



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:31 PM GMT

PDB ID : 2Q7R  
Title : Crystal structure of human FLAP with an iodinated analog of MK-591  
Authors : Ferguson, A.D.  
Deposited on : 2007-06-07  
Resolution : 4.00 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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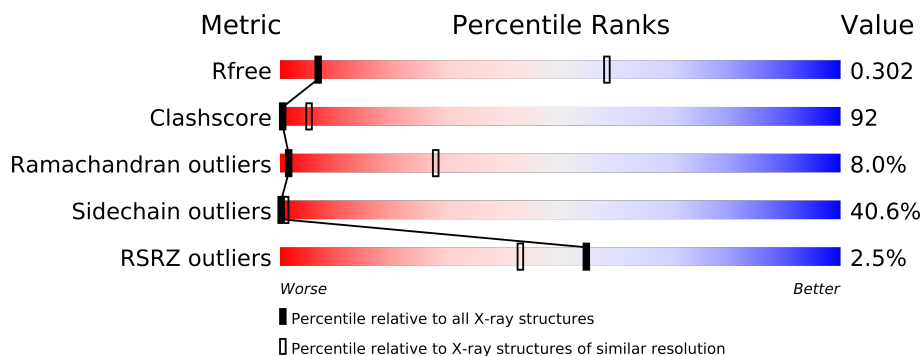
The following versions of software and data (see [references](#)) were used in the production of this report:

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 4.00 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                       | 1035 (4.52-3.46)                                      |
| Clashscore            | 79885                       | 1235 (4.50-3.50)                                      |
| Ramachandran outliers | 78287                       | 1170 (4.50-3.50)                                      |
| Sidechain outliers    | 78261                       | 1156 (4.50-3.50)                                      |
| RSRZ outliers         | 66119                       | 1035 (4.52-3.46)                                      |

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     | 161    |                  |
| 1   | B     | 161    |                  |
| 1   | C     | 161    |                  |
| 1   | D     | 161    |                  |
| 1   | E     | 161    |                  |
| 1   | F     | 161    |                  |

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|-----|----------|------------------|
| 2   | 3CS  | B     | 502 | -        | X                |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7254 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 Arachidonate 5-lipoxygenase-activatingprotein.

| Mol | Chain | Residues | Atoms |     |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|----|---------|---------|-------|
| 1   | A     | 140      | Total | C   | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 1119  | 739 | 183 | 192 | 2 | 3  |         |         |       |
| 1   | B     | 148      | Total | C   | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 1186  | 782 | 192 | 207 | 2 | 3  |         |         |       |
| 1   | C     | 149      | Total | C   | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 1193  | 786 | 193 | 209 | 2 | 3  |         |         |       |
| 1   | D     | 148      | Total | C   | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 1186  | 782 | 192 | 207 | 2 | 3  |         |         |       |
| 1   | E     | 140      | Total | C   | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 1119  | 739 | 183 | 192 | 2 | 3  |         |         |       |
| 1   | F     | 149      | Total | C   | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 1193  | 786 | 193 | 209 | 2 | 3  |         |         |       |

There are 24 discrepancies between the modelled and reference sequences:

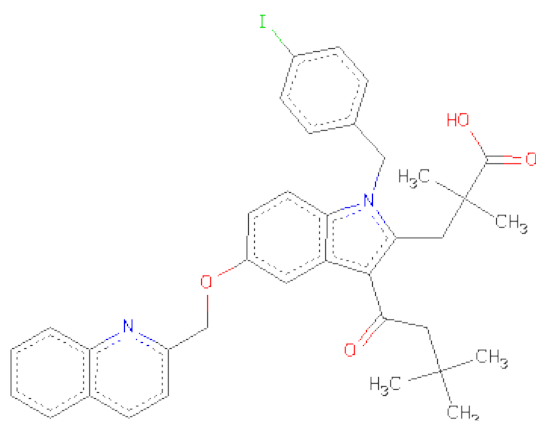
| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 1       | MSE      | MET    | MODIFIED RESIDUE | UNP P20292 |
| A     | 89      | MSE      | MET    | MODIFIED RESIDUE | UNP P20292 |
| A     | 125     | MSE      | MET    | MODIFIED RESIDUE | UNP P20292 |
| A     | 148     | ALA      | LYS    | ENGINEERED       | UNP P20292 |
| B     | 1       | MSE      | MET    | MODIFIED RESIDUE | UNP P20292 |
| B     | 89      | MSE      | MET    | MODIFIED RESIDUE | UNP P20292 |
| B     | 125     | MSE      | MET    | MODIFIED RESIDUE | UNP P20292 |
| B     | 148     | ALA      | LYS    | ENGINEERED       | UNP P20292 |
| C     | 1       | MSE      | MET    | MODIFIED RESIDUE | UNP P20292 |
| C     | 89      | MSE      | MET    | MODIFIED RESIDUE | UNP P20292 |
| C     | 125     | MSE      | MET    | MODIFIED RESIDUE | UNP P20292 |
| C     | 148     | ALA      | LYS    | ENGINEERED       | UNP P20292 |
| D     | 1       | MSE      | MET    | MODIFIED RESIDUE | UNP P20292 |
| D     | 89      | MSE      | MET    | MODIFIED RESIDUE | UNP P20292 |
| D     | 125     | MSE      | MET    | MODIFIED RESIDUE | UNP P20292 |
| D     | 148     | ALA      | LYS    | ENGINEERED       | UNP P20292 |
| E     | 1       | MSE      | MET    | MODIFIED RESIDUE | UNP P20292 |

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| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| E     | 89      | MSE      | MET    | MODIFIED RESIDUE | UNP P20292 |
| E     | 125     | MSE      | MET    | MODIFIED RESIDUE | UNP P20292 |
| E     | 148     | ALA      | LYS    | ENGINEERED       | UNP P20292 |
| F     | 1       | MSE      | MET    | MODIFIED RESIDUE | UNP P20292 |
| F     | 89      | MSE      | MET    | MODIFIED RESIDUE | UNP P20292 |
| F     | 125     | MSE      | MET    | MODIFIED RESIDUE | UNP P20292 |
| F     | 148     | ALA      | LYS    | ENGINEERED       | UNP P20292 |

- Molecule 2 is 3-[3-(3,3-DIMETHYLBUTANOYL)-1-(4-IODOBENZYL)-5-(QUINOLIN-2-YLMETHOXY)-1H-INDOL-2-YL]-2,2-DIMETHYLPROPANOICACID (three-letter code: 3CS) (formula: C<sub>36</sub>H<sub>37</sub>IN<sub>2</sub>O<sub>4</sub>).



