.98        | 0.66     |
| 5:E:137:LYS:HB2  | 5:E:192:ARG:NH2  | 2.10        | 0.66     |
| 5:J:135:THR:O    | 5:J:137:LYS:NZ   | 2.29        | 0.66     |
| 4:D:2:LYS:NZ     | 5:E:43:LEU:N     | 2.44        | 0.66     |
| 4:I:66:ASN:HB3   | 4:I:71:TYR:CD2   | 2.31        | 0.66     |
| 4:I:162:MET:CE   | 5:J:192:ARG:HB3  | 2.25        | 0.66     |
| 1:A:142:ILE:HA   | 1:A:145:ARG:HH11 | 1.60        | 0.66     |
| 2:B:96:ASP:HB3   | 2:B:99:MET:HA    | 1.77        | 0.66     |
| 5:J:144:ALA:C    | 5:J:147:PHE:HE2  | 1.98        | 0.66     |
| 1:F:193:PRO:HA   | 1:F:199:ALA:HA   | 1.76        | 0.66     |
| 1:A:117:ALA:HB2  | 2:B:60:TRP:CE2   | 2.31        | 0.66     |
| 1:F:228:THR:HG22 | 1:F:247:VAL:HG12 | 1.78        | 0.66     |
| 5:J:120:PRO:HG2  | 5:J:232:VAL:HG21 | 1.77        | 0.66     |
| 5:E:9:ARG:NH1    | 5:E:104:PRO:HB2  | 2.11        | 0.66     |
| 1:F:97:MET:HB2   | 1:F:116:TYR:CE1  | 2.31        | 0.66     |
| 1:F:70:HIS:HD2   | 1:F:73:THR:HB    | 1.58        | 0.66     |
| 4:I:60:ARG:NH2   | 4:I:80:GLN:HG2   | 2.10        | 0.66     |
| 4:D:83:ASP:O     | 4:D:106:LEU:HD23 | 1.96        | 0.66     |
| 3:H:3:PRO:HG2    | 3:H:5:THR:CG2    | 2.25        | 0.66     |
| 1:F:76:GLU:HA    | 1:F:76:GLU:OE2   | 1.96        | 0.66     |
| 4:D:94:GLN:HG3   | 4:D:97:LYS:HE2   | 1.78        | 0.65     |
| 5:J:79:GLU:HA    | 5:J:79:GLU:OE1   | 1.95        | 0.65     |
| 5:E:64:TYR:C     | 5:E:65:LYS:HD2   | 2.14        | 0.65     |
| 4:I:20:SER:O     | 4:I:21:LEU:HD23  | 1.96        | 0.65     |
| 1:F:231:VAL:HG13 | 1:F:244:TRP:CZ3  | 2.31        | 0.65     |
| 5:J:127:PRO:HD3  | 5:J:140:LEU:HD21 | 1.78        | 0.65     |
| 1:F:213:ILE:HG13 | 1:F:262:GLN:O    | 1.97        | 0.65     |
| 4:D:167:PHE:CE1  | 5:E:137:LYS:HE3  | 2.32        | 0.65     |
| 1:F:202:ARG:HH12 | 1:F:246:ALA:HB2  | 1.59        | 0.65     |
| 4:D:142:THR:HG21 | 4:D:193:PRO:HD3  | 1.79        | 0.65     |
| 5:E:32:MET:HE1   | 5:E:71:LYS:O     | 1.96        | 0.65     |
| 5:E:46:ILE:N     | 5:E:46:ILE:CD1   | 2.59        | 0.65     |
| 1:A:258:THR:HG22 | 1:A:271:THR:CG2  | 2.27        | 0.65     |
| 4:I:124:ASP:HA   | 5:J:125:PHE:CZ   | 2.31        | 0.65     |
| 1:A:68:LYS:HG2   | 5:E:54:VAL:HG22  | 1.79        | 0.65     |
| 1:A:33:PHE:HD1   | 1:A:34:VAL:N     | 1.94        | 0.65     |
| 5:E:101:TYR:CD2  | 5:E:101:TYR:N    | 2.65        | 0.65     |
| 4:I:136:THR:HG21 | 5:J:192:ARG:HH22 | 1.61        | 0.65     |
| 1:A:76:GLU:O     | 1:A:80:ILE:HG13  | 1.97        | 0.65     |
| 4:I:38:GLN:HE22  | 5:J:37:GLN:NE2   | 1.95        | 0.65     |
| 5:E:23:CYS:HB2   | 5:E:34:TRP:CZ2   | 2.31        | 0.65     |
| 1:A:154:GLU:HB2  | 4:D:51:TYR:HB2   | 1.78        | 0.64     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:J:220:TRP:HH2  | 5:J:224:ARG:HH21 | 1.42        | 0.64     |
| 5:J:180:LEU:CD1  | 5:J:180:LEU:N    | 2.59        | 0.64     |
| 4:D:114:ASN:CB   | 1:F:108:ARG:HH12 | 2.11        | 0.64     |
| 5:E:146:GLY:O    | 5:E:184:ARG:NH2  | 2.30        | 0.64     |
| 2:G:45:ARG:HE    | 2:G:81:ARG:HH22  | 1.45        | 0.64     |
| 2:B:24:ASN:N     | 2:B:24:ASN:ND2   | 2.44        | 0.64     |
| 4:D:64:GLN:NE2   | 4:I:18:ILE:HD12  | 2.11        | 0.64     |
| 4:D:31:GLN:HA    | 4:D:67:LYS:CE    | 2.28        | 0.64     |
| 4:D:2:LYS:HZ1    | 5:E:43:LEU:H     | 1.44        | 0.64     |
| 1:A:127:LYS:HD3  | 1:A:132:SER:OG   | 1.98        | 0.64     |
| 4:D:191:ILE:HD12 | 4:D:191:ILE:N    | 2.13        | 0.64     |
| 4:D:92:TYR:HE2   | 5:E:98:HIS:HB3   | 1.63        | 0.64     |
| 1:A:69:ALA:CB    | 5:E:51:ASN:HB2   | 2.28        | 0.64     |
| 1:A:242:GLN:OE1  | 2:B:10:TYR:HE2   | 1.81        | 0.64     |
| 1:A:75:ARG:HD3   | 1:A:75:ARG:O     | 1.98        | 0.64     |
| 1:A:235:PRO:CG   | 2:B:65:LEU:HD13  | 2.28        | 0.64     |
| 5:E:48:TYR:CE2   | 5:E:56:ASP:HB2   | 2.33        | 0.63     |
| 1:A:13:SER:OG    | 1:A:15:PRO:HD3   | 1.97        | 0.63     |
| 1:A:229:GLU:OE2  | 1:A:230:LEU:N    | 2.31        | 0.63     |
| 1:F:159:TYR:O    | 1:F:163:THR:OG1  | 2.15        | 0.63     |
| 5:J:159:ASN:HD21 | 5:J:204:HIS:N    | 1.94        | 0.63     |
| 2:G:21:ASN:CG    | 2:G:22:PHE:H     | 2.01        | 0.63     |
| 1:A:56:GLY:O     | 1:A:59:TYR:HB3   | 1.98        | 0.63     |
| 1:A:21:ARG:CZ    | 1:A:39:ASP:HB2   | 2.28        | 0.63     |
| 1:A:158:ALA:HB1  | 4:D:67:LYS:HZ1   | 1.63        | 0.63     |
| 1:A:126:LEU:HD13 | 1:A:133:TRP:CZ3  | 2.34        | 0.63     |
| 1:A:228:THR:HG22 | 1:A:247:VAL:HG12 | 1.79        | 0.63     |
| 5:E:194:SER:OG   | 5:E:197:PHE:HB2  | 1.98        | 0.63     |
| 5:J:206:ARG:HG3  | 5:J:235:GLU:HB3  | 1.80        | 0.63     |
| 2:B:10:TYR:OH    | 2:B:26:TYR:HB2   | 1.99        | 0.63     |
| 4:D:92:TYR:CE2   | 5:E:98:HIS:HB3   | 2.33        | 0.63     |
| 5:J:154:LEU:HG   | 5:J:209:VAL:HG22 | 1.81        | 0.63     |
| 5:E:164:HIS:O    | 5:E:167:VAL:HG13 | 1.98        | 0.63     |
| 4:D:191:ILE:CD1  | 4:D:191:ILE:H    | 2.10        | 0.63     |
| 1:A:68:LYS:CG    | 5:E:54:VAL:HG22  | 2.29        | 0.63     |
| 4:I:167:PHE:HZ   | 5:J:192:ARG:NH1  | 1.85        | 0.63     |
| 1:F:146:LYS:CB   | 1:F:146:LYS:HZ2  | 2.12        | 0.63     |
| 1:A:162:GLY:O    | 1:A:165:VAL:HG23 | 1.99        | 0.63     |
| 4:I:136:THR:HG21 | 5:J:192:ARG:NH2  | 2.14        | 0.63     |
| 1:F:202:ARG:HH11 | 1:F:202:ARG:HG3  | 1.63        | 0.63     |
| 4:D:80:GLN:HB2   | 4:D:83:ASP:OD2   | 1.98        | 0.63     |
| 5:J:177:GLN:HG3  | 5:J:180:LEU:HD22 | 1.81        | 0.63     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:I:97:LYS:HB3   | 5:J:48:TYR:CE2   | 2.34        | 0.63     |
| 2:G:12:ARG:HG2   | 2:G:13:HIS:N     | 2.14        | 0.63     |
| 4:I:60:ARG:HH21  | 4:I:80:GLN:HG2   | 1.62        | 0.62     |
| 1:A:108:ARG:O    | 1:A:110:LEU:HD13 | 1.99        | 0.62     |
| 4:D:185:ASN:HA   | 4:D:188:ASN:HD21 | 1.64        | 0.62     |
| 3:C:4:LEU:HB3    | 3:C:6:PHE:CE2    | 2.33        | 0.62     |
| 4:I:92:TYR:HA    | 4:I:97:LYS:O     | 1.98        | 0.62     |
| 2:B:35:ILE:HD11  | 2:B:82:VAL:HG13  | 1.80        | 0.62     |
| 1:A:79:ARG:HH11  | 1:A:79:ARG:HB2   | 1.65        | 0.62     |
| 4:D:147:SER:OG   | 4:D:152:VAL:HG13 | 1.99        | 0.62     |
| 1:A:111:ARG:NH2  | 1:A:128:GLU:HA   | 2.14        | 0.62     |
| 1:F:127:LYS:CE   | 1:F:134:THR:HB   | 2.30        | 0.62     |
| 4:D:48:MET:HE3   | 4:D:63:ALA:N     | 2.15        | 0.62     |
| 4:D:31:GLN:HB3   | 4:D:67:LYS:HZ3   | 1.63        | 0.62     |
| 5:J:36:ARG:HG3   | 5:J:87:SER:OG    | 2.00        | 0.62     |
| 4:I:50:ILE:HD12  | 4:I:51:TYR:N     | 2.14        | 0.62     |
| 4:D:182:ALA:HB3  | 4:D:185:ASN:HD21 | 1.63        | 0.62     |
| 1:F:150:ALA:O    | 1:F:151:HIS:HB2  | 1.99        | 0.62     |
| 1:F:158:ALA:CB   | 4:I:31:GLN:HB2   | 2.29        | 0.62     |
| 5:E:239:ARG:HH11 | 5:E:239:ARG:HG3  | 1.64        | 0.62     |
| 1:A:65:GLY:O     | 5:E:54:VAL:HG11  | 2.00        | 0.62     |
| 5:E:150:ASP:OD1  | 5:E:150:ASP:O    | 2.17        | 0.62     |
| 4:I:138:PHE:CZ   | 4:I:170:ASN:HB3  | 2.35        | 0.62     |
| 4:I:34:PHE:CZ    | 5:J:98:HIS:HB2   | 2.34        | 0.62     |
| 2:B:33:SER:HB2   | 2:B:54:LEU:HD11  | 1.81        | 0.62     |
| 1:F:175:GLY:O    | 1:F:179:LEU:HG   | 1.99        | 0.62     |
| 2:B:2:GLN:HG3    | 2:B:31:HIS:O     | 1.99        | 0.62     |
| 5:J:177:GLN:CB   | 5:J:180:LEU:HD13 | 2.12        | 0.62     |
| 1:F:115:GLN:HG3  | 2:G:60:TRP:HH2   | 1.63        | 0.62     |
| 1:F:33:PHE:CD2   | 1:F:34:VAL:HG13  | 2.24        | 0.62     |
| 4:D:108:VAL:HG12 | 4:D:108:VAL:O    | 1.97        | 0.62     |
| 5:E:4:VAL:HG13   | 5:E:23:CYS:SG    | 2.40        | 0.62     |
| 1:A:99:PHE:CD1   | 1:A:114:HIS:HD2  | 2.18        | 0.62     |
| 5:E:48:TYR:HE1   | 5:E:50:MET:HE2   | 1.65        | 0.62     |
| 4:I:88:LEU:HB3   | 4:I:103:GLY:HA2  | 1.81        | 0.62     |
| 1:F:234:ARG:HG2  | 1:F:242:GLN:HG3  | 1.82        | 0.62     |
| 5:E:128:SER:O    | 5:E:132:ILE:HD12 | 1.99        | 0.62     |
| 5:J:102:PHE:HD2  | 5:J:102:PHE:N    | 1.97        | 0.62     |
| 1:A:111:ARG:NH1  | 1:A:128:GLU:OE1  | 2.33        | 0.62     |
| 2:G:57:SER:O     | 2:G:59:ASP:O     | 2.18        | 0.62     |
| 3:H:6:PHE:CZ     | 5:J:98:HIS:HD2   | 2.18        | 0.61     |
| 1:A:193:PRO:HA   | 1:A:199:ALA:HA   | 1.81        | 0.61     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:D:88:LEU:N     | 4:D:88:LEU:HD23  | 2.15        | 0.61     |
| 1:A:80:ILE:HG23  | 1:A:83:ARG:HH22  | 1.62        | 0.61     |
| 1:F:146:LYS:HB2  | 1:F:146:LYS:HZ2  | 1.65        | 0.61     |
| 1:A:7:TYR:CE2    | 3:C:2:PHE:HA     | 2.35        | 0.61     |
| 1:A:155:GLN:OE1  | 3:C:8:TRP:HZ2    | 1.83        | 0.61     |
| 3:H:3:PRO:HG2    | 3:H:5:THR:HG22   | 1.81        | 0.61     |
| 5:E:168:CYS:O    | 5:E:190:ARG:HD2  | 2.00        | 0.61     |
| 1:F:51:TRP:HZ2   | 1:F:179:LEU:HD21 | 1.65        | 0.61     |
| 4:I:38:GLN:HB2   | 4:I:44:PRO:HG3   | 1.82        | 0.61     |
| 1:A:111:ARG:HD3  | 1:A:128:GLU:OE2  | 1.99        | 0.61     |
| 2:G:17:ASN:HA    | 2:G:72:PRO:O     | 1.99        | 0.61     |
| 5:E:52:VAL:HA    | 5:E:68:ARG:HG3   | 1.82        | 0.61     |
| 1:F:158:ALA:HB3  | 4:I:31:GLN:HB2   | 1.83        | 0.61     |
| 4:D:112:ILE:CD1  | 4:D:170:ASN:HD21 | 2.14        | 0.61     |
| 4:D:92:TYR:HA    | 4:D:97:LYS:O     | 2.00        | 0.61     |
| 1:A:34:VAL:HG21  | 1:A:45:MET:CE    | 2.30        | 0.61     |
| 1:F:63:GLU:O     | 1:F:67:VAL:HG12  | 2.00        | 0.61     |
| 1:F:168:LEU:O    | 1:F:172:LEU:HG   | 2.01        | 0.61     |
| 4:I:129:ASP:OD1  | 4:I:130:LYS:HG3  | 2.01        | 0.61     |
| 2:B:51:HIS:CD2   | 2:B:64:LEU:HD21  | 2.33        | 0.61     |
| 5:E:52:VAL:HG13  | 5:E:68:ARG:O     | 1.99        | 0.61     |
| 1:F:75:ARG:HH11  | 1:F:75:ARG:CG    | 2.11        | 0.61     |
| 5:J:4:VAL:HG21   | 5:J:102:PHE:C    | 2.21        | 0.61     |
| 1:A:26:GLY:O     | 1:A:32:GLN:OE1   | 2.18        | 0.61     |
| 1:F:191:HIS:HE1  | 1:F:193:PRO:HG3  | 1.65        | 0.61     |
| 5:E:32:MET:SD    | 5:E:68:ARG:CZ    | 2.89        | 0.61     |
| 1:F:99:PHE:HE2   | 1:F:159:TYR:CE2  | 2.19        | 0.60     |
| 5:J:163:VAL:O    | 5:J:164:HIS:ND1  | 2.34        | 0.60     |
| 4:D:135:PHE:HB2  | 4:D:187:PHE:CE2  | 2.35        | 0.60     |
| 1:F:233:THR:HG23 | 1:F:243:LYS:HD2  | 1.83        | 0.60     |
| 5:J:230:GLN:HE22 | 5:J:232:VAL:CG1  | 2.10        | 0.60     |
| 1:A:133:TRP:CZ2  | 1:A:152:VAL:HB   | 2.36        | 0.60     |
| 5:E:19:LEU:HD12  | 5:E:19:LEU:C     | 2.22        | 0.60     |
| 4:D:18:ILE:HD11  | 4:D:77:ARG:HG2   | 1.83        | 0.60     |
| 2:B:23:LEU:HD11  | 2:B:39:LEU:HD22  | 1.83        | 0.60     |
| 2:G:12:ARG:CD    | 2:G:22:PHE:HB2   | 2.31        | 0.60     |
| 1:F:267:PRO:HG2  | 1:F:268:LYS:H    | 1.65        | 0.60     |
| 4:I:81:PRO:HA    | 4:I:108:VAL:HB   | 1.83        | 0.60     |
| 2:B:33:SER:HB3   | 2:B:62:PHE:CD1   | 2.36        | 0.60     |
| 4:I:41:GLY:C     | 4:I:42:LYS:HE2   | 2.21        | 0.60     |
| 5:J:38:ASP:H     | 5:J:44:ARG:HH22  | 1.47        | 0.60     |
| 2:G:80:CYS:O     | 2:G:92:ILE:HA    | 2.02        | 0.60     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:I:91:THR:OG1   | 4:I:93:ASN:ND2   | 2.34        | 0.60     |
| 4:I:149:ASP:HB3  | 4:I:152:VAL:HG11 | 1.81        | 0.60     |
| 4:D:154:ILE:HD11 | 4:D:187:PHE:CD1  | 2.35        | 0.60     |
| 1:A:192:HIS:HD2  | 1:A:202:ARG:HH21 | 1.50        | 0.60     |
| 5:E:190:ARG:H    | 5:E:190:ARG:HD2  | 1.63        | 0.60     |
| 1:F:144:LYS:O    | 1:F:148:GLU:HG3  | 2.01        | 0.60     |
| 1:F:70:HIS:O     | 1:F:73:THR:HB    | 2.02        | 0.60     |
| 1:F:155:GLN:HE22 | 5:J:98:HIS:CE1   | 2.19        | 0.60     |
| 1:A:250:PRO:O    | 1:A:253:GLU:HB2  | 2.01        | 0.60     |
| 1:A:238:ASP:OD2  | 2:B:12:ARG:HD3   | 2.01        | 0.60     |
| 5:J:12:ILE:HD11  | 5:J:213:GLY:O    | 2.01        | 0.60     |
| 1:F:260:HIS:CE1  | 1:F:271:THR:HG23 | 2.37        | 0.60     |
| 1:F:249:VAL:HG22 | 1:F:257:TYR:CE1  | 2.37        | 0.60     |
| 1:A:99:PHE:HD1   | 1:A:114:HIS:HD2  | 1.49        | 0.60     |
| 4:I:158:CYS:HB3  | 5:J:190:ARG:HH12 | 1.66        | 0.60     |
| 4:D:60:ARG:HH22  | 4:D:83:ASP:CG    | 2.04        | 0.60     |
| 1:A:127:LYS:HB2  | 1:A:129:ASP:OD1  | 2.01        | 0.60     |
| 5:E:206:ARG:NH1  | 5:E:208:GLN:OE1  | 2.35        | 0.60     |
| 2:B:7:ILE:N      | 2:B:7:ILE:HD12   | 2.16        | 0.60     |
| 1:F:43:GLN:HA    | 1:F:43:GLN:HE21  | 1.67        | 0.60     |
| 1:F:70:HIS:HE1   | 1:F:97:MET:SD    | 2.25        | 0.60     |
| 4:I:190:SER:O    | 4:I:192:ILE:HG23 | 2.02        | 0.60     |
| 1:A:261:VAL:HG12 | 1:A:266:LEU:HD11 | 1.83        | 0.60     |