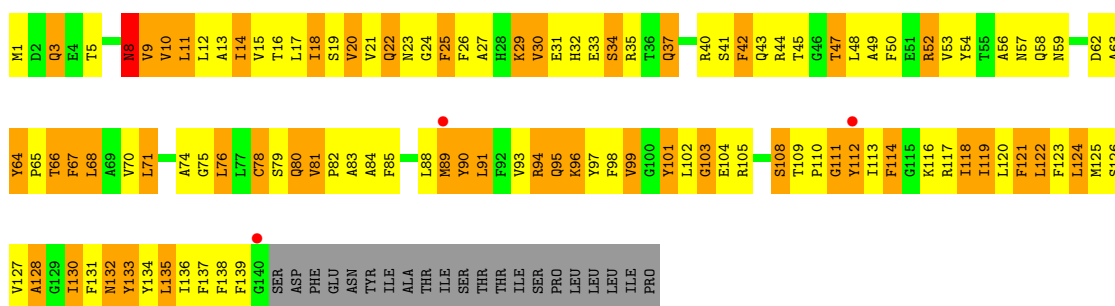
| Mol | Chain | Residues | Atoms       |         |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|---------|---------|
| 2   | C     | 1        | Total<br>43 | C<br>36 | I<br>1 | N<br>2 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>36 | I<br>1 | N<br>2 | O<br>4 | 0       | 0       |
| 2   | A     | 1        | Total<br>43 | C<br>36 | I<br>1 | N<br>2 | O<br>4 | 0       | 0       |
| 2   | F     | 1        | Total<br>43 | C<br>36 | I<br>1 | N<br>2 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>36 | I<br>1 | N<br>2 | O<br>4 | 0       | 0       |
| 2   | E     | 1        | Total<br>43 | C<br>36 | I<br>1 | N<br>2 | O<br>4 | 0       | 0       |

### 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.

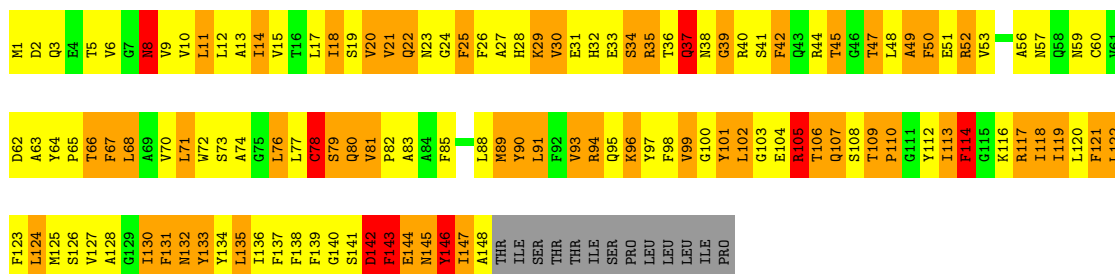
- Molecule 1: Arachidonate 5-lipoxygenase-activatingprotein

Chain A:



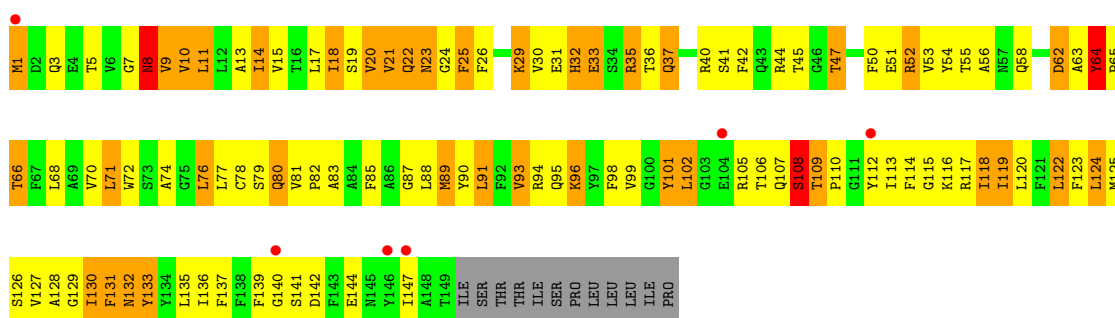
- Molecule 1: Arachidonate 5-lipoxygenase-activatingprotein

Chain B:



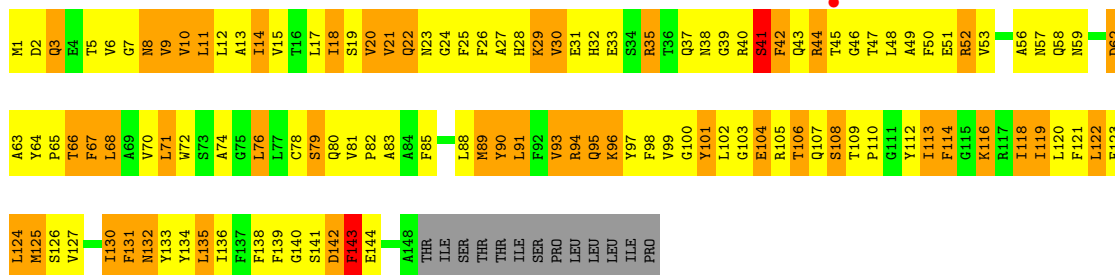
- Molecule 1: Arachidonate 5-lipoxygenase-activatingprotein

Chain C:



- Molecule 1: Arachidonate 5-lipoxygenase-activatingprotein

Chain D: 



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 4 21 2  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 180.66Å 180.66Å 139.99Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 20.00 – 4.00<br>45.18 – 4.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.5 (20.00-4.00)<br>99.5 (45.18-4.00)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.11  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.40 (at 4.00Å)   | Xtriage          |
| Refinement program  | BUSTER-TNT 2.1.1  | Depositor        |
| R, $R_{free}$   | 0.268 , 0.281<br>0.282 , 0.302                              | Depositor<br>DCC |
| $R_{free}$ test set   | 1020 reflections (5.10%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 135.6   | Xtriage          |
| Anisotropy  | 0.053   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 90.1   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Outliers  | 0 of 20007 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.88  | EDS              |
| Total number of atoms   | 7254  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 120.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.11% 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

Bond lengths and bond angles in the following residue types are not validated in this section: 3CS

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     | 0.37         | 0/1146      | 0.63        | 0/1550        |
| 1   | B     | 0.35         | 0/1215      | 0.52        | 0/1644        |
| 1   | C     | 0.39         | 0/1222      | 0.64        | 2/1654 (0.1%) |
| 1   | D     | 0.36         | 0/1215      | 0.54        | 0/1644        |
| 1   | E     | 0.34         | 0/1146      | 0.59        | 2/1550 (0.1%) |
| 1   | F     | 0.40         | 0/1222      | 0.63        | 0/1654        |
| All | All   | 0.37         | 0/7166      | 0.59        | 4/9696 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 109 | THR  | N-CA-C | 7.89  | 132.30      | 111.00   |
| 1   | E     | 109 | THR  | C-N-CD | -7.12 | 104.94      | 120.60   |
| 1   | C     | 108 | SER  | N-CA-C | -6.82 | 92.60       | 111.00   |
| 1   | E     | 104 | GLU  | N-CA-C | 5.15  | 124.92      | 111.00   |

There are no chirality outliers.

There are no planarity outliers.

### 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     | 1119  | 0        | 1116     | 234     | 0            |
| 1   | B     | 1186  | 0        | 1171     | 248     | 0            |
| 1   | C     | 1193  | 0        | 1178     | 212     | 0            |
| 1   | D     | 1186  | 0        | 1171     | 261     | 0            |
| 1   | E     | 1119  | 0        | 1116     | 217     | 0            |
| 1   | F     | 1193  | 0        | 1178     | 254     | 0            |
| 2   | A     | 43    | 0        | 36       | 29      | 0            |
| 2   | B     | 43    | 0        | 36       | 19      | 0            |
| 2   | C     | 43    | 0        | 36       | 21      | 0            |
| 2   | D     | 43    | 0        | 36       | 28      | 0            |
| 2   | E     | 43    | 0        | 36       | 23      | 0            |
| 2   | F     | 43    | 0        | 36       | 21      | 0            |
| All | All   | 7254  | 0        | 7146     | 1321    | 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 92.

All (1321) close contacts within the same asymmetric unit are listed below.

| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:120:LEU:HD23 | 2:B:502:3CS:H302 | 1.21        | 1.18     |
| 1:F:81:VAL:HG13  | 1:F:82:PRO:HD3   | 1.22        | 1.17     |
| 1:F:74:ALA:HB1   | 1:F:125:MSE:HE2  | 1.19        | 1.16     |
| 1:F:120:LEU:HD23 | 2:F:504:3CS:H302 | 1.14        | 1.13     |
| 1:B:83:ALA:HB2   | 1:B:125:MSE:HE1  | 1.19        | 1.13     |
| 1:A:120:LEU:HD23 | 2:A:503:3CS:H302 | 1.29        | 1.11     |
| 1:C:11:LEU:HD22  | 1:C:11:LEU:H     | 1.12        | 1.10     |
| 1:F:119:ILE:HD11 | 2:F:504:3CS:H12  | 1.25        | 1.09     |
| 1:A:119:ILE:HD11 | 2:A:503:3CS:H12  | 1.32        | 1.09     |
| 1:F:53:VAL:HG23  | 1:F:102:LEU:HD21 | 1.35        | 1.08     |
| 1:D:74:ALA:HB1   | 1:D:125:MSE:HE2  | 1.30        | 1.07     |
| 1:F:83:ALA:HB2   | 1:F:125:MSE:HE1  | 1.35        | 1.06     |
| 1:F:94:ARG:HA    | 1:F:114:PHE:CZ   | 1.90        | 1.06     |
| 1:D:108:SER:HA   | 1:E:40:ARG:HD2   | 1.41        | 1.02     |
| 1:B:94:ARG:HG2   | 1:B:114:PHE:HE2  | 1.21        | 1.02     |
| 1:F:11:LEU:H     | 1:F:11:LEU:HD22  | 1.22        | 1.02     |
| 2:F:504:3CS:H301 | 2:F:504:3CS:H372 | 1.40        | 1.02     |
| 1:C:83:ALA:HB2   | 1:C:125:MSE:HE1  | 1.35        | 1.02     |
| 1:B:11:LEU:HD22  | 1:B:11:LEU:H     | 1.23        | 1.01     |
| 1:C:108:SER:O    | 1:C:110:PRO:HD2  | 1.59        | 1.01     |
| 1:B:124:LEU:HA   | 1:B:127:VAL:HG12 | 1.43        | 1.00     |
| 1:C:11:LEU:HD21  | 1:C:80:GLN:HE21  | 1.25        | 0.99     |
| 1:A:83:ALA:HB2   | 1:A:125:MSE:HE1  | 1.44        | 0.99     |
| 1:E:52:ARG:HE    | 1:E:104:GLU:HB2  | 1.27        | 0.98     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:C:52:ARG:HB3   | 1:C:102:LEU:HB2  | 1.41        | 0.97     |
| 2:E:506:3CS:H323 | 2:E:506:3CS:H372 | 1.47        | 0.96     |
| 1:E:81:VAL:HG13  | 1:E:82:PRO:HD3   | 1.47        | 0.96     |
| 1:A:94:ARG:HG2   | 1:A:114:PHE:HE2  | 1.30        | 0.96     |
| 1:C:85:PHE:CZ    | 1:C:89:MSE:HE2   | 2.01        | 0.96     |
| 1:D:81:VAL:HG23  | 1:D:82:PRO:HD3   | 1.46        | 0.95     |
| 1:A:94:ARG:HG2   | 1:A:114:PHE:CE2  | 2.01        | 0.95     |
| 1:C:74:ALA:HB1   | 1:C:125:MSE:HE2  | 1.48        | 0.95     |
| 1:B:145:ASN:ND2  | 1:B:145:ASN:H    | 1.64        | 0.95     |
| 1:D:11:LEU:H     | 1:D:11:LEU:HD22  | 1.30        | 0.94     |
| 1:B:74:ALA:HB1   | 1:B:125:MSE:HE2  | 1.46        | 0.94     |
| 1:F:94:ARG:HA    | 1:F:114:PHE:CE2  | 2.03        | 0.94     |
| 1:B:81:VAL:HG13  | 1:B:82:PRO:HD3   | 1.51        | 0.93     |
| 1:D:20:VAL:HG22  | 1:F:66:THR:HG22  | 1.51        | 0.93     |
| 1:A:124:LEU:HA   | 1:A:127:VAL:HG12 | 1.51        | 0.92     |
| 1:C:52:ARG:HH21  | 1:C:105:ARG:HA   | 1.33        | 0.92     |
| 1:E:124:LEU:HA   | 1:E:127:VAL:HG12 | 1.49        | 0.92     |
| 1:E:120:LEU:HD22 | 2:E:506:3CS:H313 | 1.52        | 0.92     |
| 1:C:124:LEU:HA   | 1:C:127:VAL:HG12 | 1.50        | 0.92     |
| 1:D:45:THR:HB    | 1:F:44:ARG:HG3   | 1.50        | 0.92     |
| 1:D:43:GLN:HA    | 1:D:44:ARG:HH21  | 1.34        | 0.91     |
| 1:D:124:LEU:HA   | 1:D:127:VAL:HG12 | 1.50        | 0.91     |
| 1:B:83:ALA:HB2   | 1:B:125:MSE:CE   | 1.99        | 0.91     |
| 1:F:124:LEU:HA   | 1:F:127:VAL:HG12 | 1.53        | 0.90     |
| 1:B:79:SER:HB3   | 1:B:82:PRO:HG2   | 1.54        | 0.90     |
| 1:D:120:LEU:HD23 | 2:D:505:3CS:H301 | 1.51        | 0.90     |
| 1:D:89:MSE:HB3   | 1:D:118:ILE:HD11 | 1.54        | 0.90     |
| 1:B:94:ARG:HG2   | 1:B:114:PHE:CE2  | 2.08        | 0.89     |
| 1:E:83:ALA:HB2   | 1:E:125:MSE:HE1  | 1.52        | 0.89     |
| 1:A:21:VAL:HG22  | 2:C:501:3CS:H341 | 1.53        | 0.89     |
| 1:D:108:SER:CA   | 1:E:40:ARG:HD2   | 2.03        | 0.89     |
| 1:E:44:ARG:HH12  | 1:F:43:GLN:HB2   | 1.38        | 0.88     |
| 1:F:25:PHE:HE1   | 1:F:29:LYS:HG2   | 1.37        | 0.88     |
| 1:D:101:TYR:HA   | 1:D:109:THR:CG2  | 2.04        | 0.88     |
| 1:D:31:GLU:HG2   | 1:F:113:ILE:HD11 | 1.55        | 0.88     |
| 1:D:79:SER:HB3   | 1:D:82:PRO:HG2   | 1.54        | 0.87     |
| 1:B:70:VAL:HB    | 1:B:122:LEU:HB3  | 1.57        | 0.87     |
| 1:E:35:ARG:HA    | 1:E:35:ARG:HE    | 1.40        | 0.87     |
| 1:D:35:ARG:HE    | 1:D:35:ARG:HA    | 1.38        | 0.87     |