| 1:A:189:MET:SD   | 1:A:201:LEU:HD22 | 2.42        | 0.60     |
| 1:F:81:ALA:HB1   | 1:F:118:TYR:CE2  | 2.37        | 0.60     |
| 5:E:49:SER:CB    | 5:E:68:ARG:HD3   | 2.32        | 0.59     |
| 2:G:45:ARG:HB2   | 2:G:81:ARG:HH22  | 1.66        | 0.59     |
| 1:F:117:ALA:HB2  | 2:G:60:TRP:CD2   | 2.37        | 0.59     |
| 5:J:200:ASN:ND2  | 5:J:202:ARG:HB3  | 2.16        | 0.59     |
| 2:B:24:ASN:H     | 2:B:24:ASN:ND2   | 1.99        | 0.59     |
| 1:A:33:PHE:CD1   | 1:A:34:VAL:HG13  | 2.37        | 0.59     |
| 4:D:71:TYR:C     | 4:D:71:TYR:HD2   | 2.04        | 0.59     |
| 5:E:82:SER:HB2   | 5:E:85:GLN:HG3   | 1.84        | 0.59     |
| 1:A:104:GLY:N    | 1:A:110:LEU:HD13 | 2.18        | 0.59     |
| 4:D:94:GLN:HB3   | 4:D:97:LYS:CE    | 2.32        | 0.59     |
| 1:A:25:VAL:HB    | 1:A:32:GLN:NE2   | 2.13        | 0.59     |
| 5:J:230:GLN:NE2  | 5:J:232:VAL:HG22 | 2.17        | 0.59     |
| 5:E:82:SER:O     | 5:E:110:VAL:HG21 | 2.02        | 0.59     |
| 2:G:21:ASN:HB3   | 2:G:70:PHE:CE1   | 2.38        | 0.59     |
| 1:F:259:CYS:HB3  | 1:F:272:LEU:HB2  | 1.83        | 0.59     |
| 2:B:17:ASN:HA    | 2:B:72:PRO:O     | 2.02        | 0.59     |
| 5:E:39:PRO:O     | 5:E:41:LEU:HD22  | 2.03        | 0.59     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:F:36:PHE:HB2   | 1:F:45:MET:CE    | 2.33        | 0.59     |
| 1:F:152:VAL:HA   | 1:F:155:GLN:HG3  | 1.84        | 0.59     |
| 4:I:13:VAL:HG13  | 4:I:14:PRO:HD2   | 1.85        | 0.59     |
| 5:J:41:LEU:HB3   | 5:J:44:ARG:CZ    | 2.32        | 0.59     |
| 4:I:93:ASN:O     | 4:I:95:GLY:N     | 2.35        | 0.59     |
| 4:I:6:GLN:NE2    | 4:I:102:GLN:HB2  | 2.18        | 0.59     |
| 3:C:5:THR:HA     | 3:C:8:TRP:CZ3    | 2.36        | 0.59     |
| 5:E:11:LEU:CD2   | 5:E:19:LEU:HD22  | 2.32        | 0.59     |
| 4:D:14:PRO:HB2   | 4:I:71:TYR:OH    | 2.02        | 0.59     |
| 2:B:39:LEU:HD12  | 2:B:49:VAL:CG2   | 2.33        | 0.59     |
| 1:F:273:ARG:HH11 | 1:F:273:ARG:HG3  | 1.68        | 0.59     |
| 2:B:21:ASN:ND2   | 2:B:22:PHE:H     | 2.01        | 0.59     |
| 4:D:89:TRP:HZ3   | 4:D:91:THR:HG21  | 1.67        | 0.59     |
| 1:A:152:VAL:CG1  | 1:A:156:GLN:NE2  | 2.66        | 0.58     |
| 5:J:230:GLN:HE21 | 5:J:232:VAL:HG22 | 1.67        | 0.58     |
| 1:F:268:LYS:HD2  | 1:F:269:PRO:CD   | 2.31        | 0.58     |
| 5:J:138:ALA:O    | 5:J:192:ARG:HA   | 2.02        | 0.58     |
| 5:E:198:TRP:CZ2  | 5:E:239:ARG:HB3  | 2.38        | 0.58     |
| 4:D:148:LYS:CD   | 4:D:189:ASN:OD1  | 2.51        | 0.58     |
| 1:F:181:ARG:NH1  | 1:F:181:ARG:HG2  | 2.18        | 0.58     |
| 4:D:152:VAL:HG13 | 4:D:152:VAL:O    | 2.03        | 0.58     |
| 4:I:161:ASP:CB   | 4:I:168:LYS:HE2  | 2.26        | 0.58     |
| 5:E:138:ALA:O    | 5:E:192:ARG:HA   | 2.03        | 0.58     |
| 5:E:154:LEU:HD23 | 5:E:154:LEU:C    | 2.23        | 0.58     |
| 1:F:54:GLN:OE1   | 1:F:174:ASN:ND2  | 2.36        | 0.58     |
| 4:I:74:LEU:HG    | 4:I:75:LEU:N     | 2.18        | 0.58     |
| 1:A:242:GLN:HE22 | 2:B:10:TYR:HD2   | 1.51        | 0.58     |
| 5:J:132:ILE:HG23 | 5:J:195:ALA:HB1  | 1.86        | 0.58     |
| 5:E:217:ASN:HD22 | 5:E:217:ASN:N    | 1.99        | 0.58     |
| 5:J:6:GLN:OE1    | 5:J:91:CYS:N     | 2.35        | 0.58     |
| 2:G:23:LEU:HG    | 2:G:70:PHE:CE1   | 2.39        | 0.58     |
| 1:F:244:TRP:C    | 1:F:244:TRP:HE3  | 2.07        | 0.58     |
| 4:I:155:THR:CG2  | 4:I:173:VAL:H    | 2.16        | 0.58     |
| 1:F:5:MET:O      | 1:F:6:ARG:HD3    | 2.03        | 0.58     |
| 1:A:98:MET:O     | 1:A:114:HIS:HA   | 2.03        | 0.58     |
| 5:E:101:TYR:HD2  | 5:E:101:TYR:N    | 2.01        | 0.58     |
| 1:A:231:VAL:O    | 1:A:243:LYS:CE   | 2.52        | 0.58     |
| 4:I:93:ASN:C     | 4:I:95:GLY:H     | 2.07        | 0.58     |
| 5:J:132:ILE:HD12 | 5:J:132:ILE:N    | 2.18        | 0.58     |
| 4:I:163:ARG:HG2  | 5:J:165:SER:OG   | 2.03        | 0.58     |
| 4:D:94:GLN:HB2   | 4:D:97:LYS:HG3   | 1.85        | 0.58     |
| 1:A:157:ARG:HA   | 1:A:160:LEU:HD12 | 1.86        | 0.58     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:24:ASN:H     | 2:B:24:ASN:HD22  | 1.52        | 0.58     |
| 2:B:57:SER:O     | 2:B:59:ASP:O     | 2.22        | 0.58     |
| 5:E:20:THR:O     | 5:E:20:THR:HG23  | 2.04        | 0.58     |
| 2:G:11:SER:HB2   | 2:G:21:ASN:OD1   | 2.03        | 0.58     |
| 4:D:93:ASN:O     | 4:D:95:GLY:N     | 2.36        | 0.58     |
| 5:J:126:GLU:HA   | 5:J:140:LEU:HD23 | 1.84        | 0.58     |
| 1:F:142:ILE:O    | 1:F:146:LYS:HG3  | 2.04        | 0.58     |
| 1:A:5:MET:SD     | 1:A:171:TYR:HE2  | 2.27        | 0.58     |
| 2:B:1:ILE:HD12   | 2:B:1:ILE:O      | 2.03        | 0.58     |
| 4:I:121:GLN:HB2  | 4:I:183:CYS:SG   | 2.43        | 0.58     |
| 3:H:2:PHE:CG     | 3:H:3:PRO:HD2    | 2.39        | 0.57     |
| 1:A:6:ARG:HG2    | 1:A:6:ARG:HH11   | 1.70        | 0.57     |
| 4:I:162:MET:HE1  | 5:J:192:ARG:HB3  | 1.86        | 0.57     |
| 1:F:233:THR:OG1  | 1:F:243:LYS:HD2  | 2.04        | 0.57     |
| 5:E:37:GLN:HG3   | 5:E:43:LEU:CD1   | 2.34        | 0.57     |
| 4:D:31:GLN:HB3   | 4:D:67:LYS:HZ1   | 1.67        | 0.57     |
| 1:A:117:ALA:HB2  | 2:B:60:TRP:CD2   | 2.39        | 0.57     |
| 1:A:255:GLN:O    | 1:A:273:ARG:HD3  | 2.03        | 0.57     |
| 4:I:94:GLN:HB2   | 4:I:99:ILE:HD11  | 1.87        | 0.57     |
| 5:J:108:LEU:HD12 | 5:J:108:LEU:O    | 2.05        | 0.57     |
| 2:B:83:ASN:HD22  | 2:B:84:HIS:N     | 2.02        | 0.57     |
| 5:E:118:PHE:CE1  | 5:E:224:ARG:CZ   | 2.87        | 0.57     |
| 4:D:149:ASP:HB3  | 4:D:152:VAL:CG1  | 2.35        | 0.57     |
| 4:I:97:LYS:HE3   | 5:J:48:TYR:CE2   | 2.38        | 0.57     |
| 4:I:182:ALA:O    | 4:I:185:ASN:ND2  | 2.37        | 0.57     |
| 4:I:11:LEU:HD12  | 4:I:12:SER:H     | 1.69        | 0.57     |
| 1:A:227:ASP:O    | 1:A:248:VAL:HG23 | 2.03        | 0.57     |
| 1:A:200:THR:CG2  | 1:A:202:ARG:NH1  | 2.65        | 0.57     |
| 5:J:135:THR:O    | 5:J:136:GLN:HB2  | 2.04        | 0.57     |
| 4:D:158:CYS:HB3  | 5:E:190:ARG:NH1  | 2.19        | 0.57     |
| 5:E:118:PHE:HE1  | 5:E:224:ARG:CZ   | 2.17        | 0.57     |
| 4:D:131:SER:HB2  | 4:D:181:PHE:CE2  | 2.40        | 0.57     |
| 5:J:206:ARG:HH11 | 5:J:233:SER:HB3  | 1.70        | 0.57     |
| 2:B:23:LEU:HD11  | 2:B:39:LEU:CD2   | 2.34        | 0.57     |
| 4:I:122:LEU:CD1  | 5:J:141:VAL:HB   | 2.33        | 0.57     |
| 5:E:37:GLN:HG2   | 5:E:42:GLY:C     | 2.26        | 0.57     |
| 3:H:3:PRO:O      | 3:H:5:THR:HG23   | 2.04        | 0.57     |
| 5:J:9:ARG:HH11   | 5:J:9:ARG:CB     | 2.18        | 0.57     |
| 4:I:50:ILE:O     | 4:I:50:ILE:HG13  | 2.04        | 0.57     |
| 1:A:68:LYS:HE3   | 5:E:53:GLU:O     | 2.05        | 0.57     |
| 1:F:130:LEU:HD13 | 1:F:160:LEU:HD12 | 1.87        | 0.57     |
| 5:E:135:THR:HG21 | 5:E:192:ARG:NH1  | 2.20        | 0.57     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:D:158:CYS:CB   | 5:E:190:ARG:NH1  | 2.68        | 0.57     |
| 5:E:23:CYS:HB2   | 5:E:34:TRP:HZ2   | 1.70        | 0.57     |
| 4:I:11:LEU:HD12  | 4:I:12:SER:N     | 2.19        | 0.57     |
| 4:I:78:ASP:OD1   | 4:I:80:GLN:NE2   | 2.38        | 0.56     |
| 4:D:123:ARG:HB3  | 5:E:126:GLU:HB2  | 1.87        | 0.56     |
| 1:F:156:GLN:OE1  | 3:H:8:TRP:HH2    | 1.88        | 0.56     |
| 5:J:206:ARG:NH1  | 5:J:233:SER:CB   | 2.64        | 0.56     |
| 4:I:53:ASN:C     | 4:I:53:ASN:HD22  | 2.09        | 0.56     |
| 1:A:147:TRP:CE3  | 1:A:152:VAL:HG11 | 2.40        | 0.56     |
| 4:D:94:GLN:CG    | 4:D:97:LYS:HE2   | 2.34        | 0.56     |
| 5:E:30:GLU:O     | 5:E:68:ARG:NH2   | 2.38        | 0.56     |
| 5:J:154:LEU:CD2  | 5:J:155:SER:H    | 2.18        | 0.56     |
| 5:J:170:ASP:OD1  | 5:J:190:ARG:NH2  | 2.39        | 0.56     |
| 1:A:33:PHE:CE1   | 1:A:34:VAL:HG22  | 2.40        | 0.56     |
| 1:A:35:ARG:HH12  | 1:A:48:ARG:CZ    | 2.18        | 0.56     |
| 2:B:56:PHE:C     | 2:B:63:TYR:CE2   | 2.79        | 0.56     |
| 1:A:103:VAL:C    | 1:A:110:LEU:HD22 | 2.26        | 0.56     |
| 4:I:177:ASN:HD22 | 4:I:178:LYS:N    | 2.03        | 0.56     |
| 1:F:143:THR:HA   | 1:F:146:LYS:HD3  | 1.88        | 0.56     |
| 4:D:48:MET:HE3   | 4:D:63:ALA:H     | 1.69        | 0.56     |
| 4:I:22:ASN:N     | 4:I:22:ASN:OD1   | 2.38        | 0.56     |
| 1:F:120:GLY:HA3  | 2:G:31:HIS:NE2   | 2.20        | 0.56     |
| 1:A:234:ARG:HG3  | 1:A:242:GLN:HG3  | 1.87        | 0.56     |
| 4:I:122:LEU:HD12 | 4:I:132:VAL:HB   | 1.87        | 0.56     |
| 1:F:7:TYR:HE2    | 3:H:2:PHE:N      | 2.04        | 0.56     |
| 5:J:230:GLN:NE2  | 5:J:232:VAL:HG13 | 2.16        | 0.56     |
| 1:A:209:TYR:HD1  | 1:A:241:PHE:CE1  | 2.22        | 0.56     |
| 4:D:167:PHE:HD2  | 4:D:168:LYS:H    | 1.52        | 0.56     |
| 2:B:57:SER:N     | 2:B:63:TYR:HE2   | 2.02        | 0.56     |
| 4:I:35:TRP:CB    | 4:I:47:ILE:HD11  | 2.35        | 0.56     |
| 4:I:149:ASP:HB3  | 4:I:152:VAL:HG12 | 1.86        | 0.56     |
| 1:F:254:GLU:OE2  | 1:F:274:TRP:HD1  | 1.89        | 0.56     |
| 4:I:176:SER:HB3  | 4:I:181:PHE:CG   | 2.41        | 0.56     |
| 1:F:33:PHE:CE2   | 1:F:34:VAL:HG22  | 2.40        | 0.56     |
| 1:F:117:ALA:HB2  | 2:G:60:TRP:CE2   | 2.40        | 0.56     |
| 4:I:167:PHE:C    | 4:I:167:PHE:CD2  | 2.79        | 0.56     |
| 1:F:244:TRP:HE1  | 2:G:99:MET:CG    | 2.18        | 0.56     |
| 1:A:108:ARG:HH22 | 4:I:114:ASN:HB2  | 1.70        | 0.56     |
| 1:F:141:GLN:O    | 1:F:145:ARG:HG3  | 2.04        | 0.56     |
| 1:F:233:THR:HG23 | 1:F:243:LYS:CB   | 2.34        | 0.56     |
| 4:D:89:TRP:CZ2   | 4:D:101:GLY:HA3  | 2.40        | 0.56     |
| 4:D:197:PHE:CZ   | 4:D:199:PRO:HA   | 2.40        | 0.56     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:J:38:ASP:HB2   | 5:J:44:ARG:HH22  | 1.71        | 0.56     |
| 5:J:49:SER:OG    | 5:J:68:ARG:HG2   | 2.06        | 0.56     |
| 5:E:180:LEU:HD12 | 5:E:180:LEU:N    | 2.21        | 0.56     |
| 5:J:120:PRO:HB3  | 5:J:147:PHE:CD2  | 2.41        | 0.56     |
| 4:D:93:ASN:C     | 4:D:95:GLY:H     | 2.10        | 0.56     |
| 5:E:143:LEU:HD12 | 5:E:188:SER:HB3  | 1.87        | 0.56     |
| 5:J:127:PRO:HD2  | 5:J:198:TRP:CZ2  | 2.41        | 0.56     |
| 2:G:5:PRO:HD3    | 2:G:84:HIS:HD2   | 1.71        | 0.56     |
| 4:I:38:GLN:HE22  | 5:J:37:GLN:HE21  | 1.52        | 0.56     |
| 5:J:64:TYR:HB3   | 5:J:76:LEU:HD11  | 1.88        | 0.56     |
| 1:A:235:PRO:HG2  | 2:B:65:LEU:CD1   | 2.35        | 0.56     |
| 1:F:249:VAL:HG22 | 1:F:257:TYR:CD1  | 2.40        | 0.56     |
| 2:B:80:CYS:O     | 2:B:92:ILE:HA    | 2.06        | 0.56     |
| 5:E:48:TYR:CZ    | 5:E:56:ASP:HB2   | 2.42        | 0.55     |
| 1:A:202:ARG:HG3  | 1:A:246:ALA:HB2  | 1.88        | 0.55     |
| 5:J:211:PHE:CE2  | 5:J:213:GLY:HA3  | 2.41        | 0.55     |
| 1:F:14:ARG:CZ    | 1:F:21:ARG:HB2   | 2.37        | 0.55     |
| 1:A:97:MET:CE    | 1:A:99:PHE:HB2   | 2.36        | 0.55     |
| 4:D:91:THR:HG23  | 4:D:93:ASN:ND2   | 2.21        | 0.55     |
| 4:I:77:ARG:HG3   | 4:I:77:ARG:HH11  | 1.71        | 0.55     |
| 1:F:244:TRP:HE1  | 2:G:99:MET:HG3   | 1.72        | 0.55     |
| 1:A:14:ARG:NH2   | 1:A:19:GLU:O     | 2.37        | 0.55     |
| 4:I:123:ARG:HD3  | 5:J:126:GLU:OE2  | 2.06        | 0.55     |
| 5:J:200:ASN:O    | 5:J:238:GLY:HA3  | 2.06        | 0.55     |
| 2:B:10:TYR:N     | 2:B:10:TYR:CD1   | 2.75        | 0.55     |
| 5:J:36:ARG:NE    | 5:J:87:SER:CB    | 2.70        | 0.55     |
| 5:E:132:ILE:HG21 | 5:E:199:GLN:HE22 | 1.72        | 0.55     |
| 5:E:118:PHE:HB3  | 5:E:184:ARG:NH2  | 2.21        | 0.55     |
| 1:A:96:GLN:OE1   | 2:B:60:TRP:HB3   | 2.06        | 0.55     |
| 1:F:227:ASP:O    | 1:F:248:VAL:HG23 | 2.07        | 0.55     |
| 1:F:115:GLN:CG   | 2:G:60:TRP:HH2   | 2.19        | 0.55     |
| 4:I:160:LEU:HB3  | 5:J:168:CYS:HB2  | 1.89        | 0.55     |
| 1:F:218:GLN:HB2  | 1:F:258:THR:OG1  | 2.07        | 0.55     |
| 4:D:38:GLN:NE2   | 4:D:42:LYS:O     | 2.39        | 0.55     |
| 1:A:55:GLU:O     | 1:A:60:TRP:CZ2   | 2.60        | 0.55     |
| 4:I:50:ILE:CD1   | 4:I:65:LEU:HD22  | 2.36        | 0.55     |
| 1:A:123:TYR:CZ   | 1:A:140:ALA:HA   | 2.41        | 0.55     |
| 1:F:19:GLU:CG    | 1:F:75:ARG:HE    | 2.15        | 0.55     |
| 4:D:112:ILE:CG1  | 4:D:170:ASN:HD21 | 2.18        | 0.55     |
| 1:A:156:GLN:O    | 1:A:160:LEU:CD2  | 2.54        | 0.55     |
| 5:J:205:PHE:HD2  | 5:J:236:ALA:O    | 1.88        | 0.55     |
| 5:J:126:GLU:HA   | 5:J:140:LEU:CD2  | 2.36        | 0.55     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:D:39:TYR:CE1   | 4:D:85:ALA:HB2   | 2.41        | 0.55     |
| 5:J:27:MET:O     | 5:J:28:ASN:HB3   | 2.07        | 0.55     |
| 5:E:77:ILE:C     | 5:E:78:LEU:HD12  | 2.27        | 0.55     |