| 1:D:83:ALA:HB2   | 1:D:125:MSE:HE1  | 1.57        | 0.87     |
| 1:A:52:ARG:NH2   | 1:A:108:SER:HB3  | 1.89        | 0.86     |
| 1:C:11:LEU:CD2   | 1:C:80:GLN:HE21  | 1.89        | 0.86     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:8:ASN:ND2    | 1:B:8:ASN:H      | 1.70        | 0.86     |
| 1:F:96:LYS:HD2   | 1:F:96:LYS:N     | 1.90        | 0.85     |
| 1:E:89:MSE:HB3   | 1:E:118:ILE:HD11 | 1.57        | 0.85     |
| 1:F:120:LEU:HD23 | 2:F:504:3CS:C30  | 2.04        | 0.85     |
| 1:C:52:ARG:HB3   | 1:C:102:LEU:CB   | 2.05        | 0.85     |
| 1:F:89:MSE:HB3   | 1:F:118:ILE:HD11 | 1.59        | 0.85     |
| 1:A:8:ASN:ND2    | 1:A:8:ASN:H      | 1.74        | 0.85     |
| 1:A:96:LYS:N     | 1:A:96:LYS:HD2   | 1.92        | 0.85     |
| 1:F:19:SER:HB3   | 1:F:91:LEU:HD11  | 1.57        | 0.85     |
| 1:E:11:LEU:HD22  | 1:E:11:LEU:H     | 1.40        | 0.85     |
| 1:E:53:VAL:CG2   | 1:E:102:LEU:HD23 | 2.07        | 0.85     |
| 1:A:120:LEU:HA   | 2:A:503:3CS:H313 | 1.56        | 0.84     |
| 1:B:96:LYS:HD2   | 1:B:96:LYS:N     | 1.92        | 0.84     |
| 1:A:42:PHE:HD2   | 1:A:50:PHE:HZ    | 1.21        | 0.84     |
| 1:E:44:ARG:NH1   | 1:F:43:GLN:HB2   | 1.91        | 0.84     |
| 1:F:119:ILE:HD11 | 2:F:504:3CS:C12  | 2.05        | 0.83     |
| 1:A:102:LEU:HG   | 1:A:103:GLY:H    | 1.42        | 0.83     |
| 1:C:96:LYS:N     | 1:C:96:LYS:HD2   | 1.92        | 0.83     |
| 1:D:96:LYS:HD2   | 1:D:96:LYS:N     | 1.91        | 0.83     |
| 1:B:120:LEU:HD23 | 2:B:502:3CS:C30  | 2.08        | 0.83     |
| 1:C:70:VAL:HB    | 1:C:122:LEU:HB3  | 1.60        | 0.82     |
| 1:B:144:GLU:HB3  | 1:B:146:TYR:CZ   | 2.15        | 0.82     |
| 1:A:89:MSE:HB3   | 1:A:118:ILE:HD11 | 1.59        | 0.82     |
| 1:F:53:VAL:CG2   | 1:F:102:LEU:HD21 | 2.09        | 0.82     |
| 1:A:44:ARG:HE    | 1:C:45:THR:HG21  | 1.43        | 0.82     |
| 1:D:94:ARG:HG2   | 1:D:114:PHE:CZ   | 2.15        | 0.82     |
| 1:B:8:ASN:N      | 1:B:8:ASN:ND2    | 2.28        | 0.82     |
| 1:A:20:VAL:HG22  | 1:C:66:THR:HG22  | 1.60        | 0.81     |
| 1:A:120:LEU:HD23 | 2:A:503:3CS:C30  | 2.08        | 0.81     |
| 1:A:119:ILE:HD11 | 2:A:503:3CS:C12  | 2.09        | 0.81     |
| 1:D:70:VAL:HB    | 1:D:122:LEU:HB3  | 1.61        | 0.81     |
| 2:B:502:3CS:H301 | 2:B:502:3CS:H372 | 1.61        | 0.81     |
| 1:B:90:TYR:HE1   | 1:B:94:ARG:HG3   | 1.45        | 0.80     |
| 1:B:124:LEU:HA   | 1:B:127:VAL:CG1  | 2.11        | 0.80     |
| 1:A:123:PHE:HD1  | 1:A:124:LEU:HD13 | 1.46        | 0.80     |
| 1:A:31:GLU:HG2   | 1:C:113:ILE:HD11 | 1.63        | 0.80     |
| 1:E:116:LYS:HA   | 1:E:119:ILE:CD1  | 2.10        | 0.80     |
| 1:B:101:TYR:OH   | 1:C:42:PHE:HB3   | 1.81        | 0.80     |
| 1:B:52:ARG:HE    | 1:B:103:GLY:HA2  | 1.46        | 0.80     |
| 2:E:506:3CS:H341 | 1:F:21:VAL:HG22  | 1.62        | 0.80     |
| 1:C:30:VAL:HG22  | 1:C:53:VAL:HG12  | 1.64        | 0.80     |
| 1:C:139:PHE:HA   | 1:C:142:ASP:OD2  | 1.82        | 0.80     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:116:LYS:HE3  | 2:A:503:3CS:H391 | 1.63        | 0.79     |
| 1:B:34:SER:O     | 1:B:39:GLY:HA3   | 1.81        | 0.79     |
| 1:C:85:PHE:HZ    | 1:C:89:MSE:HE2   | 1.43        | 0.79     |
| 1:F:83:ALA:HB2   | 1:F:125:MSE:CE   | 2.11        | 0.78     |
| 1:E:101:TYR:OH   | 1:F:40:ARG:HG2   | 1.83        | 0.78     |
| 1:E:96:LYS:N     | 1:E:96:LYS:HD2   | 1.97        | 0.78     |
| 1:F:133:TYR:HE1  | 1:F:137:PHE:HB2  | 1.47        | 0.78     |
| 1:A:40:ARG:CB    | 1:C:52:ARG:HH12  | 1.97        | 0.78     |
| 1:F:81:VAL:CG1   | 1:F:82:PRO:HD3   | 2.09        | 0.78     |
| 1:A:108:SER:O    | 1:A:110:PRO:HD3  | 1.84        | 0.77     |
| 1:C:124:LEU:HA   | 1:C:127:VAL:CG1  | 2.14        | 0.77     |
| 1:B:145:ASN:HD22 | 1:B:145:ASN:H    | 1.27        | 0.77     |
| 1:D:116:LYS:HZ3  | 1:D:116:LYS:HA   | 1.48        | 0.77     |
| 1:D:81:VAL:CG2   | 1:D:82:PRO:HD3   | 2.14        | 0.77     |
| 1:F:72:TRP:O     | 1:F:76:LEU:HD22  | 1.83        | 0.77     |
| 1:D:44:ARG:N     | 1:D:44:ARG:HE    | 1.82        | 0.77     |
| 1:B:89:MSE:HB3   | 1:B:118:ILE:HD11 | 1.66        | 0.77     |
| 1:C:52:ARG:CB    | 1:C:102:LEU:HB2  | 2.15        | 0.77     |