| 2:B:21:ASN:CG    | 2:B:22:PHE:N     | 2.59        | 0.55     |
| 1:A:224:GLN:O    | 1:A:228:THR:HG21 | 2.06        | 0.55     |
| 5:E:124:VAL:HG23 | 5:E:234:ALA:HB3  | 1.88        | 0.55     |
| 4:D:167:PHE:CD1  | 5:E:137:LYS:HE3  | 2.41        | 0.55     |
| 1:F:259:CYS:O    | 1:F:272:LEU:HD12 | 2.07        | 0.55     |
| 1:F:215:LEU:HD21 | 1:F:261:VAL:HG13 | 1.88        | 0.55     |
| 4:I:30:SER:HA    | 4:I:93:ASN:OD1   | 2.07        | 0.55     |
| 4:I:50:ILE:HD13  | 4:I:65:LEU:HD22  | 1.89        | 0.55     |
| 2:G:5:PRO:HD3    | 2:G:84:HIS:CD2   | 2.42        | 0.55     |
| 1:F:168:LEU:O    | 1:F:168:LEU:HD12 | 2.06        | 0.55     |
| 4:D:27:ASP:O     | 4:D:30:SER:OG    | 2.14        | 0.54     |
| 2:B:23:LEU:HD12  | 2:B:24:ASN:N     | 2.22        | 0.54     |
| 1:A:83:ARG:NH1   | 1:A:84:TYR:CE1   | 2.74        | 0.54     |
| 5:E:170:ASP:HB2  | 5:E:187:LEU:CD1  | 2.35        | 0.54     |
| 5:E:127:PRO:HG3  | 5:E:139:THR:O    | 2.07        | 0.54     |
| 2:G:10:TYR:CD1   | 2:G:10:TYR:N     | 2.75        | 0.54     |
| 5:E:131:GLU:HG2  | 5:E:137:LYS:O    | 2.07        | 0.54     |
| 4:D:2:LYS:NZ     | 5:E:43:LEU:H     | 2.04        | 0.54     |
| 5:E:49:SER:HB3   | 5:E:68:ARG:HH11  | 1.72        | 0.54     |
| 1:F:115:GLN:HG3  | 2:G:60:TRP:CZ2   | 2.42        | 0.54     |
| 1:A:231:VAL:O    | 1:A:243:LYS:NZ   | 2.40        | 0.54     |
| 4:I:36:TYR:OH    | 5:J:100:GLN:HB2  | 2.08        | 0.54     |
| 1:A:152:VAL:HG12 | 1:A:156:GLN:NE2  | 2.20        | 0.54     |
| 2:G:79:ALA:HB2   | 2:G:94:LYS:HA    | 1.89        | 0.54     |
| 1:A:157:ARG:HA   | 1:A:160:LEU:HD11 | 1.88        | 0.54     |
| 4:I:159:VAL:HG12 | 4:I:168:LYS:HZ1  | 1.70        | 0.54     |
| 5:J:172:GLN:OE1  | 5:J:173:PRO:HD2  | 2.06        | 0.54     |
| 5:J:25:GLN:NE2   | 5:J:29:HIS:H     | 2.05        | 0.54     |
| 1:F:35:ARG:C     | 1:F:35:ARG:HD2   | 2.28        | 0.54     |
| 2:G:31:HIS:CE1   | 2:G:60:TRP:O     | 2.59        | 0.54     |
| 4:I:185:ASN:HD22 | 4:I:186:ALA:N    | 2.05        | 0.54     |
| 5:E:211:PHE:HD2  | 5:E:230:GLN:HG2  | 1.73        | 0.54     |
| 3:C:4:LEU:HB3    | 3:C:6:PHE:HE2    | 1.71        | 0.54     |
| 5:J:38:ASP:N     | 5:J:44:ARG:HH22  | 2.05        | 0.54     |
| 1:F:45:MET:HG3   | 1:F:60:TRP:CZ3   | 2.38        | 0.54     |
| 4:I:160:LEU:HD11 | 4:I:167:PHE:CE2  | 2.35        | 0.54     |
| 4:I:122:LEU:HD11 | 5:J:141:VAL:HB   | 1.90        | 0.54     |
| 5:J:41:LEU:CB    | 5:J:44:ARG:CZ    | 2.86        | 0.54     |
| 5:J:49:SER:OG    | 5:J:68:ARG:NH1   | 2.40        | 0.54     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:56:PHE:CB    | 2:B:61:SER:O     | 2.56        | 0.54     |
| 1:A:108:ARG:NH2  | 4:I:114:ASN:CB   | 2.70        | 0.54     |
| 5:E:118:PHE:CE1  | 5:E:224:ARG:NH2  | 2.75        | 0.54     |
| 4:D:133:CYS:SG   | 4:D:181:PHE:CE1  | 3.01        | 0.54     |
| 4:D:23:CYS:HB2   | 4:D:72:VAL:CG1   | 2.38        | 0.54     |
| 5:J:153:GLU:HG2  | 5:J:212:TYR:HE2  | 1.73        | 0.54     |
| 4:I:191:ILE:O    | 4:I:191:ILE:HG13 | 2.08        | 0.54     |
| 2:G:45:ARG:HH21  | 2:G:81:ARG:HH12  | 1.55        | 0.54     |
| 5:E:168:CYS:O    | 5:E:190:ARG:CD   | 2.56        | 0.54     |
| 4:I:32:SER:HG    | 4:I:51:TYR:HE1   | 1.55        | 0.54     |
| 4:D:149:ASP:HB3  | 4:D:152:VAL:HG11 | 1.90        | 0.54     |
| 1:F:235:PRO:HG2  | 2:G:65:LEU:HD13  | 1.89        | 0.54     |
| 4:D:50:ILE:HD11  | 4:D:65:LEU:CB    | 2.38        | 0.54     |
| 1:A:83:ARG:HH11  | 1:A:83:ARG:HG2   | 1.72        | 0.54     |
| 4:D:187:PHE:O    | 4:D:190:SER:OG   | 2.26        | 0.54     |
| 1:A:68:LYS:CE    | 5:E:53:GLU:O     | 2.56        | 0.53     |
| 2:B:35:ILE:HG12  | 2:B:37:VAL:HG23  | 1.89        | 0.53     |
| 4:I:178:LYS:HG2  | 4:I:180:ASP:HB2  | 1.88        | 0.53     |
| 4:I:162:MET:HE2  | 5:J:192:ARG:HB3  | 1.87        | 0.53     |
| 1:A:75:ARG:HH11  | 1:A:79:ARG:HE    | 1.56        | 0.53     |
| 4:D:89:TRP:CE2   | 4:D:101:GLY:HA3  | 2.44        | 0.53     |
| 4:I:80:GLN:HB2   | 4:I:83:ASP:OD2   | 2.07        | 0.53     |
| 1:F:191:HIS:HB3  | 1:F:274:TRP:CH2  | 2.43        | 0.53     |
| 3:C:3:PRO:HG2    | 3:C:5:THR:HG23   | 1.90        | 0.53     |
| 5:J:38:ASP:N     | 5:J:44:ARG:NH2   | 2.53        | 0.53     |
| 4:I:178:LYS:HG2  | 4:I:180:ASP:H    | 1.73        | 0.53     |
| 4:D:94:GLN:HB3   | 4:D:97:LYS:HE2   | 1.88        | 0.53     |
| 1:A:26:GLY:CA    | 1:A:33:PHE:CE1   | 2.89        | 0.53     |
| 4:D:123:ARG:NH1  | 5:E:239:ARG:NE   | 2.57        | 0.53     |
| 1:A:154:GLU:HG3  | 4:D:51:TYR:CD2   | 2.43        | 0.53     |
| 5:E:35:TYR:HA    | 5:E:46:ILE:CD1   | 2.37        | 0.53     |
| 1:F:99:PHE:CE2   | 3:H:3:PRO:HG3    | 2.43        | 0.53     |
| 1:A:215:LEU:HD12 | 1:A:243:LYS:CD   | 2.37        | 0.53     |
| 5:E:117:VAL:HG12 | 5:E:227:PRO:HB2  | 1.89        | 0.53     |
| 1:A:123:TYR:CD2  | 1:A:124:ILE:HG22 | 2.44        | 0.53     |
| 5:E:11:LEU:HD23  | 5:E:19:LEU:HD22  | 1.91        | 0.53     |
| 4:I:66:ASN:OD1   | 4:I:69:SER:N     | 2.31        | 0.53     |
| 2:B:39:LEU:HD12  | 2:B:49:VAL:HG21  | 1.91        | 0.53     |
| 4:D:62:THR:O     | 4:D:75:LEU:HD12  | 2.09        | 0.53     |
| 4:D:111:ASN:OD1  | 4:I:68:ALA:HB3   | 2.09        | 0.53     |
| 1:A:176:LYS:HD2  | 1:A:180:GLN:NE2  | 2.23        | 0.53     |
| 2:B:41:LYS:HA    | 2:B:78:TYR:HD2   | 1.74        | 0.53     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:E:32:MET:SD    | 5:E:71:LYS:O     | 2.66        | 0.53     |
| 1:A:208:PHE:CE2  | 1:A:241:PHE:HB2  | 2.44        | 0.53     |
| 5:E:167:VAL:HA   | 5:E:190:ARG:O    | 2.09        | 0.53     |
| 2:B:56:PHE:CD2   | 2:B:62:PHE:CE2   | 2.97        | 0.53     |
| 4:I:178:LYS:HE3  | 4:I:180:ASP:CB   | 2.37        | 0.53     |
| 5:E:97:SER:OG    | 5:E:98:HIS:N     | 2.33        | 0.53     |
| 5:J:47:TYR:CD1   | 5:J:66:VAL:HG22  | 2.43        | 0.53     |
| 5:J:132:ILE:HG23 | 5:J:195:ALA:CB   | 2.38        | 0.53     |
| 1:F:226:GLN:O    | 1:F:227:ASP:HB2  | 2.08        | 0.53     |
| 5:E:220:TRP:CH2  | 5:E:222:GLN:HG3  | 2.43        | 0.53     |
| 1:F:98:MET:O     | 1:F:114:HIS:HA   | 2.08        | 0.53     |
| 5:J:64:TYR:CD1   | 5:J:78:LEU:HD13  | 2.44        | 0.53     |
| 5:E:37:GLN:HB2   | 5:E:43:LEU:HD12  | 1.90        | 0.53     |
| 4:D:96:GLY:HA3   | 5:E:50:MET:CE    | 2.39        | 0.53     |
| 1:F:70:HIS:ND1   | 3:H:2:PHE:HZ     | 2.01        | 0.53     |
| 1:A:242:GLN:OE1  | 2:B:10:TYR:CE2   | 2.61        | 0.53     |
| 4:D:88:LEU:H     | 4:D:88:LEU:HD23  | 1.73        | 0.53     |
| 4:I:50:ILE:C     | 4:I:50:ILE:CD1   | 2.72        | 0.52     |
| 4:D:114:ASN:CB   | 1:F:108:ARG:HH22 | 2.20        | 0.52     |
| 1:F:35:ARG:HD2   | 1:F:36:PHE:N     | 2.24        | 0.52     |
| 1:F:96:GLN:NE2   | 2:G:56:PHE:CD2   | 2.77        | 0.52     |
| 4:I:46:LEU:HD11  | 5:J:99:GLU:HG2   | 1.92        | 0.52     |
| 4:D:182:ALA:HB3  | 4:D:185:ASN:ND2  | 2.25        | 0.52     |
| 5:J:25:GLN:NE2   | 5:J:29:HIS:HB2   | 2.25        | 0.52     |
| 3:H:9:CYS:SG     | 5:J:30:GLU:OE1   | 2.67        | 0.52     |
| 4:D:94:GLN:HB2   | 4:D:99:ILE:HD11  | 1.92        | 0.52     |
| 4:I:88:LEU:N     | 4:I:88:LEU:CD2   | 2.63        | 0.52     |
| 1:A:8:PHE:HB2    | 1:A:25:VAL:HG22  | 1.92        | 0.52     |
| 4:I:120:TYR:CE1  | 5:J:131:GLU:CA   | 2.90        | 0.52     |
| 1:F:231:VAL:HG22 | 1:F:244:TRP:O    | 2.09        | 0.52     |
| 4:D:123:ARG:CZ   | 5:E:239:ARG:CZ   | 2.87        | 0.52     |
| 4:I:132:VAL:HG23 | 5:J:125:PHE:CE1  | 2.44        | 0.52     |
| 1:A:15:PRO:HG2   | 1:A:91:GLY:O     | 2.09        | 0.52     |
| 4:D:72:VAL:O     | 4:D:72:VAL:HG13  | 2.08        | 0.52     |
| 1:A:130:LEU:CB   | 1:A:157:ARG:HG3  | 2.39        | 0.52     |
| 1:A:66:LYS:HG3   | 5:E:50:MET:CE    | 2.40        | 0.52     |
| 5:J:41:LEU:HB3   | 5:J:44:ARG:NH1   | 2.24        | 0.52     |
| 5:E:132:ILE:H    | 5:E:132:ILE:HD12 | 1.73        | 0.52     |
| 4:D:69:SER:O     | 4:D:70:GLN:HB2   | 2.10        | 0.52     |
| 1:F:155:GLN:O    | 4:I:31:GLN:NE2   | 2.42        | 0.52     |
| 5:J:200:ASN:HD22 | 5:J:203:ASN:CG   | 2.13        | 0.52     |
| 5:J:167:VAL:HA   | 5:J:190:ARG:O    | 2.09        | 0.52     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:55:GLU:CB    | 1:A:59:TYR:CD2   | 2.93        | 0.52     |
| 4:D:153:TYR:HB2  | 4:D:175:TRP:CE2  | 2.45        | 0.52     |
| 1:F:190:THR:O    | 1:F:201:LEU:HD23 | 2.09        | 0.52     |
| 1:F:72:GLN:O     | 1:F:72:GLN:OE1   | 2.28        | 0.52     |
| 1:A:133:TRP:HZ2  | 1:A:152:VAL:HB   | 1.74        | 0.52     |
| 3:C:6:PHE:CD1    | 5:E:31:TYR:HB2   | 2.45        | 0.52     |
| 2:G:96:ASP:HB3   | 2:G:99:MET:HA    | 1.91        | 0.52     |
| 5:E:37:GLN:CB    | 5:E:43:LEU:HD12  | 2.39        | 0.52     |
| 5:E:135:THR:HG21 | 5:E:192:ARG:HH12 | 1.74        | 0.52     |
| 5:E:135:THR:HG22 | 5:E:137:LYS:CG   | 2.35        | 0.52     |
| 2:B:55:SER:OG    | 2:B:63:TYR:CE1   | 2.62        | 0.52     |
| 4:I:35:TRP:HB2   | 4:I:48:MET:HB3   | 1.91        | 0.52     |
| 2:G:1:ILE:O      | 2:G:1:ILE:HD12   | 2.10        | 0.52     |
| 1:A:123:TYR:HD2  | 1:A:124:ILE:HG22 | 1.75        | 0.52     |
| 1:A:130:LEU:HB3  | 1:A:157:ARG:HG3  | 1.91        | 0.52     |
| 5:E:9:ARG:HH12   | 5:E:104:PRO:C    | 2.12        | 0.52     |
| 4:D:39:TYR:OH    | 4:D:82:SER:O     | 2.18        | 0.52     |
| 5:J:83:PRO:HA    | 5:J:110:VAL:HB   | 1.92        | 0.52     |
| 1:A:160:LEU:O    | 1:A:165:VAL:HG22 | 2.09        | 0.52     |
| 5:J:41:LEU:CB    | 5:J:44:ARG:NH1   | 2.72        | 0.52     |
| 1:F:95:LEU:HD12  | 1:F:117:ALA:O    | 2.10        | 0.52     |
| 5:J:206:ARG:HB3  | 5:J:206:ARG:CZ   | 2.39        | 0.52     |
| 4:I:53:ASN:ND2   | 4:I:65:LEU:O     | 2.43        | 0.52     |
| 5:E:37:GLN:HG2   | 5:E:42:GLY:O     | 2.10        | 0.52     |
| 4:D:53:ASN:HD21  | 4:D:67:LYS:HB2   | 1.74        | 0.52     |
| 2:G:13:HIS:N     | 2:G:21:ASN:HD21  | 2.08        | 0.52     |
| 2:B:57:SER:N     | 2:B:63:TYR:CE2   | 2.78        | 0.52     |
| 2:G:19:LYS:O     | 2:G:72:PRO:HD2   | 2.09        | 0.52     |
| 5:J:70:GLU:HG3   | 5:J:73:ASN:H     | 1.74        | 0.51     |
| 4:D:3:GLU:HG3    | 4:D:4:VAL:HG12   | 1.91        | 0.51     |
| 1:A:242:GLN:NE2  | 2:B:10:TYR:CD2   | 2.78        | 0.51     |
| 1:A:209:TYR:CD1  | 1:A:210:PRO:HA   | 2.44        | 0.51     |
| 5:E:161:LYS:HB2  | 5:E:161:LYS:HZ2  | 1.75        | 0.51     |
| 4:I:33:PHE:O     | 4:I:50:ILE:HG23  | 2.10        | 0.51     |
| 4:I:149:ASP:O    | 4:I:152:VAL:CG1  | 2.58        | 0.51     |
| 4:I:124:ASP:HA   | 5:J:125:PHE:CE1  | 2.45        | 0.51     |
| 1:F:104:GLY:N    | 1:F:110:LEU:HD23 | 2.24        | 0.51     |
| 1:F:159:TYR:CZ   | 3:H:3:PRO:HB3    | 2.46        | 0.51     |
| 2:G:1:ILE:HD12   | 2:G:1:ILE:C      | 2.31        | 0.51     |
| 1:F:5:MET:SD     | 1:F:171:TYR:HE2  | 2.33        | 0.51     |
| 5:E:37:GLN:HG3   | 5:E:43:LEU:HD12  | 1.90        | 0.51     |
| 5:J:19:LEU:HD12  | 5:J:19:LEU:H     | 1.76        | 0.51     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:E:158:VAL:CG2  | 5:E:163:VAL:HG21 | 2.38        | 0.51     |
| 5:J:220:TRP:HH2  | 5:J:224:ARG:NH2  | 2.08        | 0.51     |
| 5:E:136:GLN:HA   | 5:E:136:GLN:OE1  | 2.10        | 0.51     |
| 5:J:131:GLU:HG2  | 5:J:137:LYS:O    | 2.10        | 0.51     |
| 4:D:157:LYS:H    | 4:D:157:LYS:CD   | 2.23        | 0.51     |
| 5:J:25:GLN:OE1   | 5:J:27:MET:N     | 2.43        | 0.51     |
| 5:E:153:GLU:HB2  | 5:E:210:GLN:HB3  | 1.92        | 0.51     |
| 5:J:49:SER:CB    | 5:J:68:ARG:HH11  | 2.24        | 0.51     |
| 4:I:14:PRO:HA    | 4:I:109:LYS:HB2  | 1.93        | 0.51     |
| 1:F:261:VAL:CG2  | 1:F:272:LEU:HD11 | 2.41        | 0.51     |
| 5:E:45:GLN:C     | 5:E:46:ILE:HD12  | 2.31        | 0.51     |
| 1:F:70:HIS:HB2   | 3:H:2:PHE:HE2    | 1.76        | 0.51     |
| 4:I:77:ARG:O     | 4:I:78:ASP:HB3   | 2.11        | 0.51     |
| 2:G:4:THR:OG1    | 2:G:5:PRO:HD2    | 2.10        | 0.51     |
| 1:F:191:HIS:CE1  | 1:F:193:PRO:HG3  | 2.45        | 0.51     |
| 4:D:131:SER:HB2  | 4:D:181:PHE:HE2  | 1.76        | 0.51     |
| 5:J:206:ARG:HH11 | 5:J:206:ARG:HG2  | 1.75        | 0.51     |
| 5:E:200:ASN:O    | 5:E:238:GLY:HA3  | 2.11        | 0.51     |
| 5:E:12:ILE:HD11  | 5:E:213:GLY:HA2  | 1.93        | 0.51     |
| 1:A:99:PHE:HD1   | 1:A:114:HIS:CD2  | 2.28        | 0.50     |
| 5:J:40:GLY:C     | 5:J:41:LEU:HD22  | 2.32        | 0.50     |
| 2:G:23:LEU:HG    | 2:G:70:PHE:CZ    | 2.46        | 0.50     |
| 5:E:187:LEU:HG   | 5:E:188:SER:N    | 2.26        | 0.50     |
| 4:I:173:VAL:HG12 | 4:I:175:TRP:CE3  | 2.45        | 0.50     |
| 5:E:47:TYR:CZ    | 5:E:57:LYS:HB3   | 2.45        | 0.50     |
| 5:E:62:GLU:HA    | 5:E:62:GLU:OE1   | 2.11        | 0.50     |
| 5:E:78:LEU:N     | 5:E:78:LEU:CD1   | 2.73        | 0.50     |
| 4:I:160:LEU:CD1  | 4:I:160:LEU:C    | 2.79        | 0.50     |
| 5:J:77:ILE:N     | 5:J:77:ILE:CD1   | 2.71        | 0.50     |
| 5:J:36:ARG:HE    | 5:J:87:SER:CB    | 2.25        | 0.50     |
| 5:J:144:ALA:O    | 5:J:147:PHE:HE2  | 1.95        | 0.50     |
| 1:F:27:TYR:CE2   | 1:F:32:GLN:N     | 2.79        | 0.50     |
| 1:F:80:ILE:HG23  | 1:F:83:ARG:NH2   | 2.26        | 0.50     |
| 5:E:4:VAL:HG11   | 5:E:91:CYS:O     | 2.11        | 0.50     |
| 1:A:22:PHE:CE1   | 1:A:71:SER:HA    | 2.46        | 0.50     |
| 5:J:47:TYR:CD1   | 5:J:66:VAL:CG2   | 2.95        | 0.50     |
| 4:I:50:ILE:O     | 4:I:50:ILE:CG1   | 2.59        | 0.50     |
| 5:J:23:CYS:HB2   | 5:J:34:TRP:CZ2   | 2.46        | 0.50     |
| 4:D:37:ARG:HB2   | 4:D:47:ILE:HD13  | 1.93        | 0.50     |
| 5:E:46:ILE:HG23  | 5:E:60:VAL:O     | 2.11        | 0.50     |
| 2:G:40:LEU:HD21  | 2:G:81:ARG:HE    | 1.76        | 0.50     |
| 5:E:96:ALA:O     | 5:E:97:SER:HB3   | 2.10        | 0.50     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:F:7:TYR:HE2    | 3:H:2:PHE:CA     | 2.25        | 0.50     |
| 1:F:10:THR:HB    | 1:F:23:ILE:CG2   | 2.31        | 0.50     |
| 1:A:75:ARG:CD    | 1:A:79:ARG:HD2   | 2.42        | 0.50     |
| 4:I:65:LEU:HD21  | 4:I:67:LYS:HG3   | 1.93        | 0.50     |
| 4:D:147:SER:CB   | 4:D:152:VAL:HG13 | 2.41        | 0.50     |
| 5:E:208:GLN:HG2  | 5:E:233:SER:OG   | 2.10        | 0.50     |
| 4:I:176:SER:HB3  | 4:I:181:PHE:CD2  | 2.46        | 0.50     |
| 5:E:77:ILE:H     | 5:E:77:ILE:HD12  | 1.77        | 0.50     |
| 2:G:40:LEU:HD21  | 2:G:81:ARG:NE    | 2.27        | 0.50     |
| 1:F:244:TRP:C    | 1:F:244:TRP:CE3  | 2.85        | 0.50     |
| 5:E:211:PHE:HB3  | 5:E:230:GLN:O    | 2.11        | 0.50     |
| 5:J:139:THR:OG1  | 5:J:192:ARG:HB2  | 2.12        | 0.50     |
| 2:B:84:HIS:HB3   | 2:B:86:THR:HG23  | 1.92        | 0.50     |
| 4:D:185:ASN:CA   | 4:D:188:ASN:ND2  | 2.75        | 0.50     |
| 5:J:70:GLU:CD    | 5:J:73:ASN:HD22  | 2.15        | 0.50     |
| 5:J:128:SER:OG   | 5:J:130:ALA:HB3  | 2.12        | 0.50     |
| 5:J:173:PRO:CA   | 5:J:187:LEU:HD13 | 2.36        | 0.50     |
| 4:I:30:SER:O     | 4:I:67:LYS:NZ    | 2.41        | 0.50     |
| 4:I:33:PHE:H     | 4:I:50:ILE:HG13  | 1.76        | 0.50     |
| 4:D:39:TYR:CD1   | 4:D:85:ALA:HB2   | 2.46        | 0.50     |
| 1:F:220:ASP:OD2  | 1:F:256:ARG:HD3  | 2.11        | 0.50     |
| 4:I:88:LEU:HB3   | 4:I:103:GLY:CA   | 2.41        | 0.50     |
| 1:F:99:PHE:HZ    | 1:F:156:GLN:CD   | 2.15        | 0.50     |
| 5:J:200:ASN:HB3  | 5:J:203:ASN:OD1  | 2.12        | 0.50     |
| 5:J:164:HIS:O    | 5:J:167:VAL:HG13 | 2.12        | 0.50     |
| 1:A:45:MET:SD    | 1:A:63:GLU:HB3   | 2.52        | 0.50     |
| 3:C:2:PHE:CG     | 3:C:3:PRO:HD2    | 2.46        | 0.49     |
| 1:A:68:LYS:HD3   | 5:E:54:VAL:HA    | 1.93        | 0.49     |
| 5:J:96:ALA:O     | 5:J:97:SER:OG    | 2.29        | 0.49     |
| 4:I:152:VAL:HG13 | 4:I:152:VAL:O    | 2.11        | 0.49     |
| 5:J:176:GLU:O    | 5:J:178:PRO:HD3  | 2.12        | 0.49     |
| 2:B:79:ALA:HB2   | 2:B:94:LYS:HA    | 1.94        | 0.49     |
| 1:A:152:VAL:HG13 | 1:A:156:GLN:HE21 | 1.77        | 0.49     |
| 1:A:159:TYR:CE2  | 1:A:163:THR:HB   | 2.46        | 0.49     |
| 1:A:156:GLN:NE2  | 3:C:8:TRP:CH2    | 2.79        | 0.49     |
| 1:A:3:HIS:HB3    | 1:A:29:ASP:OD2   | 2.12        | 0.49     |
| 1:A:75:ARG:HD3   | 1:A:75:ARG:C     | 2.32        | 0.49     |
| 5:J:36:ARG:HE    | 5:J:87:SER:HB2   | 1.77        | 0.49     |
| 2:G:23:LEU:HD21  | 2:G:95:TRP:CE3   | 2.47        | 0.49     |
| 5:E:132:ILE:CG2  | 5:E:195:ALA:HB1  | 2.40        | 0.49     |
| 5:E:140:LEU:HD12 | 5:E:140:LEU:N    | 2.27        | 0.49     |
| 1:A:2:SER:O      | 1:A:3:HIS:ND1    | 2.45        | 0.49     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:D:12:SER:HB2   | 4:D:109:LYS:CE   | 2.41        | 0.49     |
| 2:B:41:LYS:HG3   | 2:B:78:TYR:HE2   | 1.77        | 0.49     |
| 1:F:147:TRP:CD1  | 1:F:147:TRP:N    | 2.74        | 0.49     |
| 1:A:130:LEU:HD13 | 1:A:160:LEU:HD12 | 1.92        | 0.49     |
| 5:J:156:TRP:NE1  | 5:J:189:SER:OG   | 2.44        | 0.49     |
| 5:E:157:TRP:CE3  | 5:E:162:GLU:N    | 2.80        | 0.49     |
| 1:A:9:SER:OG     | 1:A:97:MET:HB3   | 2.12        | 0.49     |
| 4:I:136:THR:CG2  | 5:J:192:ARG:HH22 | 2.25        | 0.49     |
| 1:A:104:GLY:H    | 1:A:110:LEU:HD13 | 1.75        | 0.49     |
| 5:E:36:ARG:NE    | 5:E:38:ASP:OD2   | 2.46        | 0.49     |
| 4:I:161:ASP:HB2  | 4:I:168:LYS:NZ   | 2.28        | 0.49     |
| 4:I:134:LEU:HD21 | 5:J:139:THR:HG21 | 1.94        | 0.49     |
| 5:E:132:ILE:N    | 5:E:132:ILE:HD12 | 2.27        | 0.49     |
| 1:F:143:THR:HG23 | 1:F:146:LYS:HD3  | 1.93        | 0.49     |
| 4:D:139:ASP:O    | 4:D:142:THR:OG1  | 2.30        | 0.49     |
| 4:D:149:ASP:O    | 4:D:152:VAL:HG12 | 2.13        | 0.49     |
| 4:D:133:CYS:SG   | 4:D:181:PHE:CZ   | 3.06        | 0.49     |
| 5:E:72:ARG:HB2   | 5:E:73:ASN:HD22  | 1.76        | 0.49     |
| 5:J:90:PHE:CE1   | 5:J:105:GLY:HA3  | 2.48        | 0.49     |
| 5:J:147:PHE:CZ   | 5:J:186:ALA:HA   | 2.47        | 0.49     |
| 4:I:177:ASN:HD22 | 4:I:177:ASN:C    | 2.16        | 0.49     |
| 4:D:141:GLN:OE1  | 4:D:141:GLN:HA   | 2.13        | 0.49     |
| 5:J:97:SER:O     | 5:J:98:HIS:ND1   | 2.46        | 0.49     |
| 4:I:171:SER:OG   | 5:J:190:ARG:NH1  | 2.46        | 0.49     |
| 1:A:55:GLU:OE2   | 1:A:170:ARG:NH2  | 2.46        | 0.49     |
| 4:I:47:ILE:HD12  | 4:I:47:ILE:C     | 2.33        | 0.49     |
| 4:I:91:THR:O     | 4:I:91:THR:HG23  | 2.13        | 0.49     |
| 1:F:51:TRP:HE1   | 1:F:179:LEU:HD21 | 1.78        | 0.49     |
| 1:A:111:ARG:CZ   | 1:A:128:GLU:HA   | 2.43        | 0.49     |
| 2:B:92:ILE:N     | 2:B:92:ILE:HD12  | 2.28        | 0.49     |
| 5:E:32:MET:SD    | 5:E:68:ARG:NH2   | 2.85        | 0.49     |
| 5:E:107:ARG:NH1  | 5:E:151:HIS:NE2  | 2.60        | 0.49     |
| 1:F:35:ARG:NH1   | 1:F:35:ARG:HG2   | 2.26        | 0.49     |
| 3:H:4:LEU:HD21   | 4:I:96:GLY:HA2   | 1.95        | 0.49     |
| 4:D:89:TRP:CZ3   | 4:D:91:THR:HG22  | 2.48        | 0.49     |
| 1:F:272:LEU:H    | 1:F:272:LEU:HD12 | 1.77        | 0.49     |
| 1:F:143:THR:HG23 | 3:H:10:PHE:HA    | 1.95        | 0.49     |
| 5:E:51:ASN:O     | 5:E:68:ARG:HG2   | 2.13        | 0.48     |
| 2:G:54:LEU:HD12  | 2:G:55:SER:N     | 2.27        | 0.48     |
| 1:A:26:GLY:O     | 1:A:33:PHE:CD1   | 2.66        | 0.48     |
| 4:D:192:ILE:HG13 | 4:D:193:PRO:N    | 2.28        | 0.48     |
| 5:J:158:VAL:HG12 | 5:J:158:VAL:O    | 2.13        | 0.48     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:I:4:VAL:HG22   | 4:I:5:GLU:CD     | 2.33        | 0.48     |
| 2:G:12:ARG:HG2   | 2:G:13:HIS:H     | 1.78        | 0.48     |
| 4:I:147:SER:OG   | 4:I:152:VAL:O    | 2.21        | 0.48     |
| 5:J:78:LEU:HD11  | 5:J:85:GLN:NE2   | 2.28        | 0.48     |
| 1:F:202:ARG:HD3  | 1:F:244:TRP:NE1  | 2.28        | 0.48     |
| 4:I:122:LEU:HD11 | 5:J:141:VAL:CG2  | 2.42        | 0.48     |
| 4:I:47:ILE:HD12  | 4:I:48:MET:CB    | 2.43        | 0.48     |
| 1:A:106:ASP:OD1  | 1:A:108:ARG:HB2  | 2.13        | 0.48     |
| 1:F:51:TRP:CE2   | 1:F:179:LEU:HD21 | 2.48        | 0.48     |
| 2:B:7:ILE:C      | 2:B:8:GLN:HE21   | 2.17        | 0.48     |
| 4:D:30:SER:C     | 4:D:31:GLN:HG3   | 2.32        | 0.48     |
| 5:E:7:ASN:OD1    | 5:E:8:PRO:HA     | 2.13        | 0.48     |
| 2:G:10:TYR:O     | 2:G:24:ASN:ND2   | 2.46        | 0.48     |
| 2:G:81:ARG:CA    | 2:G:92:ILE:HG12  | 2.41        | 0.48     |
| 5:E:143:LEU:CD1  | 5:E:188:SER:HB3  | 2.43        | 0.48     |
| 4:D:36:TYR:CD1   | 4:D:46:LEU:HA    | 2.49        | 0.48     |
| 1:A:66:LYS:HG3   | 5:E:50:MET:HE1   | 1.95        | 0.48     |
| 3:H:8:TRP:CD1    | 3:H:8:TRP:N      | 2.78        | 0.48     |
| 4:I:167:PHE:CZ   | 4:I:169:SER:HB3  | 2.49        | 0.48     |
| 1:A:35:ARG:NH1   | 1:A:48:ARG:CD    | 2.77        | 0.48     |
| 1:F:242:GLN:O    | 1:F:243:LYS:HB2  | 2.14        | 0.48     |
| 1:A:55:GLU:HB2   | 1:A:59:TYR:CD2   | 2.49        | 0.48     |
| 4:I:46:LEU:CD2   | 5:J:99:GLU:HB3   | 2.40        | 0.48     |
| 2:B:83:ASN:HD22  | 2:B:83:ASN:C     | 2.15        | 0.48     |
| 4:D:134:LEU:HD11 | 4:D:171:SER:HB2  | 1.96        | 0.48     |
| 4:D:192:ILE:HD11 | 4:D:196:THR:HB   | 1.96        | 0.48     |
| 5:J:177:GLN:HB2  | 5:J:183:SER:HB2  | 1.95        | 0.48     |
| 1:F:108:ARG:NH1  | 1:F:108:ARG:HG3  | 2.27        | 0.48     |
| 4:I:160:LEU:C    | 4:I:168:LYS:HZ3  | 2.17        | 0.48     |
| 4:I:162:MET:HG3  | 5:J:166:GLY:HA2  | 1.96        | 0.48     |
| 4:I:77:ARG:HG3   | 4:I:77:ARG:NH1   | 2.28        | 0.48     |
| 4:I:36:TYR:CE1   | 5:J:102:PHE:CE2  | 3.02        | 0.48     |
| 1:F:213:ILE:HG13 | 1:F:263:HIS:HB2  | 1.94        | 0.48     |
| 2:G:30:PHE:O     | 2:G:62:PHE:HD1   | 1.96        | 0.48     |
| 1:A:73:THR:HG23  | 5:E:30:GLU:OE1   | 2.12        | 0.48     |
| 2:G:3:ARG:HD2    | 2:G:29:GLY:O     | 2.13        | 0.48     |
| 5:J:205:PHE:HE2  | 5:J:237:TRP:C    | 2.16        | 0.48     |
| 1:F:231:VAL:CG2  | 1:F:244:TRP:H    | 2.27        | 0.48     |
| 5:E:152:VAL:HA   | 5:E:210:GLN:O    | 2.14        | 0.48     |
| 5:J:35:TYR:CD1   | 5:J:45:GLN:HA    | 2.48        | 0.48     |
| 5:E:19:LEU:HD11  | 5:E:78:LEU:HD13  | 1.92        | 0.48     |
| 5:J:205:PHE:CE2  | 5:J:238:GLY:N    | 2.75        | 0.48     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:J:125:PHE:O    | 5:J:140:LEU:HD23 | 2.14        | 0.48     |
| 4:D:192:ILE:HD11 | 4:D:196:THR:HG21 | 1.96        | 0.48     |
| 5:E:237:TRP:N    | 5:E:237:TRP:CD1  | 2.82        | 0.48     |
| 5:E:92:ALA:HB1   | 5:E:100:GLN:CG   | 2.30        | 0.47     |
| 1:A:242:GLN:O    | 1:A:243:LYS:HB2  | 2.13        | 0.47     |
| 2:B:22:PHE:C     | 2:B:70:PHE:HE1   | 2.17        | 0.47     |
| 1:F:133:TRP:HB2  | 1:F:144:LYS:HG3  | 1.95        | 0.47     |
| 2:B:26:TYR:HD1   | 2:B:64:LEU:O     | 1.97        | 0.47     |
| 4:I:114:ASN:HD22 | 4:I:114:ASN:C    | 2.18        | 0.47     |
| 4:D:192:ILE:CD1  | 4:D:196:THR:HG21 | 2.44        | 0.47     |
| 1:A:72:GLN:HB2   | 5:E:51:ASN:CG    | 2.35        | 0.47     |
| 5:E:49:SER:HB2   | 5:E:74:PHE:CE1   | 2.49        | 0.47     |
| 4:I:99:ILE:HD12  | 4:I:99:ILE:N     | 2.30        | 0.47     |
| 4:I:92:TYR:OH    | 5:J:98:HIS:O     | 2.32        | 0.47     |
| 5:J:162:GLU:CG   | 5:J:164:HIS:CE1  | 2.98        | 0.47     |
| 5:J:108:LEU:C    | 5:J:108:LEU:CD1  | 2.82        | 0.47     |
| 4:I:132:VAL:HG23 | 5:J:125:PHE:CD1  | 2.49        | 0.47     |
| 1:F:51:TRP:CD1   | 1:F:175:GLY:CA   | 2.97        | 0.47     |
| 2:B:41:LYS:HA    | 2:B:78:TYR:CD2   | 2.49        | 0.47     |
| 4:D:164:SER:OG   | 4:D:165:MET:HG2  | 2.15        | 0.47     |
| 1:F:15:PRO:HG2   | 1:F:91:GLY:O     | 2.14        | 0.47     |
| 1:A:139:ALA:HA   | 1:A:142:ILE:CD1  | 2.44        | 0.47     |
| 5:J:218:ASP:N    | 5:J:218:ASP:OD1  | 2.47        | 0.47     |
| 5:E:84:ASN:N     | 5:E:84:ASN:HD22  | 2.12        | 0.47     |
| 4:D:94:GLN:CB    | 4:D:97:LYS:CE    | 2.89        | 0.47     |
| 5:E:32:MET:CE    | 5:E:71:LYS:O     | 2.62        | 0.47     |
| 4:D:114:ASN:OD1  | 1:F:108:ARG:NH1  | 2.47        | 0.47     |
| 2:G:13:HIS:HB2   | 2:G:21:ASN:HD21  | 1.76        | 0.47     |
| 1:A:209:TYR:CD1  | 1:A:241:PHE:HE1  | 2.27        | 0.47     |
| 1:F:202:ARG:NH1  | 1:F:244:TRP:CZ3  | 2.82        | 0.47     |
| 1:A:229:GLU:O    | 1:A:230:LEU:HD12 | 2.14        | 0.47     |
| 4:D:48:MET:CE    | 4:D:63:ALA:N     | 2.77        | 0.47     |
| 1:A:194:ILE:HD11 | 1:A:198:GLU:HB3  | 1.96        | 0.47     |
| 5:E:36:ARG:HB2   | 5:E:89:TYR:CE1   | 2.49        | 0.47     |
| 1:F:99:PHE:HZ    | 1:F:156:GLN:OE1  | 1.98        | 0.47     |
| 3:H:2:PHE:CD1    | 3:H:3:PRO:HD2    | 2.50        | 0.47     |
| 5:J:204:HIS:NE2  | 5:J:235:GLU:HB2  | 2.30        | 0.47     |
| 1:A:200:THR:HG21 | 1:A:202:ARG:HH22 | 1.79        | 0.47     |
| 5:J:86:THR:HA    | 5:J:108:LEU:HD12 | 1.96        | 0.47     |
| 4:D:81:PRO:HA    | 4:D:108:VAL:CG1  | 2.44        | 0.47     |
| 1:F:168:LEU:HD11 | 1:F:172:LEU:HD21 | 1.96        | 0.47     |
| 4:D:35:TRP:O     | 4:D:46:LEU:HD12  | 2.15        | 0.47     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:87:GLN:NE2   | 1:A:118:TYR:OH   | 2.47        | 0.47     |
| 5:E:31:TYR:C     | 5:E:32:MET:HG3   | 2.34        | 0.47     |
| 5:E:86:THR:CG2   | 5:E:109:THR:HA   | 2.29        | 0.47     |
| 5:J:97:SER:OG    | 5:J:98:HIS:N     | 2.47        | 0.47     |
| 1:F:150:ALA:HB3  | 1:F:152:VAL:HG23 | 1.95        | 0.47     |