| 1:F:8:ASN:ND2    | 1:F:8:ASN:H      | 1.82        | 0.77     |
| 1:B:120:LEU:HA   | 2:B:502:3CS:H313 | 1.65        | 0.76     |
| 1:A:70:VAL:HB    | 1:A:122:LEU:HB3  | 1.68        | 0.76     |
| 1:F:74:ALA:HB1   | 1:F:125:MSE:CE   | 2.10        | 0.76     |
| 1:F:43:GLN:O     | 1:F:45:THR:HG23  | 1.86        | 0.76     |
| 1:E:124:LEU:HA   | 1:E:127:VAL:CG1  | 2.15        | 0.76     |
| 1:D:66:THR:HG22  | 1:E:20:VAL:HG22  | 1.67        | 0.76     |
| 1:C:119:ILE:HD11 | 2:C:501:3CS:H12  | 1.66        | 0.76     |
| 1:A:11:LEU:HD23  | 1:A:80:GLN:HG2   | 1.67        | 0.76     |
| 1:D:44:ARG:HB3   | 1:E:44:ARG:NH2   | 2.01        | 0.76     |
| 1:A:8:ASN:ND2    | 1:A:8:ASN:N      | 2.30        | 0.75     |
| 1:A:110:PRO:HB3  | 1:B:42:PHE:H     | 1.51        | 0.75     |
| 1:D:101:TYR:HA   | 1:D:109:THR:HG23 | 1.69        | 0.75     |
| 1:A:34:SER:HB2   | 1:A:42:PHE:HE2   | 1.50        | 0.75     |
| 1:B:8:ASN:N      | 1:B:8:ASN:HD22   | 1.82        | 0.75     |
| 1:A:78:CYS:HB3   | 1:A:125:MSE:HE3  | 1.68        | 0.75     |
| 1:D:74:ALA:CB    | 1:D:125:MSE:HE2  | 2.14        | 0.75     |
| 1:B:19:SER:HB3   | 1:B:91:LEU:HD11  | 1.67        | 0.74     |
| 1:E:30:VAL:HG22  | 1:E:53:VAL:HG12  | 1.69        | 0.74     |
| 1:B:11:LEU:HD23  | 1:B:80:GLN:NE2   | 2.02        | 0.74     |
| 1:C:63:ALA:HB2   | 1:C:114:PHE:CE2  | 2.23        | 0.74     |
| 1:E:120:LEU:CD2  | 2:E:506:3CS:H313 | 2.16        | 0.74     |
| 1:A:85:PHE:HZ    | 1:A:89:MSE:HE2   | 1.51        | 0.74     |
| 1:D:116:LYS:HE3  | 2:D:505:3CS:C15  | 2.18        | 0.74     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:F:74:ALA:CB    | 1:F:125:MSE:HE2  | 2.11        | 0.74     |
| 1:A:83:ALA:HB2   | 1:A:125:MSE:CE   | 2.16        | 0.74     |
| 1:A:19:SER:HB3   | 1:A:91:LEU:HD11  | 1.69        | 0.74     |
| 1:D:105:ARG:O    | 1:D:107:GLN:N    | 2.21        | 0.74     |
| 1:A:85:PHE:CZ    | 1:A:89:MSE:HE2   | 2.23        | 0.74     |
| 2:C:501:3CS:H23  | 2:C:501:3CS:O42  | 1.88        | 0.74     |
| 1:C:11:LEU:HD22  | 1:C:11:LEU:N     | 1.95        | 0.74     |
| 1:C:89:MSE:HB3   | 1:C:118:ILE:HD11 | 1.69        | 0.74     |
| 1:E:70:VAL:HB    | 1:E:122:LEU:HB3  | 1.69        | 0.74     |
| 1:E:66:THR:HG22  | 1:F:20:VAL:HG22  | 1.67        | 0.74     |
| 1:B:33:GLU:HG3   | 1:B:49:ALA:O     | 1.88        | 0.73     |
| 1:B:26:PHE:HA    | 1:B:98:PHE:HE2   | 1.53        | 0.73     |
| 1:A:42:PHE:HD2   | 1:A:50:PHE:CZ    | 2.05        | 0.73     |
| 1:E:53:VAL:HG22  | 1:E:102:LEU:HD23 | 1.70        | 0.73     |
| 1:A:8:ASN:N      | 1:A:8:ASN:HD22   | 1.83        | 0.73     |
| 1:E:116:LYS:HA   | 1:E:119:ILE:HD11 | 1.68        | 0.73     |
| 1:B:11:LEU:HD23  | 1:B:80:GLN:HE22  | 1.53        | 0.73     |
| 1:A:120:LEU:HD13 | 1:A:124:LEU:CD2  | 2.18        | 0.73     |
| 1:A:120:LEU:CD2  | 2:A:503:3CS:H302 | 2.14        | 0.73     |
| 1:B:83:ALA:CB    | 1:B:125:MSE:HE1  | 2.11        | 0.73     |
| 1:D:120:LEU:HD23 | 2:D:505:3CS:C30  | 2.19        | 0.73     |
| 1:C:120:LEU:HD13 | 1:C:124:LEU:CD2  | 2.19        | 0.73     |
| 1:F:94:ARG:HA    | 1:F:114:PHE:HZ   | 1.48        | 0.73     |
| 1:D:19:SER:HB3   | 1:D:91:LEU:HD11  | 1.70        | 0.73     |
| 1:A:44:ARG:NE    | 1:C:45:THR:HG21  | 2.04        | 0.73     |
| 1:C:10:VAL:HG13  | 1:C:14:ILE:CD1   | 2.19        | 0.72     |
| 1:D:20:VAL:HG22  | 1:F:66:THR:CG2   | 2.19        | 0.72     |
| 1:A:44:ARG:HE    | 1:C:45:THR:CG2   | 2.01        | 0.72     |
| 1:C:8:ASN:H      | 1:C:8:ASN:ND2    | 1.86        | 0.72     |
| 2:A:503:3CS:H382 | 2:A:503:3CS:H23  | 1.71        | 0.72     |
| 1:C:19:SER:HB3   | 1:C:91:LEU:HD11  | 1.70        | 0.72     |
| 1:D:116:LYS:HZ1  | 2:D:505:3CS:C16  | 2.03        | 0.72     |
| 1:A:43:GLN:HE22  | 1:C:54:TYR:HB3   | 1.55        | 0.72     |
| 1:F:17:LEU:O     | 1:F:20:VAL:HG12  | 1.89        | 0.72     |
| 1:A:21:VAL:CG2   | 2:C:501:3CS:H341 | 2.20        | 0.72     |
| 2:D:505:3CS:C23  | 2:D:505:3CS:H371 | 2.20        | 0.72     |
| 1:F:42:PHE:CD1   | 1:F:43:GLN:N     | 2.58        | 0.72     |
| 1:E:83:ALA:HB2   | 1:E:125:MSE:CE   | 2.18        | 0.72     |
| 1:D:124:LEU:HA   | 1:D:127:VAL:CG1  | 2.20        | 0.72     |
| 1:E:48:LEU:HD11  | 1:E:52:ARG:HD2   | 1.72        | 0.72     |