| 5:J:49:SER:HB3   | 5:J:68:ARG:NH1   | 2.29        | 0.47     |
| 4:I:135:PHE:CE1  | 4:I:138:PHE:HB3  | 2.49        | 0.47     |
| 4:I:162:MET:HG3  | 5:J:166:GLY:CA   | 2.45        | 0.47     |
| 5:E:177:GLN:O    | 5:E:183:SER:HB2  | 2.14        | 0.47     |
| 5:J:76:LEU:C     | 5:J:77:ILE:HD12  | 2.34        | 0.47     |
| 5:J:18:LYS:HB2   | 5:J:79:GLU:O     | 2.15        | 0.47     |
| 1:A:258:THR:CG2  | 1:A:271:THR:CG2  | 2.93        | 0.47     |
| 1:A:26:GLY:CA    | 1:A:33:PHE:HE1   | 2.25        | 0.47     |
| 1:F:233:THR:CG2  | 1:F:243:LYS:HD2  | 2.44        | 0.47     |
| 1:A:185:PRO:HG3  | 1:A:213:ILE:HD12 | 1.95        | 0.47     |
| 4:I:110:PRO:HD2  | 4:I:140:SER:OG   | 2.14        | 0.47     |
| 4:D:123:ARG:NH1  | 5:E:239:ARG:CZ   | 2.78        | 0.47     |
| 4:I:50:ILE:HD12  | 4:I:51:TYR:CA    | 2.44        | 0.47     |
| 1:F:51:TRP:CZ2   | 1:F:179:LEU:CD2  | 2.98        | 0.47     |
| 4:D:80:GLN:C     | 4:D:108:VAL:HG11 | 2.35        | 0.47     |
| 4:D:13:VAL:O     | 4:D:108:VAL:HA   | 2.15        | 0.47     |
| 5:E:19:LEU:HD11  | 5:E:78:LEU:CD2   | 2.42        | 0.47     |
| 1:F:33:PHE:CD2   | 1:F:34:VAL:HG22  | 2.50        | 0.47     |
| 4:I:135:PHE:CZ   | 4:I:138:PHE:HB3  | 2.50        | 0.47     |
| 2:B:12:ARG:H     | 2:B:21:ASN:HD21  | 1.63        | 0.47     |
| 4:D:162:MET:CE   | 5:E:192:ARG:HG2  | 2.45        | 0.47     |
| 5:E:199:GLN:HA   | 5:E:239:ARG:O    | 2.14        | 0.47     |
| 4:D:12:SER:HA    | 4:D:109:LYS:NZ   | 2.27        | 0.47     |
| 4:I:4:VAL:HG13   | 4:I:5:GLU:HG2    | 1.96        | 0.47     |
| 1:A:130:LEU:HB3  | 1:A:157:ARG:CG   | 2.45        | 0.47     |
| 5:E:11:LEU:O     | 5:E:108:LEU:HD12 | 2.15        | 0.47     |
| 1:A:49:ALA:HB1   | 1:A:51:TRP:CE2   | 2.50        | 0.47     |
| 4:D:154:ILE:HD11 | 4:D:187:PHE:HD1  | 1.77        | 0.47     |
| 4:D:25:TYR:CD2   | 4:D:33:PHE:CE1   | 3.03        | 0.47     |
| 2:G:12:ARG:CG    | 2:G:13:HIS:N     | 2.78        | 0.47     |
| 1:F:203:CYS:SG   | 1:F:272:LEU:HD22 | 2.55        | 0.47     |
| 1:F:202:ARG:NH1  | 1:F:202:ARG:HG3  | 2.27        | 0.47     |
| 5:J:9:ARG:HH11   | 5:J:9:ARG:CG     | 2.28        | 0.47     |
| 1:F:4:SER:OG     | 1:F:6:ARG:NE     | 2.47        | 0.47     |
| 4:I:6:GLN:HE21   | 4:I:102:GLN:HB2  | 1.77        | 0.47     |
| 4:D:36:TYR:CE1   | 4:D:46:LEU:HB2   | 2.50        | 0.47     |
| 1:F:162:GLY:O    | 1:F:163:THR:C    | 2.53        | 0.46     |

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| Atom-1          | Atom-2           | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 2:B:50:GLU:HB3  | 2:B:67:TYR:CE1   | 2.50        | 0.46     |
| 1:A:83:ARG:HH12 | 1:A:84:TYR:HE1   | 1.56        | 0.46     |
| 5:J:86:THR:HA   | 5:J:108:LEU:CD1  | 2.45        | 0.46     |
| 5:E:128:SER:O   | 5:E:132:ILE:CD1  | 2.63        | 0.46     |
| 1:A:159:TYR:CD1 | 4:D:31:GLN:NE2   | 2.83        | 0.46     |
| 1:A:234:ARG:NH2 | 2:B:10:TYR:CB    | 2.78        | 0.46     |
| 2:B:23:LEU:O    | 2:B:67:TYR:HA    | 2.15        | 0.46     |
| 1:F:51:TRP:NE1  | 1:F:179:LEU:HD21 | 2.29        | 0.46     |
| 1:F:244:TRP:O   | 1:F:244:TRP:HE3  | 1.97        | 0.46     |
| 1:A:129:ASP:OD2 | 1:A:131:ARG:HB2  | 2.15        | 0.46     |
| 1:A:13:SER:HA   | 1:A:20:PRO:HG3   | 1.97        | 0.46     |
| 2:B:8:GLN:O     | 2:B:25:CYS:HA    | 2.16        | 0.46     |
| 5:J:25:GLN:OE1  | 5:J:28:ASN:N     | 2.49        | 0.46     |
| 5:J:215:SER:C   | 5:J:217:ASN:H    | 2.18        | 0.46     |
| 1:F:7:TYR:CD2   | 3:H:2:PHE:HD1    | 2.33        | 0.46     |
| 4:I:92:TYR:CE2  | 5:J:98:HIS:HB3   | 2.51        | 0.46     |
| 4:I:9:GLY:HA2   | 4:I:10:PRO:HD3   | 1.68        | 0.46     |
| 4:D:48:MET:HG2  | 4:D:63:ALA:HB2   | 1.97        | 0.46     |
| 4:D:34:PHE:CD2  | 4:D:34:PHE:N     | 2.83        | 0.46     |
| 4:I:118:ALA:HB2 | 4:I:197:PHE:HB3  | 1.97        | 0.46     |
| 5:E:31:TYR:CD2  | 5:E:100:GLN:NE2  | 2.84        | 0.46     |
| 1:F:158:ALA:HB1 | 4:I:31:GLN:HB2   | 1.98        | 0.46     |
| 5:J:154:LEU:CD2 | 5:J:209:VAL:HG22 | 2.46        | 0.46     |
| 5:E:135:THR:O   | 5:E:136:GLN:HB2  | 2.15        | 0.46     |
| 1:F:51:TRP:HZ2  | 1:F:179:LEU:CD2  | 2.26        | 0.46     |
| 5:E:115:LYS:NZ  | 5:E:118:PHE:HZ   | 2.13        | 0.46     |
| 4:D:23:CYS:HB2  | 4:D:72:VAL:HG12  | 1.98        | 0.46     |
| 4:D:36:TYR:HD1  | 4:D:46:LEU:N     | 2.14        | 0.46     |
| 5:E:52:VAL:O    | 5:E:54:VAL:HG23  | 2.16        | 0.46     |
| 5:E:32:MET:HG2  | 5:E:93:SER:OG    | 2.15        | 0.46     |
| 1:A:33:PHE:CG   | 1:A:34:VAL:HG13  | 2.50        | 0.46     |
| 4:D:89:TRP:CZ3  | 4:D:91:THR:CG2   | 2.94        | 0.46     |
| 4:I:123:ARG:CB  | 5:J:126:GLU:HB2  | 2.41        | 0.46     |
| 5:E:6:GLN:NE2   | 5:E:34:TRP:CZ3   | 2.84        | 0.46     |
| 5:E:107:ARG:CZ  | 5:E:150:ASP:OD1  | 2.64        | 0.46     |
| 2:G:56:PHE:CB   | 2:G:61:SER:O     | 2.58        | 0.46     |
| 2:B:52:SER:O    | 2:B:64:LEU:HD21  | 2.16        | 0.46     |
| 5:J:19:LEU:N    | 5:J:19:LEU:HD12  | 2.30        | 0.46     |
| 1:A:55:GLU:O    | 1:A:60:TRP:HZ2   | 1.98        | 0.46     |
| 1:F:122:ASP:O   | 1:F:136:ALA:CB   | 2.64        | 0.46     |
| 5:J:60:VAL:HG23 | 5:J:60:VAL:O     | 2.16        | 0.46     |
| 5:E:25:GLN:HB3  | 5:E:25:GLN:HE21  | 1.53        | 0.46     |

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| Atom-1           | Atom-2          | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 4:D:96:GLY:HA3   | 5:E:50:MET:HE1  | 1.96        | 0.46     |
| 5:E:32:MET:HB2   | 5:E:68:ARG:NH1  | 2.31        | 0.46     |
| 1:A:4:SER:N      | 1:A:29:ASP:OD1  | 2.49        | 0.46     |
| 4:D:14:PRO:HB2   | 4:I:71:TYR:CE1  | 2.48        | 0.46     |
| 5:J:49:SER:CB    | 5:J:68:ARG:NH1  | 2.79        | 0.46     |
| 1:F:51:TRP:CD1   | 1:F:175:GLY:HA3 | 2.51        | 0.46     |
| 1:F:76:GLU:O     | 1:F:80:ILE:HG13 | 2.15        | 0.46     |
| 4:I:192:ILE:HG13 | 4:I:193:PRO:O   | 2.16        | 0.46     |
| 4:D:133:CYS:SG   | 4:D:181:PHE:HE1 | 2.39        | 0.46     |
| 5:E:53:GLU:OE1   | 5:E:69:LYS:HA   | 2.16        | 0.46     |
| 4:D:114:ASN:HB3  | 1:F:108:ARG:NH1 | 2.23        | 0.46     |
| 3:H:6:PHE:CZ     | 5:J:98:HIS:CD2  | 3.02        | 0.46     |
| 4:I:28:ARG:HA    | 4:I:70:GLN:NE2  | 2.30        | 0.46     |
| 4:I:160:LEU:CD1  | 4:I:162:MET:HE3 | 2.42        | 0.46     |
| 5:E:117:VAL:HG12 | 5:E:227:PRO:CB  | 2.46        | 0.46     |
| 2:B:83:ASN:ND2   | 2:B:83:ASN:C    | 2.68        | 0.46     |
| 4:D:187:PHE:HB3  | 4:D:190:SER:OG  | 2.16        | 0.46     |
| 5:J:124:VAL:HG23 | 5:J:234:ALA:HB3 | 1.98        | 0.46     |
| 1:F:13:SER:O     | 1:F:92:SER:HB2  | 2.16        | 0.46     |
| 1:F:120:GLY:CA   | 2:G:31:HIS:NE2  | 2.79        | 0.46     |
| 4:D:156:ASP:OD2  | 4:D:157:LYS:HD3 | 2.15        | 0.46     |
| 1:F:93:HIS:HB3   | 1:F:118:TYR:CE1 | 2.51        | 0.46     |
| 5:E:36:ARG:NH2   | 5:E:87:SER:HB2  | 2.23        | 0.45     |
| 4:D:189:ASN:HD22 | 4:D:189:ASN:HA  | 1.66        | 0.45     |
| 4:D:88:LEU:CD2   | 4:D:88:LEU:N    | 2.78        | 0.45     |
| 1:F:35:ARG:O     | 1:F:45:MET:SD   | 2.74        | 0.45     |
| 4:I:69:SER:O     | 4:I:70:GLN:HB2  | 2.16        | 0.45     |
| 5:J:218:ASP:O    | 5:J:226:LYS:NZ  | 2.42        | 0.45     |
| 1:A:152:VAL:HG13 | 1:A:156:GLN:NE2 | 2.30        | 0.45     |
| 1:F:98:MET:HB3   | 1:F:115:GLN:HG2 | 1.98        | 0.45     |
| 5:J:154:LEU:HD22 | 5:J:155:SER:H   | 1.81        | 0.45     |
| 4:I:159:VAL:N    | 5:J:168:CYS:SG  | 2.88        | 0.45     |
| 1:A:190:THR:HG21 | 2:B:98:ASP:CG   | 2.36        | 0.45     |
| 5:J:199:GLN:HA   | 5:J:239:ARG:O   | 2.15        | 0.45     |
| 4:D:192:ILE:HD11 | 4:D:196:THR:CB  | 2.46        | 0.45     |
| 4:I:135:PHE:HB2  | 4:I:187:PHE:CE2 | 2.51        | 0.45     |
| 2:G:37:VAL:HG13  | 2:G:80:CYS:SG   | 2.56        | 0.45     |
| 1:A:185:PRO:HG3  | 1:A:213:ILE:CD1 | 2.46        | 0.45     |
| 1:A:219:ARG:HG3  | 1:A:257:TYR:CE1 | 2.52        | 0.45     |
| 2:B:5:PRO:O      | 2:B:7:ILE:HD12  | 2.17        | 0.45     |
| 1:F:240:THR:C    | 1:F:241:PHE:CD1 | 2.90        | 0.45     |
| 3:C:3:PRO:HG2    | 3:C:5:THR:CG2   | 2.46        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:J:97:SER:C     | 5:J:98:HIS:ND1   | 2.70        | 0.45     |
| 5:J:154:LEU:HD22 | 5:J:155:SER:N    | 2.31        | 0.45     |
| 5:J:82:SER:HB2   | 5:J:84:ASN:OD1   | 2.16        | 0.45     |
| 2:G:23:LEU:O     | 2:G:67:TYR:HA    | 2.17        | 0.45     |
| 2:G:81:ARG:CB    | 2:G:92:ILE:HG12  | 2.47        | 0.45     |
| 1:A:53:GLU:HA    | 1:A:60:TRP:HH2   | 1.81        | 0.45     |
| 1:A:51:TRP:CZ3   | 1:A:52:ILE:HD13  | 2.52        | 0.45     |
| 2:G:62:PHE:N     | 2:G:62:PHE:CD1   | 2.84        | 0.45     |
| 1:F:50:PRO:HA    | 1:F:53:GLU:OE1   | 2.15        | 0.45     |
| 2:B:23:LEU:HG    | 2:B:23:LEU:O     | 2.17        | 0.45     |
| 2:G:40:LEU:HD11  | 2:G:81:ARG:HB2   | 1.99        | 0.45     |
| 2:G:45:ARG:HB2   | 2:G:81:ARG:NH2   | 2.30        | 0.45     |
| 4:D:91:THR:CG2   | 4:D:91:THR:O     | 2.63        | 0.45     |
| 1:F:202:ARG:HD2  | 1:F:204:TRP:CE2  | 2.51        | 0.45     |
| 1:F:43:GLN:HE21  | 1:F:43:GLN:CA    | 2.28        | 0.45     |
| 5:E:72:ARG:H     | 5:E:72:ARG:HD2   | 1.81        | 0.45     |
| 5:E:79:GLU:C     | 5:E:81:PRO:HD3   | 2.37        | 0.45     |
| 5:E:49:SER:CB    | 5:E:74:PHE:CE1   | 3.00        | 0.45     |
| 5:E:108:LEU:HD12 | 5:E:109:THR:H    | 1.82        | 0.45     |
| 1:F:99:PHE:CE2   | 1:F:159:TYR:CE2  | 3.03        | 0.45     |
| 1:F:117:ALA:CB   | 2:G:60:TRP:CD2   | 2.99        | 0.45     |
| 4:I:160:LEU:C    | 4:I:168:LYS:NZ   | 2.70        | 0.45     |
| 4:I:33:PHE:HB2   | 4:I:50:ILE:HG12  | 1.99        | 0.45     |
| 5:J:210:GLN:HE21 | 5:J:231:ILE:HG12 | 1.81        | 0.45     |
| 1:F:256:ARG:HG2  | 1:F:256:ARG:HH11 | 1.82        | 0.45     |
| 1:A:145:ARG:O    | 1:A:148:GLU:HB2  | 2.17        | 0.45     |
| 5:E:88:LEU:CD1   | 5:E:107:ARG:HG2  | 2.41        | 0.45     |
| 5:J:11:LEU:HD12  | 5:J:12:ILE:H     | 1.80        | 0.45     |
| 1:A:186:LYS:HB2  | 1:A:186:LYS:HZ3  | 1.80        | 0.45     |
| 3:C:7:GLY:N      | 5:E:30:GLU:HG3   | 2.25        | 0.45     |
| 5:J:52:VAL:HG13  | 5:J:68:ARG:O     | 2.17        | 0.45     |
| 5:J:20:THR:OG1   | 5:J:77:ILE:HG13  | 2.17        | 0.45     |
| 5:E:124:VAL:HG23 | 5:E:234:ALA:CB   | 2.46        | 0.45     |
| 5:J:210:GLN:NE2  | 5:J:231:ILE:CG1  | 2.80        | 0.45     |
| 1:A:188:HIS:CE1  | 1:A:204:TRP:CB   | 3.00        | 0.45     |
| 1:A:43:GLN:NE2   | 1:A:43:GLN:HA    | 2.32        | 0.45     |
| 1:F:99:PHE:CE1   | 1:F:114:HIS:CG   | 3.04        | 0.45     |
| 4:D:89:TRP:HZ3   | 4:D:91:THR:HG22  | 1.77        | 0.45     |
| 4:D:154:ILE:O    | 4:D:154:ILE:HG22 | 2.17        | 0.45     |
| 5:E:38:ASP:OD2   | 5:E:44:ARG:NH2   | 2.44        | 0.44     |
| 1:F:70:HIS:HD2   | 1:F:73:THR:CB    | 2.27        | 0.44     |
| 5:J:154:LEU:HD23 | 5:J:155:SER:H    | 1.81        | 0.44     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:200:THR:HG21 | 1:A:202:ARG:CZ   | 2.47        | 0.44     |
| 2:G:21:ASN:CG    | 2:G:22:PHE:N     | 2.69        | 0.44     |
| 5:E:127:PRO:HG3  | 5:E:139:THR:C    | 2.38        | 0.44     |
| 4:I:21:LEU:HD23  | 4:I:21:LEU:N     | 2.32        | 0.44     |
| 4:D:139:ASP:C    | 4:D:141:GLN:H    | 2.20        | 0.44     |
| 4:I:102:GLN:OE1  | 4:I:102:GLN:C    | 2.56        | 0.44     |
| 5:E:215:SER:C    | 5:E:217:ASN:H    | 2.20        | 0.44     |
| 5:J:210:GLN:HG2  | 5:J:212:TYR:CE2  | 2.52        | 0.44     |
| 4:I:116:ASP:N    | 4:I:117:PRO:HD3  | 2.32        | 0.44     |
| 1:A:97:MET:HE2   | 1:A:99:PHE:HB2   | 1.99        | 0.44     |
| 4:D:17:ALA:HB2   | 4:I:71:TYR:OH    | 2.18        | 0.44     |
| 4:I:161:ASP:HB2  | 4:I:168:LYS:HG2  | 2.00        | 0.44     |
| 1:F:272:LEU:CD1  | 1:F:272:LEU:N    | 2.74        | 0.44     |
| 1:F:56:GLY:O     | 1:F:59:TYR:HB3   | 2.17        | 0.44     |
| 4:D:12:SER:CB    | 4:D:109:LYS:HZ1  | 2.30        | 0.44     |
| 1:F:82:LEU:HD23  | 1:F:87:GLN:HB2   | 2.00        | 0.44     |
| 3:H:7:GLY:HA2    | 5:J:30:GLU:CG    | 2.48        | 0.44     |
| 4:I:23:CYS:HB3   | 4:I:89:TRP:CZ2   | 2.52        | 0.44     |
| 4:I:87:TYR:C     | 4:I:88:LEU:HD23  | 2.37        | 0.44     |
| 1:F:202:ARG:HD3  | 1:F:244:TRP:CG   | 2.52        | 0.44     |
| 1:A:57:PRO:CA    | 1:A:60:TRP:HD1   | 2.26        | 0.44     |
| 4:D:136:THR:OG1  | 4:D:137:ASP:N    | 2.50        | 0.44     |
| 4:D:15:GLU:HG3   | 4:D:16:GLY:N     | 2.33        | 0.44     |
| 1:A:68:LYS:HB3   | 5:E:54:VAL:HG22  | 1.99        | 0.44     |
| 3:C:4:LEU:O      | 5:E:98:HIS:NE2   | 2.50        | 0.44     |
| 4:I:182:ALA:H    | 4:I:185:ASN:HD21 | 1.66        | 0.44     |
| 1:A:75:ARG:NH1   | 1:A:79:ARG:NE    | 2.62        | 0.44     |
| 5:J:18:LYS:HG2   | 5:J:19:LEU:N     | 2.32        | 0.44     |
| 1:A:208:PHE:CZ   | 1:A:241:PHE:HB2  | 2.52        | 0.44     |
| 5:E:159:ASN:OD1  | 5:E:203:ASN:ND2  | 2.50        | 0.44     |
| 1:F:146:LYS:HB3  | 1:F:146:LYS:HZ3  | 1.82        | 0.44     |
| 4:D:192:ILE:HD11 | 4:D:196:THR:CG2  | 2.47        | 0.44     |
| 5:E:218:ASP:O    | 5:E:226:LYS:NZ   | 2.43        | 0.44     |
| 5:E:85:GLN:O     | 5:E:89:TYR:OH    | 2.23        | 0.44     |
| 1:A:234:ARG:O    | 1:A:242:GLN:HG3  | 2.17        | 0.44     |
| 5:J:36:ARG:NH2   | 5:J:84:ASN:O     | 2.46        | 0.44     |
| 1:A:63:GLU:O     | 1:A:67:VAL:HG12  | 2.17        | 0.44     |
| 1:A:249:VAL:CG1  | 1:A:257:TYR:CE2  | 2.95        | 0.44     |
| 4:D:158:CYS:HB2  | 5:E:190:ARG:NH1  | 2.32        | 0.44     |
| 2:B:56:PHE:HD2   | 2:B:62:PHE:CE2   | 2.36        | 0.44     |
| 4:I:93:ASN:C     | 4:I:95:GLY:N     | 2.70        | 0.44     |
| 1:F:51:TRP:CZ2   | 1:F:179:LEU:CD1  | 3.00        | 0.44     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:D:75:LEU:N     | 4:D:75:LEU:HD12  | 2.32        | 0.44     |
| 5:J:152:VAL:HG12 | 5:J:210:GLN:O    | 2.17        | 0.44     |
| 2:B:14:PRO:O     | 2:B:16:GLU:HG2   | 2.18        | 0.44     |
| 1:F:189:MET:HB2  | 1:F:189:MET:HE2  | 1.82        | 0.44     |
| 1:A:66:LYS:HB2   | 1:A:66:LYS:HE3   | 1.74        | 0.44     |
| 5:J:162:GLU:CG   | 5:J:164:HIS:HE1  | 2.30        | 0.44     |
| 4:I:185:ASN:HD22 | 4:I:185:ASN:C    | 2.20        | 0.44     |
| 1:F:204:TRP:HH2  | 2:G:99:MET:CE    | 2.31        | 0.44     |
| 5:E:203:ASN:HB3  | 5:E:205:PHE:CZ   | 2.53        | 0.44     |
| 1:F:260:HIS:CE1  | 1:F:271:THR:CG2  | 3.00        | 0.44     |
| 3:C:4:LEU:CD2    | 4:D:96:GLY:HA2   | 2.46        | 0.44     |
| 1:F:156:GLN:OE1  | 3:H:8:TRP:CH2    | 2.70        | 0.44     |
| 1:F:99:PHE:CE2   | 3:H:3:PRO:HB3    | 2.53        | 0.44     |
| 1:A:200:THR:CG2  | 1:A:202:ARG:HH22 | 2.31        | 0.44     |
| 4:D:138:PHE:O    | 4:D:170:ASN:ND2  | 2.51        | 0.44     |
| 4:I:38:GLN:CG    | 4:I:44:PRO:HG3   | 2.48        | 0.44     |
| 5:E:8:PRO:O      | 5:E:106:THR:HG23 | 2.17        | 0.44     |
| 1:A:68:LYS:NZ    | 5:E:53:GLU:O     | 2.51        | 0.44     |
| 5:J:154:LEU:CD2  | 5:J:155:SER:N    | 2.81        | 0.44     |
| 1:A:202:ARG:HH11 | 1:A:246:ALA:HB2  | 1.83        | 0.44     |
| 1:A:219:ARG:HG3  | 1:A:257:TYR:HE1  | 1.83        | 0.44     |
| 1:F:67:VAL:HG13  | 1:F:68:LYS:N     | 2.33        | 0.44     |
| 1:F:144:LYS:O    | 1:F:148:GLU:CG   | 2.65        | 0.44     |
| 1:A:111:ARG:NH2  | 1:A:128:GLU:CA   | 2.79        | 0.44     |
| 3:C:4:LEU:HD22   | 3:C:6:PHE:HE2    | 1.83        | 0.44     |
| 1:F:106:ASP:CG   | 1:F:108:ARG:HB2  | 2.38        | 0.44     |
| 4:D:115:PRO:HD2  | 1:F:108:ARG:NH2  | 2.32        | 0.44     |
| 2:B:23:LEU:N     | 2:B:70:PHE:CE1   | 2.85        | 0.44     |
| 1:F:202:ARG:HD3  | 1:F:244:TRP:CE2  | 2.52        | 0.44     |
| 1:F:244:TRP:CE3  | 1:F:244:TRP:O    | 2.71        | 0.44     |
| 1:F:51:TRP:C     | 1:F:51:TRP:HE3   | 2.22        | 0.44     |
| 5:E:70:GLU:HB3   | 5:E:72:ARG:HD2   | 2.00        | 0.44     |
| 1:A:207:GLY:HA2  | 1:A:240:THR:HB   | 2.00        | 0.44     |
| 5:J:148:TYR:HB2  | 5:J:184:ARG:HG3  | 2.00        | 0.44     |
| 1:A:126:LEU:HD13 | 1:A:133:TRP:CE3  | 2.52        | 0.43     |
| 5:E:86:THR:O     | 5:E:87:SER:HB2   | 2.18        | 0.43     |
| 1:A:159:TYR:CD1  | 4:D:31:GLN:OE1   | 2.70        | 0.43     |
| 1:A:65:GLY:HA2   | 5:E:54:VAL:CG1   | 2.48        | 0.43     |
| 5:J:41:LEU:N     | 5:J:41:LEU:HD22  | 2.33        | 0.43     |
| 1:F:106:ASP:OD2  | 1:F:108:ARG:CB   | 2.58        | 0.43     |
| 2:G:54:LEU:HA    | 2:G:64:LEU:HD21  | 2.00        | 0.43     |
| 2:G:22:PHE:HD2   | 2:G:67:TYR:HD2   | 1.64        | 0.43     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:109:PHE:O    | 1:A:110:LEU:HD12 | 2.17        | 0.43     |
| 4:D:11:LEU:HG    | 4:D:12:SER:N     | 2.31        | 0.43     |
| 1:A:11:SER:OG    | 1:A:78:LEU:HD11  | 2.18        | 0.43     |
| 4:I:4:VAL:HG22   | 4:I:5:GLU:N      | 2.33        | 0.43     |
| 1:A:121:LYS:HD3  | 1:A:122:ASP:H    | 1.84        | 0.43     |
| 1:A:150:ALA:HB1  | 5:E:96:ALA:HB1   | 1.99        | 0.43     |
| 4:I:87:TYR:CE2   | 4:I:106:LEU:HB3  | 2.53        | 0.43     |
| 4:I:88:LEU:HD12  | 4:I:100:PHE:CD1  | 2.53        | 0.43     |
| 1:F:8:PHE:CD2    | 1:F:25:VAL:HG23  | 2.40        | 0.43     |
| 4:I:37:ARG:CZ    | 4:I:39:TYR:OH    | 2.66        | 0.43     |
| 5:E:181:ASN:N    | 5:E:181:ASN:OD1  | 2.51        | 0.43     |
| 4:D:53:ASN:HA    | 4:D:65:LEU:HD23  | 1.99        | 0.43     |
| 5:J:43:LEU:HD12  | 5:J:44:ARG:N     | 2.32        | 0.43     |
| 4:I:109:LYS:HD2  | 4:I:140:SER:OG   | 2.18        | 0.43     |
| 1:A:170:ARG:HH11 | 1:A:170:ARG:HG3  | 1.84        | 0.43     |
| 1:A:50:PRO:HA    | 1:A:53:GLU:OE2   | 2.19        | 0.43     |
| 4:I:38:GLN:CB    | 4:I:44:PRO:HG3   | 2.48        | 0.43     |
| 3:C:4:LEU:CD2    | 3:C:6:PHE:HE2    | 2.30        | 0.43     |
| 4:I:160:LEU:O    | 4:I:168:LYS:HA   | 2.19        | 0.43     |
| 1:F:22:PHE:CE2   | 1:F:71:SER:HB3   | 2.52        | 0.43     |
| 1:F:231:VAL:HG13 | 1:F:244:TRP:CH2  | 2.54        | 0.43     |
| 1:A:19:GLU:CA    | 1:A:19:GLU:OE2   | 2.54        | 0.43     |
| 1:A:268:LYS:HG3  | 1:A:269:PRO:HD2  | 2.01        | 0.43     |
| 5:J:150:ASP:C    | 5:J:151:HIS:HD2  | 2.22        | 0.43     |
| 4:I:124:ASP:OD2  | 5:J:125:PHE:CZ   | 2.72        | 0.43     |
| 4:D:157:LYS:CD   | 4:D:157:LYS:N    | 2.82        | 0.43     |
| 4:D:110:PRO:HG2  | 4:D:112:ILE:HD11 | 2.00        | 0.43     |
| 1:A:133:TRP:HB2  | 1:A:144:LYS:HG3  | 2.00        | 0.43     |
| 5:E:6:GLN:OE1    | 5:E:91:CYS:N     | 2.46        | 0.43     |
| 1:A:147:TRP:CZ2  | 3:C:8:TRP:HB3    | 2.54        | 0.43     |
| 1:A:33:PHE:CD1   | 1:A:33:PHE:C     | 2.91        | 0.43     |
| 1:A:48:ARG:HD2   | 1:A:48:ARG:HA    | 1.63        | 0.43     |
| 1:A:208:PHE:HZ   | 1:A:233:THR:HG23 | 1.84        | 0.43     |
| 2:B:56:PHE:CD2   | 2:B:62:PHE:HE2   | 2.36        | 0.43     |
| 1:F:205:ALA:O    | 1:F:208:PHE:HE1  | 2.02        | 0.43     |
| 5:E:9:ARG:HB3    | 5:E:10:TYR:CD2   | 2.54        | 0.43     |
| 4:D:81:PRO:N     | 4:D:108:VAL:HG11 | 2.34        | 0.43     |
| 5:J:152:VAL:HA   | 5:J:210:GLN:O    | 2.19        | 0.43     |
| 1:A:44:ARG:HA    | 1:A:64:THR:HG23  | 2.00        | 0.43     |
| 4:D:161:ASP:OD2  | 4:D:163:ARG:HG2  | 2.19        | 0.43     |
| 5:J:46:ILE:O     | 5:J:58:GLY:N     | 2.41        | 0.43     |
| 1:A:162:GLY:O    | 1:A:163:THR:C    | 2.57        | 0.43     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:158:ALA:HB1  | 4:D:31:GLN:CB    | 2.49        | 0.43     |
| 5:J:38:ASP:CB    | 5:J:44:ARG:HH22  | 2.30        | 0.43     |
| 1:F:234:ARG:HG3  | 1:F:242:GLN:CG   | 2.38        | 0.43     |
| 5:J:127:PRO:HD2  | 5:J:198:TRP:CE2  | 2.54        | 0.43     |
| 1:A:191:HIS:CE1  | 1:A:193:PRO:HG3  | 2.54        | 0.43     |
| 1:F:201:LEU:HD23 | 1:F:201:LEU:HA   | 1.94        | 0.43     |
| 1:A:82:LEU:HD22  | 1:A:87:GLN:HB2   | 2.01        | 0.43     |
| 4:D:116:ASP:N    | 4:D:117:PRO:HD3  | 2.33        | 0.43     |
| 4:D:194:GLU:HA   | 4:D:194:GLU:OE1  | 2.19        | 0.43     |
| 5:E:176:GLU:O    | 5:E:178:PRO:HD3  | 2.18        | 0.43     |
| 1:A:130:LEU:O    | 1:A:157:ARG:HG3  | 2.18        | 0.43     |
| 5:E:19:LEU:HD12  | 5:E:19:LEU:O     | 2.19        | 0.43     |
| 1:F:7:TYR:HE1    | 1:F:33:PHE:CZ    | 2.36        | 0.43     |
| 1:F:99:PHE:HE1   | 1:F:114:HIS:CG   | 2.37        | 0.43     |
| 4:I:94:GLN:CB    | 4:I:97:LYS:HD3   | 2.30        | 0.43     |
| 5:J:203:ASN:O    | 5:J:205:PHE:CE2  | 2.72        | 0.43     |
| 2:B:23:LEU:HD21  | 2:B:39:LEU:HD13  | 2.01        | 0.43     |
| 2:G:9:VAL:HA     | 2:G:24:ASN:O     | 2.18        | 0.43     |
| 5:E:132:ILE:HG23 | 5:E:195:ALA:HB2  | 1.99        | 0.43     |
| 4:I:36:TYR:CD1   | 4:I:46:LEU:N     | 2.87        | 0.43     |
| 1:F:218:GLN:OE1  | 1:F:223:ASP:N    | 2.52        | 0.43     |
| 4:D:111:ASN:HA   | 4:D:111:ASN:HD22 | 1.48        | 0.43     |
| 1:F:104:GLY:CA   | 1:F:110:LEU:HD23 | 2.49        | 0.43     |
| 1:A:44:ARG:HG2   | 1:A:64:THR:HG21  | 2.01        | 0.43     |
| 1:A:98:MET:SD    | 1:A:99:PHE:N     | 2.91        | 0.42     |
| 1:A:200:THR:HG21 | 1:A:202:ARG:NH2  | 2.34        | 0.42     |
| 1:A:11:SER:HA    | 1:A:21:ARG:O     | 2.19        | 0.42     |
| 1:A:111:ARG:HD3  | 1:A:128:GLU:CD   | 2.39        | 0.42     |
| 4:I:42:LYS:N     | 4:I:42:LYS:HE2   | 2.34        | 0.42     |
| 4:I:193:PRO:HB2  | 4:I:196:THR:OG1  | 2.19        | 0.42     |
| 1:A:150:ALA:HB3  | 1:A:152:VAL:HG23 | 2.01        | 0.42     |
| 4:D:30:SER:HB3   | 4:D:33:PHE:CE2   | 2.54        | 0.42     |
| 4:D:32:SER:C     | 4:D:33:PHE:HD2   | 2.22        | 0.42     |
| 1:F:33:PHE:C     | 1:F:48:ARG:HB2   | 2.40        | 0.42     |
| 5:J:64:TYR:CD1   | 5:J:78:LEU:CD1   | 3.02        | 0.42     |
| 2:G:12:ARG:HD2   | 2:G:22:PHE:CB    | 2.39        | 0.42     |
| 1:F:185:PRO:HB3  | 1:F:208:PHE:CD1  | 2.54        | 0.42     |
| 4:D:112:ILE:HD13 | 4:D:112:ILE:N    | 2.34        | 0.42     |
| 5:J:132:ILE:N    | 5:J:132:ILE:CD1  | 2.82        | 0.42     |
| 5:E:79:GLU:O     | 5:E:81:PRO:HD3   | 2.18        | 0.42     |
| 4:D:43:SER:HA    | 5:E:90:PHE:CZ    | 2.55        | 0.42     |
| 1:A:161:GLU:O    | 1:A:165:VAL:HG21 | 2.20        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:E:86:THR:OG1   | 5:E:110:VAL:HG23 | 2.19        | 0.42     |
| 1:F:159:TYR:OH   | 3:H:1:ARG:O      | 2.31        | 0.42     |
| 4:I:185:ASN:ND2  | 4:I:185:ASN:C    | 2.70        | 0.42     |
| 2:B:23:LEU:CD2   | 2:B:39:LEU:HD13  | 2.50        | 0.42     |
| 5:J:79:GLU:C     | 5:J:81:PRO:HD3   | 2.40        | 0.42     |
| 1:A:213:ILE:CD1  | 1:A:263:HIS:HB2  | 2.49        | 0.42     |
| 4:I:35:TRP:O     | 4:I:47:ILE:HG13  | 2.18        | 0.42     |
| 1:A:108:ARG:O    | 1:A:110:LEU:CD1  | 2.64        | 0.42     |
| 4:D:12:SER:CB    | 4:D:109:LYS:NZ   | 2.82        | 0.42     |
| 1:F:125:ALA:O    | 1:F:134:THR:CG2  | 2.68        | 0.42     |
| 5:J:146:GLY:HA2  | 5:J:176:GLU:OE2  | 2.20        | 0.42     |
| 1:A:188:HIS:CE1  | 1:A:204:TRP:HB2  | 2.54        | 0.42     |
| 1:A:268:LYS:HA   | 1:A:268:LYS:HD2  | 1.85        | 0.42     |
| 5:E:114:LEU:HD13 | 5:E:214:LEU:HD21 | 2.02        | 0.42     |
| 1:F:137:ASP:OD1  | 1:F:137:ASP:C    | 2.56        | 0.42     |
| 4:D:25:TYR:CE2   | 4:D:33:PHE:CZ    | 3.07        | 0.42     |
| 1:A:235:PRO:HG2  | 2:B:65:LEU:HD22  | 2.01        | 0.42     |
| 1:A:220:ASP:OD1  | 1:A:256:ARG:HD3  | 2.19        | 0.42     |
| 1:A:157:ARG:CZ   | 1:A:161:GLU:OE1  | 2.67        | 0.42     |
| 5:J:177:GLN:O    | 5:J:183:SER:HB2  | 2.20        | 0.42     |
| 4:I:14:PRO:HG2   | 4:I:17:ALA:CB    | 2.49        | 0.42     |
| 4:I:124:ASP:OD2  | 5:J:125:PHE:HZ   | 2.02        | 0.42     |
| 4:I:36:TYR:CE1   | 5:J:102:PHE:HE2  | 2.35        | 0.42     |
| 1:F:127:LYS:HE3  | 1:F:133:TRP:O    | 2.19        | 0.42     |
| 4:I:163:ARG:H    | 4:I:163:ARG:HG2  | 1.42        | 0.42     |
| 2:B:41:LYS:HG3   | 2:B:78:TYR:CE2   | 2.55        | 0.42     |
| 1:A:44:ARG:HA    | 1:A:64:THR:CG2   | 2.50        | 0.42     |
| 1:A:183:ASP:HA   | 1:A:184:PRO:HD3  | 1.79        | 0.42     |
| 1:F:34:VAL:CG1   | 1:F:60:TRP:HH2   | 2.33        | 0.42     |
| 1:A:63:GLU:OE2   | 1:A:63:GLU:CA    | 2.64        | 0.42     |
| 5:E:64:TYR:CD1   | 5:E:76:LEU:HD21  | 2.55        | 0.42     |
| 5:J:131:GLU:O    | 5:J:135:THR:OG1  | 2.19        | 0.42     |
| 5:E:154:LEU:HD23 | 5:E:155:SER:CA   | 2.48        | 0.42     |
| 4:D:37:ARG:CB    | 4:D:47:ILE:HD13  | 2.49        | 0.42     |
| 1:A:98:MET:C     | 1:A:98:MET:SD    | 2.98        | 0.42     |
| 5:J:68:ARG:HG2   | 5:J:68:ARG:HH11  | 1.84        | 0.42     |
| 4:I:185:ASN:N    | 4:I:185:ASN:HD22 | 2.16        | 0.42     |
| 4:D:122:LEU:HD12 | 5:E:128:SER:N    | 2.35        | 0.42     |
| 1:F:8:PHE:O      | 1:F:24:ALA:HA    | 2.20        | 0.42     |
| 1:A:51:TRP:HZ3   | 1:A:52:ILE:HD13  | 1.85        | 0.42     |
| 4:I:89:TRP:CD1   | 4:I:89:TRP:N     | 2.88        | 0.42     |
| 1:F:115:GLN:HE21 | 1:F:115:GLN:HB3  | 1.55        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:244:TRP:HE1  | 2:B:99:MET:HG3   | 1.84        | 0.42     |
| 2:G:10:TYR:OH    | 2:G:26:TYR:HB2   | 2.20        | 0.42     |
| 1:F:22:PHE:CD2   | 1:F:71:SER:CB    | 3.00        | 0.42     |
| 1:F:202:ARG:NH1  | 1:F:244:TRP:CH2  | 2.88        | 0.42     |
| 5:E:239:ARG:NH1  | 5:E:239:ARG:HG3  | 2.33        | 0.42     |
| 2:B:35:ILE:HD11  | 2:B:82:VAL:CG1   | 2.48        | 0.42     |