| 1:E:67:PHE:HB2   | 1:E:90:TYR:HE2   | 1.54        | 0.72     |
| 1:D:45:THR:CB    | 1:F:44:ARG:HG3   | 2.19        | 0.72     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:100:GLY:O    | 1:D:109:THR:HG23 | 1.90        | 0.72     |
| 1:B:26:PHE:HA    | 1:B:98:PHE:CE2   | 2.25        | 0.72     |
| 1:A:66:THR:HG22  | 1:B:20:VAL:HG22  | 1.72        | 0.72     |
| 1:D:43:GLN:CA    | 1:D:44:ARG:HH21  | 2.01        | 0.71     |
| 1:B:124:LEU:CA   | 1:B:127:VAL:HG12 | 2.18        | 0.71     |
| 1:A:52:ARG:HG3   | 1:A:52:ARG:HH11  | 1.54        | 0.71     |
| 1:E:97:TYR:HD2   | 1:E:114:PHE:CD2  | 2.08        | 0.71     |
| 1:B:66:THR:HG22  | 1:C:20:VAL:HG22  | 1.72        | 0.71     |
| 1:C:45:THR:HG23  | 1:C:51:GLU:OE2   | 1.89        | 0.71     |
| 1:E:8:ASN:ND2    | 1:E:8:ASN:H      | 1.86        | 0.71     |
| 1:D:27:ALA:HB2   | 2:F:504:3CS:C4   | 2.20        | 0.71     |
| 1:C:14:ILE:O     | 1:C:18:ILE:HD12  | 1.89        | 0.71     |
| 1:D:112:TYR:CE2  | 1:E:30:VAL:HG11  | 2.24        | 0.71     |
| 1:E:106:THR:HG22 | 1:E:107:GLN:HG3  | 1.71        | 0.71     |
| 1:B:120:LEU:CD2  | 2:B:502:3CS:H302 | 2.13        | 0.70     |
| 1:C:35:ARG:HA    | 1:C:35:ARG:HE    | 1.55        | 0.70     |
| 1:F:8:ASN:ND2    | 1:F:8:ASN:N      | 2.37        | 0.70     |
| 1:A:40:ARG:HB3   | 1:C:52:ARG:HH12  | 1.56        | 0.70     |
| 1:D:45:THR:HG22  | 1:D:46:GLY:H     | 1.55        | 0.70     |
| 1:F:11:LEU:HD23  | 1:F:80:GLN:NE2   | 2.07        | 0.70     |
| 1:F:107:GLN:O    | 1:F:108:SER:HB2  | 1.90        | 0.70     |
| 1:A:102:LEU:HG   | 1:A:103:GLY:N    | 2.05        | 0.70     |
| 1:C:90:TYR:HB2   | 1:C:118:ILE:HG21 | 1.72        | 0.70     |
| 1:D:94:ARG:HA    | 1:D:114:PHE:HE1  | 1.55        | 0.70     |
| 1:E:119:ILE:HD11 | 2:E:506:3CS:H12  | 1.74        | 0.70     |
| 1:F:11:LEU:H     | 1:F:11:LEU:CD2   | 2.01        | 0.70     |
| 1:A:67:PHE:HB2   | 1:A:90:TYR:HE2   | 1.57        | 0.70     |
| 1:D:10:VAL:HG13  | 1:D:14:ILE:HD12  | 1.74        | 0.69     |
| 1:D:8:ASN:N      | 1:D:8:ASN:ND2    | 2.38        | 0.69     |
| 1:E:52:ARG:HE    | 1:E:104:GLU:CB   | 2.05        | 0.69     |
| 1:F:26:PHE:HA    | 1:F:98:PHE:CE2   | 2.28        | 0.69     |
| 1:B:90:TYR:CE1   | 1:B:94:ARG:HG3   | 2.26        | 0.69     |
| 1:F:79:SER:OG    | 1:F:80:GLN:N     | 2.26        | 0.69     |
| 1:B:79:SER:HB3   | 1:B:82:PRO:CG    | 2.21        | 0.69     |
| 1:B:38:ASN:O     | 1:B:40:ARG:N     | 2.25        | 0.69     |
| 1:F:11:LEU:CD2   | 1:F:80:GLN:HE22  | 2.04        | 0.69     |
| 1:C:83:ALA:CB    | 1:C:125:MSE:HE1  | 2.18        | 0.69     |
| 1:A:14:ILE:O     | 1:A:18:ILE:HD12  | 1.92        | 0.69     |
| 1:A:120:LEU:O    | 1:A:124:LEU:HD22 | 1.93        | 0.69     |
| 1:C:116:LYS:HG3  | 1:C:117:ARG:N    | 2.08        | 0.69     |
| 1:C:124:LEU:CA   | 1:C:127:VAL:HG12 | 2.21        | 0.69     |
| 1:D:101:TYR:CD1  | 1:D:109:THR:HG22 | 2.28        | 0.69     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:C:52:ARG:NH2   | 1:C:105:ARG:HA   | 2.07        | 0.69     |
| 1:C:37:GLN:HA    | 1:C:37:GLN:OE1   | 1.91        | 0.69     |
| 1:E:13:ALA:O     | 1:E:17:LEU:HD23  | 1.92        | 0.69     |
| 1:F:11:LEU:HD23  | 1:F:80:GLN:HE22  | 1.58        | 0.69     |
| 1:F:133:TYR:CE1  | 1:F:137:PHE:HB2  | 2.28        | 0.69     |
| 1:D:8:ASN:ND2    | 1:D:8:ASN:H      | 1.89        | 0.69     |
| 1:C:119:ILE:HD11 | 2:C:501:3CS:C12  | 2.23        | 0.68     |
| 1:E:120:LEU:HD13 | 1:E:124:LEU:CD2  | 2.23        | 0.68     |
| 1:A:30:VAL:CG2   | 1:A:53:VAL:HG12  | 2.24        | 0.68     |
| 1:E:42:PHE:H     | 1:E:42:PHE:HD1   | 1.41        | 0.68     |
| 1:B:30:VAL:HG22  | 1:B:53:VAL:HG12  | 1.75        | 0.68     |
| 1:F:39:GLY:O     | 1:F:41:SER:N     | 2.25        | 0.68     |
| 1:B:144:GLU:HB3  | 1:B:146:TYR:CE1  | 2.28        | 0.68     |
| 1:A:101:TYR:OH   | 1:B:42:PHE:HB3   | 1.93        | 0.68     |
| 1:D:45:THR:HG22  | 1:D:46:GLY:N     | 2.09        | 0.68     |
| 1:B:132:ASN:ND2  | 1:B:136:ILE:HD11 | 2.09        | 0.68     |
| 1:D:79:SER:HB3   | 1:D:82:PRO:CG    | 2.23        | 0.68     |
| 1:D:120:LEU:HD23 | 2:D:505:3CS:O35  | 1.94        | 0.68     |
| 1:E:114:PHE:HD1  | 1:E:114:PHE:N    | 1.92        | 0.67     |