| 2:G:35:ILE:HD11  | 2:G:84:HIS:CD2   | 2.55        | 0.42     |
| 4:D:2:LYS:NZ     | 5:E:42:GLY:HA3   | 2.35        | 0.42     |
| 4:D:60:ARG:NH2   | 4:D:83:ASP:OD2   | 2.42        | 0.42     |
| 1:A:123:TYR:CE1  | 1:A:140:ALA:HA   | 2.55        | 0.42     |
| 1:F:96:GLN:HB3   | 2:G:56:PHE:CE2   | 2.55        | 0.42     |
| 2:B:22:PHE:C     | 2:B:70:PHE:CE1   | 2.93        | 0.42     |
| 5:J:36:ARG:NH2   | 5:J:86:THR:O     | 2.53        | 0.42     |
| 5:J:89:TYR:CE2   | 5:J:108:LEU:HG   | 2.55        | 0.42     |
| 1:F:71:SER:O     | 1:F:75:ARG:HB2   | 2.20        | 0.42     |
| 4:D:122:LEU:HG   | 5:E:127:PRO:HA   | 2.01        | 0.42     |
| 2:B:33:SER:HB3   | 2:B:62:PHE:CE1   | 2.55        | 0.42     |
| 2:G:35:ILE:HD11  | 2:G:84:HIS:CG    | 2.55        | 0.42     |
| 1:F:191:HIS:HB2  | 1:F:274:TRP:CZ3  | 2.55        | 0.42     |
| 5:E:20:THR:O     | 5:E:20:THR:CG2   | 2.67        | 0.42     |
| 5:J:25:GLN:HE22  | 5:J:29:HIS:N     | 2.17        | 0.42     |
| 4:D:34:PHE:HB3   | 4:D:46:LEU:CD1   | 2.50        | 0.42     |
| 1:A:134:THR:HG23 | 1:A:134:THR:O    | 2.20        | 0.42     |
| 1:A:150:ALA:CB   | 5:E:96:ALA:HB1   | 2.50        | 0.42     |
| 1:A:123:TYR:CE2  | 3:C:10:PHE:CE2   | 3.08        | 0.42     |
| 3:C:5:THR:HG22   | 3:C:8:TRP:HZ3    | 1.84        | 0.42     |
| 4:D:94:GLN:HB2   | 4:D:97:LYS:CG    | 2.48        | 0.42     |
| 5:J:172:GLN:HA   | 5:J:173:PRO:HD3  | 1.94        | 0.42     |
| 4:I:47:ILE:HD12  | 4:I:48:MET:HB2   | 2.01        | 0.42     |
| 1:F:82:LEU:HD21  | 1:F:93:HIS:CE1   | 2.55        | 0.42     |
| 4:I:98:LEU:HD12  | 5:J:35:TYR:OH    | 2.19        | 0.41     |
| 1:A:217:TRP:CD1  | 1:A:247:VAL:HG13 | 2.54        | 0.41     |
| 1:F:8:PHE:HE2    | 1:F:27:TYR:CD1   | 2.38        | 0.41     |
| 1:F:77:ASN:HA    | 1:F:80:ILE:HD12  | 2.02        | 0.41     |
| 5:E:3:GLN:N      | 5:E:3:GLN:OE1    | 2.53        | 0.41     |
| 5:E:46:ILE:O     | 5:E:58:GLY:N     | 2.45        | 0.41     |
| 4:I:160:LEU:O    | 4:I:168:LYS:NZ   | 2.52        | 0.41     |
| 5:J:120:PRO:HG2  | 5:J:232:VAL:CG2  | 2.49        | 0.41     |
| 4:D:93:ASN:C     | 4:D:95:GLY:N     | 2.73        | 0.41     |
| 1:A:52:ILE:HA    | 1:A:52:ILE:HD12  | 1.88        | 0.41     |
| 1:F:85:TYR:HB3   | 1:F:87:GLN:HG3   | 2.01        | 0.41     |
| 5:J:29:HIS:CD2   | 5:J:95:GLY:HA3   | 2.55        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:J:176:GLU:C    | 5:J:178:PRO:HD3  | 2.39        | 0.41     |
| 1:A:232:GLU:CD   | 2:B:6:LYS:HE2    | 2.40        | 0.41     |
| 5:E:87:SER:OG    | 5:E:88:LEU:N     | 2.52        | 0.41     |
| 1:F:23:ILE:O     | 1:F:23:ILE:CG2   | 2.68        | 0.41     |
| 1:A:244:TRP:C    | 1:A:244:TRP:CE3  | 2.93        | 0.41     |
| 2:G:12:ARG:NH1   | 2:G:22:PHE:CD1   | 2.88        | 0.41     |
| 1:A:213:ILE:CG1  | 1:A:262:GLN:O    | 2.59        | 0.41     |
| 2:B:7:ILE:C      | 2:B:8:GLN:NE2    | 2.73        | 0.41     |
| 5:J:25:GLN:NE2   | 5:J:29:HIS:N     | 2.68        | 0.41     |
| 1:A:173:GLU:OE1  | 1:A:176:LYS:HD3  | 2.21        | 0.41     |
| 1:F:3:HIS:HB3    | 1:F:29:ASP:OD2   | 2.19        | 0.41     |
| 1:A:74:ASP:HB3   | 1:A:95:LEU:HD23  | 2.01        | 0.41     |
| 1:A:70:HIS:HA    | 1:A:73:THR:OG1   | 2.21        | 0.41     |
| 5:E:11:LEU:HD21  | 5:E:19:LEU:HD22  | 2.02        | 0.41     |
| 1:F:156:GLN:O    | 1:F:159:TYR:HB3  | 2.20        | 0.41     |
| 1:F:33:PHE:O     | 1:F:48:ARG:N     | 2.47        | 0.41     |
| 5:J:19:LEU:HD11  | 5:J:78:LEU:HB3   | 2.02        | 0.41     |
| 4:I:13:VAL:O     | 4:I:108:VAL:HA   | 2.21        | 0.41     |
| 1:F:204:TRP:HH2  | 2:G:99:MET:HE2   | 1.85        | 0.41     |
| 1:A:14:ARG:HB3   | 1:A:17:ARG:HB2   | 2.01        | 0.41     |
| 4:I:114:ASN:HA   | 4:I:115:PRO:HD2  | 1.94        | 0.41     |
| 5:J:132:ILE:CG2  | 5:J:195:ALA:HB1  | 2.49        | 0.41     |
| 1:A:255:GLN:HB3  | 1:A:255:GLN:HE21 | 1.71        | 0.41     |
| 5:E:7:ASN:HA     | 5:E:8:PRO:HA     | 1.64        | 0.41     |
| 5:E:82:SER:HB2   | 5:E:85:GLN:CG    | 2.50        | 0.41     |
| 5:J:204:HIS:HD2  | 5:J:236:ALA:O    | 2.03        | 0.41     |
| 5:J:191:LEU:HD12 | 5:J:192:ARG:N    | 2.35        | 0.41     |
| 5:J:144:ALA:O    | 5:J:147:PHE:CE2  | 2.73        | 0.41     |
| 5:E:220:TRP:NE1  | 5:E:226:LYS:HA   | 2.36        | 0.41     |
| 1:F:241:PHE:CD1  | 1:F:241:PHE:N    | 2.88        | 0.41     |
| 1:A:133:TRP:CZ2  | 1:A:153:ALA:N    | 2.88        | 0.41     |
| 3:C:2:PHE:CD2    | 3:C:3:PRO:O      | 2.74        | 0.41     |
| 1:A:158:ALA:HB1  | 4:D:31:GLN:HB2   | 2.03        | 0.41     |
| 5:E:77:ILE:CD1   | 5:E:77:ILE:N     | 2.77        | 0.41     |
| 4:D:14:PRO:HD2   | 4:I:71:TYR:HE1   | 1.82        | 0.41     |
| 2:B:23:LEU:C     | 2:B:23:LEU:HD12  | 2.41        | 0.41     |
| 5:E:118:PHE:O    | 5:E:147:PHE:HA   | 2.21        | 0.41     |
| 5:E:193:VAL:HG23 | 5:E:194:SER:O    | 2.20        | 0.41     |
| 5:E:25:GLN:OE1   | 5:E:29:HIS:HB2   | 2.19        | 0.41     |
| 1:A:99:PHE:CE2   | 3:C:3:PRO:HG3    | 2.55        | 0.41     |
| 1:A:218:GLN:HB2  | 1:A:260:HIS:NE2  | 2.36        | 0.41     |
| 1:A:259:CYS:O    | 1:A:271:THR:HA   | 2.19        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:E:161:LYS:HZ3  | 5:E:161:LYS:HB2  | 1.83        | 0.41     |
| 2:B:84:HIS:CB    | 2:B:87:LEU:HD12  | 2.51        | 0.41     |
| 1:F:80:ILE:CD1   | 3:H:10:PHE:H     | 2.33        | 0.41     |
| 4:D:138:PHE:HE2  | 4:D:171:SER:HA   | 1.85        | 0.41     |
| 1:A:95:LEU:HD11  | 1:A:116:TYR:CD1  | 2.54        | 0.41     |
| 4:I:141:GLN:HA   | 4:I:141:GLN:OE1  | 2.21        | 0.41     |
| 4:D:50:ILE:CD1   | 4:D:65:LEU:HB3   | 2.46        | 0.41     |
| 4:D:99:ILE:N     | 4:D:99:ILE:HD12  | 2.36        | 0.41     |
| 5:J:41:LEU:HB2   | 5:J:44:ARG:NH2   | 2.36        | 0.41     |
| 5:J:163:VAL:C    | 5:J:164:HIS:ND1  | 2.74        | 0.41     |
| 5:J:36:ARG:NE    | 5:J:87:SER:HB3   | 2.34        | 0.41     |
| 5:J:47:TYR:CE2   | 5:J:61:PRO:HB2   | 2.56        | 0.41     |
| 4:D:123:ARG:NH1  | 5:E:239:ARG:HD3  | 2.35        | 0.41     |
| 2:B:35:ILE:HD12  | 2:B:84:HIS:CD2   | 2.44        | 0.41     |
| 1:A:5:MET:SD     | 1:A:171:TYR:CE2  | 3.10        | 0.41     |
| 1:A:87:GLN:OE1   | 1:A:118:TYR:OH   | 2.31        | 0.41     |
| 1:A:68:LYS:CB    | 5:E:54:VAL:HG22  | 2.51        | 0.41     |
| 5:E:97:SER:O     | 5:E:98:HIS:ND1   | 2.54        | 0.41     |
| 1:F:34:VAL:HG12  | 1:F:60:TRP:HH2   | 1.86        | 0.41     |
| 1:F:70:HIS:ND1   | 3:H:2:PHE:CZ     | 2.70        | 0.41     |
| 1:A:217:TRP:CH2  | 1:A:259:CYS:HB2  | 2.55        | 0.41     |
| 4:I:18:ILE:HA    | 4:I:76:ILE:O     | 2.20        | 0.41     |
| 5:E:117:VAL:HG12 | 5:E:227:PRO:CG   | 2.51        | 0.41     |
| 2:G:4:THR:OG1    | 2:G:87:LEU:HD21  | 2.20        | 0.41     |
| 1:F:127:LYS:HG3  | 1:F:134:THR:HG22 | 2.02        | 0.41     |
| 2:G:30:PHE:O     | 2:G:62:PHE:CD1   | 2.73        | 0.41     |
| 1:A:95:LEU:HD11  | 1:A:116:TYR:CE1  | 2.55        | 0.41     |
| 1:F:55:GLU:OE1   | 1:F:55:GLU:HA    | 2.21        | 0.41     |
| 1:A:124:ILE:HD11 | 1:A:144:LYS:HB2  | 2.03        | 0.41     |
| 5:J:49:SER:HB3   | 5:J:68:ARG:HH11  | 1.86        | 0.41     |
| 4:I:134:LEU:CD2  | 5:J:139:THR:HG21 | 2.51        | 0.41     |
| 5:E:187:LEU:HG   | 5:E:188:SER:H    | 1.85        | 0.41     |
| 1:F:51:TRP:CD1   | 1:F:175:GLY:HA2  | 2.56        | 0.41     |
| 1:F:80:ILE:HD13  | 3:H:10:PHE:H     | 1.85        | 0.41     |
| 5:E:9:ARG:NH1    | 5:E:104:PRO:CB   | 2.81        | 0.41     |
| 1:A:5:MET:HB2    | 1:A:168:LEU:HD13 | 2.03        | 0.41     |
| 5:J:150:ASP:C    | 5:J:151:HIS:CD2  | 2.95        | 0.41     |
| 1:A:74:ASP:HA    | 1:A:77:ASN:ND2   | 2.35        | 0.41     |
| 1:F:183:ASP:HA   | 1:F:184:PRO:HD3  | 1.79        | 0.41     |
| 5:J:154:LEU:CG   | 5:J:209:VAL:HG22 | 2.49        | 0.40     |
| 5:J:118:PHE:O    | 5:J:147:PHE:HA   | 2.21        | 0.40     |
| 4:I:114:ASN:ND2  | 4:I:114:ASN:C    | 2.74        | 0.40     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:F:143:THR:HA   | 1:F:146:LYS:CD   | 2.51        | 0.40     |
| 1:A:151:HIS:O    | 1:A:154:GLU:HG2  | 2.20        | 0.40     |
| 5:E:217:ASN:ND2  | 5:E:217:ASN:N    | 2.68        | 0.40     |
| 5:E:57:LYS:H     | 5:E:57:LYS:HG2   | 1.55        | 0.40     |
| 5:E:25:GLN:OE1   | 5:E:29:HIS:N     | 2.31        | 0.40     |
| 5:E:30:GLU:HB3   | 5:E:51:ASN:ND2   | 2.36        | 0.40     |
| 5:E:97:SER:HB3   | 5:E:99:GLU:OE1   | 2.21        | 0.40     |
| 5:J:43:LEU:HD12  | 5:J:44:ARG:H     | 1.86        | 0.40     |
| 5:J:41:LEU:HB2   | 5:J:44:ARG:CZ    | 2.51        | 0.40     |
| 4:I:28:ARG:HA    | 4:I:70:GLN:HE21  | 1.84        | 0.40     |
| 1:A:34:VAL:HG21  | 1:A:45:MET:HE1   | 2.03        | 0.40     |
| 5:E:159:ASN:HD22 | 5:E:204:HIS:HB3  | 1.87        | 0.40     |
| 4:I:125:SER:N    | 5:J:125:PHE:CE2  | 2.89        | 0.40     |
| 1:F:55:GLU:OE2   | 1:F:170:ARG:NE   | 2.54        | 0.40     |
| 1:F:197:HIS:CE1  | 1:F:198:GLU:HG3  | 2.56        | 0.40     |
| 4:D:9:GLY:HA2    | 4:D:10:PRO:HD3   | 1.73        | 0.40     |
| 1:F:115:GLN:CG   | 2:G:60:TRP:CH2   | 2.93        | 0.40     |
| 4:I:94:GLN:HB3   | 4:I:97:LYS:CD    | 2.30        | 0.40     |
| 5:J:159:ASN:ND2  | 5:J:204:HIS:N    | 2.56        | 0.40     |
| 5:J:206:ARG:NH2  | 5:J:208:GLN:HE21 | 2.20        | 0.40     |
| 5:J:205:PHE:CD2  | 5:J:236:ALA:O    | 2.70        | 0.40     |
| 4:I:170:ASN:O    | 4:I:171:SER:HB3  | 2.21        | 0.40     |
| 1:A:234:ARG:NH2  | 2:B:10:TYR:CG    | 2.89        | 0.40     |
| 1:A:33:PHE:C     | 1:A:48:ARG:HB2   | 2.42        | 0.40     |
| 2:G:12:ARG:HD2   | 2:G:22:PHE:N     | 2.37        | 0.40     |
| 1:A:185:PRO:CB   | 1:A:208:PHE:HB3  | 2.38        | 0.40     |
| 5:J:47:TYR:HE2   | 5:J:61:PRO:HB2   | 1.86        | 0.40     |
| 1:F:267:PRO:CG   | 1:F:268:LYS:H    | 2.33        | 0.40     |
| 5:J:9:ARG:NH1    | 5:J:9:ARG:CG     | 2.83        | 0.40     |
| 5:J:33:SER:HA    | 5:J:74:PHE:HE2   | 1.86        | 0.40     |
| 4:D:160:LEU:HD12 | 4:D:160:LEU:O    | 2.21        | 0.40     |
| 5:J:206:ARG:HH11 | 5:J:206:ARG:CG   | 2.34        | 0.40     |
| 2:B:12:ARG:N     | 2:B:21:ASN:HD21  | 2.18        | 0.40     |
| 1:A:31:THR:OG1   | 1:A:209:TYR:OH   | 2.36        | 0.40     |
| 1:F:228:THR:HG22 | 1:F:247:VAL:CG1  | 2.46        | 0.40     |
| 1:A:191:HIS:HE1  | 1:A:193:PRO:HG3  | 1.86        | 0.40     |
| 2:G:16:GLU:OE2   | 2:G:19:LYS:NZ    | 2.47        | 0.40     |
| 1:A:181:ARG:HG2  | 1:A:181:ARG:HH11 | 1.86        | 0.40     |
| 1:A:99:PHE:CD2   | 3:C:3:PRO:HG3    | 2.57        | 0.40     |
| 5:E:99:GLU:H     | 5:E:99:GLU:HG2   | 1.59        | 0.40     |
| 1:F:7:TYR:HE2    | 3:H:2:PHE:HA     | 1.86        | 0.40     |
| 1:A:234:ARG:CZ   | 2:B:10:TYR:CG    | 3.04        | 0.40     |

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| Atom-1           | Atom-2         | Distance(Å) | Clash(Å) |
|------------------|----------------|-------------|----------|
| 2:G:95:TRP:CD1   | 2:G:95:TRP:C   | 2.92        | 0.40     |
| 5:J:156:TRP:HZ2  | 5:J:189:SER:O  | 2.05        | 0.40     |
| 4:I:122:LEU:HD11 | 5:J:141:VAL:CB | 2.50        | 0.40     |
| 1:F:80:ILE:HG21  | 3:H:10:PHE:HB2 | 2.04        | 0.40     |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 272/275 (99%)   | 259 (95%)  | 12 (4%)  | 1 (0%)   | 43          | 76  |
| 1   | F     | 272/275 (99%)   | 257 (94%)  | 14 (5%)  | 1 (0%)   | 43          | 76  |
| 2   | B     | 97/100 (97%)    | 93 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 2   | G     | 97/100 (97%)    | 93 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 3   | C     | 8/10 (80%)      | 8 (100%)   | 0        | 0        | 100         | 100 |
| 3   | H     | 8/10 (80%)      | 8 (100%)   | 0        | 0        | 100         | 100 |
| 4   | D     | 197/205 (96%)   | 167 (85%)  | 24 (12%) | 6 (3%)   | 7           | 15  |
| 4   | I     | 197/205 (96%)   | 169 (86%)  | 22 (11%) | 6 (3%)   | 7           | 15  |
| 5   | E     | 239/242 (99%)   | 223 (93%)  | 15 (6%)  | 1 (0%)   | 43          | 76  |
| 5   | J     | 239/242 (99%)   | 220 (92%)  | 18 (8%)  | 1 (0%)   | 43          | 76  |
| All | All   | 1626/1664 (98%) | 1497 (92%) | 113 (7%) | 16 (1%)  | 22          | 51  |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 94  | GLN  |
| 4   | D     | 8   | SER  |
| 4   | D     | 40  | SER  |
| 4   | I     | 7   | ASN  |
| 4   | I     | 40  | SER  |
| 4   | I     | 94  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 7   | ASN  |
| 4   | I     | 8   | SER  |
| 1   | F     | 163 | THR  |
| 1   | A     | 163 | THR  |
| 4   | D     | 27  | ASP  |
| 4   | D     | 53  | ASN  |
| 5   | E     | 222 | GLN  |
| 4   | I     | 27  | ASP  |
| 5   | J     | 222 | GLN  |
| 4   | I     | 9   | GLY  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |     |
|-----|-------|-----------------|------------|-----------|-------------|-----|
| 1   | A     | 230/231 (100%)  | 194 (84%)  | 36 (16%)  | 4           | 10  |
| 1   | F     | 230/231 (100%)  | 190 (83%)  | 40 (17%)  | 3           | 7   |
| 2   | B     | 94/95 (99%)     | 77 (82%)   | 17 (18%)  | 2           | 7   |
| 2   | G     | 94/95 (99%)     | 78 (83%)   | 16 (17%)  | 3           | 8   |
| 3   | C     | 9/9 (100%)      | 9 (100%)   | 0         | 100         | 100 |
| 3   | H     | 9/9 (100%)      | 9 (100%)   | 0         | 100         | 100 |
| 4   | D     | 177/183 (97%)   | 145 (82%)  | 32 (18%)  | 2           | 7   |
| 4   | I     | 177/183 (97%)   | 144 (81%)  | 33 (19%)  | 2           | 6   |
| 5   | E     | 214/215 (100%)  | 176 (82%)  | 38 (18%)  | 2           | 7   |
| 5   | J     | 214/215 (100%)  | 185 (86%)  | 29 (14%)  | 5           | 13  |
| All | All   | 1448/1466 (99%) | 1207 (83%) | 241 (17%) | 3           | 8   |

All (241) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 13  | SER  |
| 1   | A     | 19  | GLU  |
| 1   | A     | 20  | PRO  |
| 1   | A     | 33  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 34  | VAL  |
| 1   | A     | 39  | ASP  |
| 1   | A     | 60  | TRP  |
| 1   | A     | 74  | ASP  |
| 1   | A     | 75  | ARG  |
| 1   | A     | 79  | ARG  |
| 1   | A     | 86  | ASN  |
| 1   | A     | 89  | GLU  |
| 1   | A     | 97  | MET  |
| 1   | A     | 98  | MET  |
| 1   | A     | 116 | TYR  |
| 1   | A     | 122 | ASP  |
| 1   | A     | 157 | ARG  |
| 1   | A     | 160 | LEU  |
| 1   | A     | 163 | THR  |
| 1   | A     | 165 | VAL  |
| 1   | A     | 166 | ASP  |
| 1   | A     | 172 | LEU  |
| 1   | A     | 186 | LYS  |
| 1   | A     | 190 | THR  |
| 1   | A     | 216 | THR  |
| 1   | A     | 225 | THR  |
| 1   | A     | 229 | GLU  |
| 1   | A     | 230 | LEU  |
| 1   | A     | 231 | VAL  |
| 1   | A     | 234 | ARG  |
| 1   | A     | 238 | ASP  |
| 1   | A     | 242 | GLN  |
| 1   | A     | 247 | VAL  |
| 1   | A     | 248 | VAL  |
| 1   | A     | 255 | GLN  |
| 1   | A     | 258 | THR  |
| 2   | B     | 1   | ILE  |
| 2   | B     | 2   | GLN  |
| 2   | B     | 6   | LYS  |
| 2   | B     | 10  | TYR  |
| 2   | B     | 13  | HIS  |
| 2   | B     | 16  | GLU  |
| 2   | B     | 23  | LEU  |
| 2   | B     | 24  | ASN  |
| 2   | B     | 36  | GLU  |
| 2   | B     | 64  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 70  | PHE  |
| 2   | B     | 74  | GLU  |
| 2   | B     | 83  | ASN  |
| 2   | B     | 84  | HIS  |
| 2   | B     | 85  | VAL  |
| 2   | B     | 86  | THR  |
| 2   | B     | 87  | LEU  |
| 4   | D     | 6   | GLN  |
| 4   | D     | 7   | ASN  |
| 4   | D     | 15  | GLU  |
| 4   | D     | 20  | SER  |
| 4   | D     | 31  | GLN  |
| 4   | D     | 33  | PHE  |
| 4   | D     | 34  | PHE  |
| 4   | D     | 48  | MET  |
| 4   | D     | 50  | ILE  |
| 4   | D     | 71  | TYR  |
| 4   | D     | 73  | SER  |
| 4   | D     | 88  | LEU  |
| 4   | D     | 98  | LEU  |
| 4   | D     | 100 | PHE  |
| 4   | D     | 102 | GLN  |
| 4   | D     | 104 | THR  |
| 4   | D     | 106 | LEU  |
| 4   | D     | 111 | ASN  |
| 4   | D     | 124 | ASP  |
| 4   | D     | 139 | ASP  |
| 4   | D     | 140 | SER  |
| 4   | D     | 142 | THR  |
| 4   | D     | 151 | ASP  |
| 4   | D     | 154 | ILE  |
| 4   | D     | 156 | ASP  |
| 4   | D     | 157 | LYS  |
| 4   | D     | 162 | MET  |
| 4   | D     | 167 | PHE  |
| 4   | D     | 180 | ASP  |
| 4   | D     | 189 | ASN  |
| 4   | D     | 191 | ILE  |
| 4   | D     | 192 | ILE  |
| 5   | E     | 1   | GLU  |
| 5   | E     | 3   | GLN  |
| 5   | E     | 13  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 18  | LYS  |
| 5   | E     | 25  | GLN  |
| 5   | E     | 30  | GLU  |
| 5   | E     | 33  | SER  |
| 5   | E     | 37  | GLN  |
| 5   | E     | 46  | ILE  |
| 5   | E     | 47  | TYR  |
| 5   | E     | 50  | MET  |
| 5   | E     | 51  | ASN  |
| 5   | E     | 53  | GLU  |
| 5   | E     | 56  | ASP  |
| 5   | E     | 59  | ASP  |
| 5   | E     | 60  | VAL  |
| 5   | E     | 72  | ARG  |
| 5   | E     | 77  | ILE  |
| 5   | E     | 78  | LEU  |
| 5   | E     | 84  | ASN  |
| 5   | E     | 93  | SER  |
| 5   | E     | 99  | GLU  |
| 5   | E     | 100 | GLN  |
| 5   | E     | 101 | TYR  |
| 5   | E     | 107 | ARG  |
| 5   | E     | 120 | PRO  |
| 5   | E     | 121 | GLU  |
| 5   | E     | 149 | PRO  |
| 5   | E     | 161 | LYS  |
| 5   | E     | 167 | VAL  |
| 5   | E     | 174 | LEU  |
| 5   | E     | 181 | ASN  |
| 5   | E     | 190 | ARG  |
| 5   | E     | 199 | GLN  |
| 5   | E     | 203 | ASN  |
| 5   | E     | 216 | GLU  |
| 5   | E     | 217 | ASN  |
| 5   | E     | 241 | ASP  |
| 1   | F     | 19  | GLU  |
| 1   | F     | 35  | ARG  |
| 1   | F     | 38  | SER  |
| 1   | F     | 39  | ASP  |
| 1   | F     | 43  | GLN  |
| 1   | F     | 51  | TRP  |
| 1   | F     | 54  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 72  | GLN  |
| 1   | F     | 75  | ARG  |
| 1   | F     | 79  | ARG  |
| 1   | F     | 85  | TYR  |
| 1   | F     | 86  | ASN  |
| 1   | F     | 94  | THR  |
| 1   | F     | 98  | MET  |
| 1   | F     | 99  | PHE  |
| 1   | F     | 110 | LEU  |
| 1   | F     | 115 | GLN  |
| 1   | F     | 132 | SER  |
| 1   | F     | 134 | THR  |
| 1   | F     | 143 | THR  |
| 1   | F     | 146 | LYS  |
| 1   | F     | 155 | GLN  |
| 1   | F     | 170 | ARG  |
| 1   | F     | 174 | ASN  |
| 1   | F     | 177 | GLU  |
| 1   | F     | 186 | LYS  |
| 1   | F     | 188 | HIS  |
| 1   | F     | 214 | THR  |
| 1   | F     | 223 | ASP  |
| 1   | F     | 225 | THR  |
| 1   | F     | 233 | THR  |
| 1   | F     | 238 | ASP  |
| 1   | F     | 242 | GLN  |
| 1   | F     | 244 | TRP  |
| 1   | F     | 247 | VAL  |
| 1   | F     | 254 | GLU  |
| 1   | F     | 255 | GLN  |
| 1   | F     | 256 | ARG  |
| 1   | F     | 261 | VAL  |
| 1   | F     | 273 | ARG  |
| 2   | G     | 3   | ARG  |
| 2   | G     | 4   | THR  |
| 2   | G     | 17  | ASN  |
| 2   | G     | 24  | ASN  |
| 2   | G     | 31  | HIS  |
| 2   | G     | 35  | ILE  |
| 2   | G     | 36  | GLU  |
| 2   | G     | 40  | LEU  |
| 2   | G     | 50  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | G     | 59  | ASP  |
| 2   | G     | 62  | PHE  |
| 2   | G     | 65  | LEU  |
| 2   | G     | 68  | THR  |
| 2   | G     | 70  | PHE  |
| 2   | G     | 89  | GLN  |
| 2   | G     | 96  | ASP  |
| 4   | I     | 2   | LYS  |
| 4   | I     | 14  | PRO  |
| 4   | I     | 22  | ASN  |
| 4   | I     | 24  | THR  |
| 4   | I     | 31  | GLN  |
| 4   | I     | 32  | SER  |
| 4   | I     | 42  | LYS  |
| 4   | I     | 44  | PRO  |
| 4   | I     | 50  | ILE  |
| 4   | I     | 53  | ASN  |
| 4   | I     | 57  | GLU  |
| 4   | I     | 69  | SER  |
| 4   | I     | 71  | TYR  |
| 4   | I     | 88  | LEU  |
| 4   | I     | 89  | TRP  |
| 4   | I     | 97  | LYS  |
| 4   | I     | 98  | LEU  |
| 4   | I     | 102 | GLN  |
| 4   | I     | 105 | GLU  |
| 4   | I     | 113 | GLN  |
| 4   | I     | 114 | ASN  |
| 4   | I     | 116 | ASP  |
| 4   | I     | 128 | SER  |
| 4   | I     | 129 | ASP  |
| 4   | I     | 146 | GLN  |
| 4   | I     | 160 | LEU  |
| 4   | I     | 163 | ARG  |
| 4   | I     | 167 | PHE  |
| 4   | I     | 177 | ASN  |
| 4   | I     | 180 | ASP  |
| 4   | I     | 185 | ASN  |
| 4   | I     | 190 | SER  |
| 4   | I     | 194 | GLU  |
| 5   | J     | 1   | GLU  |
| 5   | J     | 4   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | J     | 9   | ARG  |
| 5   | J     | 12  | ILE  |
| 5   | J     | 17  | LYS  |
| 5   | J     | 18  | LYS  |
| 5   | J     | 19  | LEU  |
| 5   | J     | 25  | GLN  |
| 5   | J     | 37  | GLN  |
| 5   | J     | 55  | THR  |
| 5   | J     | 56  | ASP  |
| 5   | J     | 79  | GLU  |
| 5   | J     | 101 | TYR  |
| 5   | J     | 102 | PHE  |
| 5   | J     | 108 | LEU  |
| 5   | J     | 115 | LYS  |
| 5   | J     | 135 | THR  |
| 5   | J     | 154 | LEU  |
| 5   | J     | 167 | VAL  |
| 5   | J     | 181 | ASN  |
| 5   | J     | 182 | ASP  |
| 5   | J     | 190 | ARG  |
| 5   | J     | 205 | PHE  |
| 5   | J     | 206 | ARG  |
| 5   | J     | 215 | SER  |
| 5   | J     | 217 | ASN  |
| 5   | J     | 218 | ASP  |
| 5   | J     | 230 | GLN  |
| 5   | J     | 232 | VAL  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 32  | GLN  |
| 1   | A     | 43  | GLN  |
| 1   | A     | 77  | ASN  |
| 1   | A     | 86  | ASN  |
| 1   | A     | 114 | HIS  |
| 1   | A     | 141 | GLN  |
| 1   | A     | 155 | GLN  |
| 1   | A     | 156 | GLN  |
| 1   | A     | 180 | GLN  |
| 1   | A     | 188 | HIS  |
| 1   | A     | 192 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 218 | GLN  |
| 1   | A     | 255 | GLN  |
| 2   | B     | 8   | GLN  |
| 2   | B     | 24  | ASN  |
| 2   | B     | 51  | HIS  |
| 2   | B     | 83  | ASN  |
| 2   | B     | 84  | HIS  |
| 4   | D     | 6   | GLN  |
| 4   | D     | 64  | GLN  |
| 4   | D     | 170 | ASN  |
| 4   | D     | 185 | ASN  |
| 4   | D     | 188 | ASN  |
| 5   | E     | 51  | ASN  |
| 5   | E     | 73  | ASN  |
| 5   | E     | 84  | ASN  |
| 5   | E     | 159 | ASN  |
| 5   | E     | 199 | GLN  |
| 5   | E     | 203 | ASN  |
| 5   | E     | 208 | GLN  |
| 5   | E     | 217 | ASN  |
| 1   | F     | 32  | GLN  |
| 1   | F     | 43  | GLN  |
| 1   | F     | 86  | ASN  |
| 1   | F     | 115 | GLN  |
| 1   | F     | 141 | GLN  |
| 1   | F     | 155 | GLN  |
| 1   | F     | 156 | GLN  |
| 1   | F     | 174 | ASN  |
| 1   | F     | 188 | HIS  |
| 1   | F     | 191 | HIS  |
| 1   | F     | 255 | GLN  |
| 1   | F     | 260 | HIS  |
| 2   | G     | 2   | GLN  |
| 2   | G     | 13  | HIS  |
| 2   | G     | 21  | ASN  |
| 2   | G     | 24  | ASN  |
| 2   | G     | 31  | HIS  |
| 4   | I     | 6   | GLN  |
| 4   | I     | 53  | ASN  |
| 4   | I     | 64  | GLN  |
| 4   | I     | 70  | GLN  |
| 4   | I     | 80  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | I     | 93  | ASN  |
| 4   | I     | 113 | GLN  |
| 4   | I     | 114 | ASN  |
| 4   | I     | 177 | ASN  |
| 4   | I     | 185 | ASN  |
| 4   | I     | 188 | ASN  |
| 4   | I     | 189 | ASN  |
| 5   | J     | 37  | GLN  |
| 5   | J     | 98  | HIS  |
| 5   | J     | 151 | HIS  |
| 5   | J     | 159 | ASN  |
| 5   | J     | 181 | ASN  |
| 5   | J     | 200 | ASN  |
| 5   | J     | 208 | GLN  |
| 5   | J     | 210 | GLN  |
| 5   | J     | 217 | ASN  |
| 5   | J     | 230 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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     | 274/275 (99%)   | 0.02   | 9 (3%) 44 49  | 36, 69, 105, 120      | 0     |
| 1   | F     | 274/275 (99%)   | -0.15  | 3 (1%) 77 82  | 33, 67, 86, 91        | 0     |
| 2   | B     | 99/100 (99%)    | 0.02   | 2 (2%) 62 68  | 53, 68, 93, 97        | 0     |
| 2   | G     | 99/100 (99%)    | 0.22   | 4 (4%) 36 41  | 49, 79, 96, 101       | 0     |
| 3   | C     | 10/10 (100%)    | -0.43  | 0 100 100     | 44, 48, 56, 57        | 0     |
| 3   | H     | 10/10 (100%)    | -0.11  | 0 100 100     | 34, 40, 59, 64        | 0     |
| 4   | D     | 199/205 (97%)   | 0.05   | 3 (1%) 70 75  | 32, 61, 97, 115       | 0     |
| 4   | I     | 199/205 (97%)   | 0.09   | 4 (2%) 62 68  | 20, 64, 102, 119      | 0     |
| 5   | E     | 241/242 (99%)   | -0.25  | 0 100 100     | 35, 64, 81, 92        | 0     |
| 5   | J     | 241/242 (99%)   | -0.24  | 1 (0%) 90 93  | 29, 62, 84, 94        | 0     |
| All | All   | 1646/1664 (98%) | -0.07  | 26 (1%) 68 74 | 20, 66, 96, 120       | 0     |

All (26) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | I     | 164 | SER  | 5.2  |
| 4   | D     | 131 | SER  | 5.0  |
| 1   | A     | 199 | ALA  | 4.6  |
| 4   | I     | 165 | MET  | 4.6  |
| 1   | A     | 215 | LEU  | 4.3  |
| 1   | A     | 185 | PRO  | 4.0  |
| 4   | D     | 4   | VAL  | 3.5  |
| 1   | A     | 201 | LEU  | 3.3  |
| 1   | F     | 257 | TYR  | 3.0  |
| 1   | A     | 214 | THR  | 2.8  |
| 2   | G     | 23  | LEU  | 2.7  |
| 4   | D     | 5   | GLU  | 2.7  |
| 4   | I     | 4   | VAL  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 99  | PHE  | 2.7  |
| 2   | G     | 15  | ALA  | 2.7  |
| 2   | G     | 80  | CYS  | 2.7  |
| 1   | A     | 112 | GLY  | 2.6  |
| 2   | B     | 15  | ALA  | 2.4  |
| 1   | A     | 274 | TRP  | 2.3  |
| 1   | F     | 126 | LEU  | 2.2  |
| 1   | F     | 247 | VAL  | 2.2  |
| 4   | I     | 72  | VAL  | 2.2  |
| 2   | G     | 52  | SER  | 2.1  |
| 1   | A     | 187 | THR  | 2.1  |
| 5   | J     | 187 | LEU  | 2.0  |
| 2   | B     | 46  | ILE  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.