| 1:D:11:LEU:N     | 1:D:11:LEU:HD22  | 2.06        | 0.67     |
| 1:F:96:LYS:H     | 1:F:96:LYS:HD2   | 1.56        | 0.67     |
| 1:D:124:LEU:CA   | 1:D:127:VAL:HG12 | 2.24        | 0.67     |
| 1:E:81:VAL:HG13  | 1:E:82:PRO:CD    | 2.23        | 0.67     |
| 1:E:102:LEU:O    | 1:E:102:LEU:HD22 | 1.94        | 0.67     |
| 1:A:26:PHE:HA    | 1:A:98:PHE:CE2   | 2.30        | 0.67     |
| 1:D:10:VAL:HG13  | 1:D:14:ILE:CD1   | 2.25        | 0.67     |
| 1:A:133:TYR:HA   | 1:A:136:ILE:HD12 | 1.76        | 0.67     |
| 1:C:120:LEU:O    | 1:C:124:LEU:HD22 | 1.95        | 0.67     |
| 1:C:8:ASN:N      | 1:C:8:ASN:ND2    | 2.42        | 0.67     |
| 1:D:13:ALA:O     | 1:D:17:LEU:HD23  | 1.94        | 0.67     |
| 1:B:89:MSE:O     | 1:B:93:VAL:HG23  | 1.95        | 0.67     |
| 1:A:11:LEU:HD22  | 1:A:80:GLN:NE2   | 2.09        | 0.67     |
| 1:A:14:ILE:HG22  | 1:A:15:VAL:N     | 2.10        | 0.67     |
| 1:D:79:SER:CB    | 1:D:82:PRO:HG2   | 2.25        | 0.67     |
| 1:C:32:HIS:O     | 1:C:36:THR:HG23  | 1.95        | 0.67     |
| 1:B:71:LEU:O     | 1:B:71:LEU:HD22  | 1.95        | 0.67     |
| 1:F:23:ASN:OD1   | 1:F:94:ARG:NH2   | 2.27        | 0.67     |
| 1:B:11:LEU:CD2   | 1:B:80:GLN:HE22  | 2.07        | 0.67     |
| 1:A:10:VAL:HG13  | 1:A:14:ILE:CD1   | 2.23        | 0.67     |
| 1:A:103:GLY:O    | 1:A:104:GLU:HG3  | 1.95        | 0.67     |
| 1:F:25:PHE:CE1   | 1:F:29:LYS:HG2   | 2.26        | 0.66     |
| 1:F:6:VAL:O      | 1:F:10:VAL:HG23  | 1.96        | 0.66     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:17:LEU:O     | 1:B:20:VAL:HG12  | 1.95        | 0.66     |
| 1:F:52:ARG:HG3   | 1:F:52:ARG:HH11  | 1.60        | 0.66     |
| 1:D:42:PHE:HE2   | 1:F:112:TYR:HA   | 1.58        | 0.66     |
| 1:D:35:ARG:NE    | 1:D:35:ARG:HA    | 2.11        | 0.66     |
| 1:F:104:GLU:O    | 1:F:105:ARG:HG2  | 1.94        | 0.66     |
| 1:B:117:ARG:HH12 | 1:F:141:SER:CB   | 2.08        | 0.66     |
| 2:A:503:3CS:H382 | 2:A:503:3CS:H182 | 1.76        | 0.66     |
| 1:C:11:LEU:HD21  | 1:C:80:GLN:NE2   | 2.06        | 0.66     |
| 1:B:35:ARG:O     | 1:B:37:GLN:N     | 2.28        | 0.66     |
| 1:E:8:ASN:ND2    | 1:E:8:ASN:N      | 2.42        | 0.66     |
| 1:B:141:SER:OG   | 1:B:142:ASP:N    | 2.29        | 0.66     |
| 1:A:124:LEU:CA   | 1:A:127:VAL:HG12 | 2.26        | 0.66     |
| 1:F:126:SER:O    | 1:F:130:ILE:HB   | 1.96        | 0.66     |
| 1:D:42:PHE:CE2   | 1:F:112:TYR:HA   | 2.31        | 0.65     |
| 1:E:35:ARG:HA    | 1:E:35:ARG:NE    | 2.11        | 0.65     |
| 1:A:34:SER:CB    | 1:A:42:PHE:HE2   | 2.09        | 0.65     |
| 1:A:124:LEU:HA   | 1:A:127:VAL:CG1  | 2.24        | 0.65     |
| 1:C:25:PHE:HE1   | 1:C:29:LYS:HG2   | 1.62        | 0.65     |
| 1:F:124:LEU:HA   | 1:F:127:VAL:CG1  | 2.25        | 0.65     |
| 1:F:120:LEU:CD2  | 2:F:504:3CS:H302 | 2.08        | 0.65     |
| 1:C:18:ILE:CG2   | 1:C:91:LEU:HD23  | 2.25        | 0.65     |
| 1:D:110:PRO:HG3  | 1:E:40:ARG:HD3   | 1.78        | 0.65     |
| 1:D:44:ARG:NH1   | 1:F:51:GLU:HG2   | 2.11        | 0.65     |
| 1:A:99:VAL:O     | 1:A:102:LEU:HB3  | 1.96        | 0.65     |
| 1:B:112:TYR:CD2  | 1:C:30:VAL:HG11  | 2.31        | 0.65     |
| 1:B:132:ASN:HD21 | 1:B:136:ILE:HD11 | 1.60        | 0.65     |
| 2:A:503:3CS:C38  | 2:A:503:3CS:H23  | 2.27        | 0.65     |
| 1:E:81:VAL:CG1   | 1:E:82:PRO:HD3   | 2.24        | 0.65     |
| 1:D:11:LEU:HD23  | 1:D:80:GLN:NE2   | 2.10        | 0.65     |
| 1:B:44:ARG:O     | 1:B:45:THR:HB    | 1.95        | 0.65     |
| 1:F:120:LEU:HD13 | 1:F:124:LEU:HD22 | 1.77        | 0.65     |
| 1:F:124:LEU:CA   | 1:F:127:VAL:HG12 | 2.25        | 0.65     |
| 1:F:26:PHE:HA    | 1:F:98:PHE:HE2   | 1.60        | 0.65     |
| 2:C:501:3CS:H371 | 2:C:501:3CS:C23  | 2.27        | 0.65     |
| 1:A:34:SER:HB2   | 1:A:42:PHE:CE2   | 2.29        | 0.65     |
| 1:D:30:VAL:HG22  | 1:D:53:VAL:HG12  | 1.78        | 0.65     |
| 1:E:37:GLN:HE21  | 1:E:37:GLN:HA    | 1.61        | 0.65     |
| 1:C:11:LEU:HD23  | 1:C:80:GLN:CG    | 2.27        | 0.65     |
| 1:A:42:PHE:CE1   | 1:C:112:TYR:HE1  | 2.15        | 0.64     |
| 1:E:124:LEU:CA   | 1:E:127:VAL:HG12 | 2.22        | 0.64     |
| 1:E:125:MSE:O    | 1:E:128:ALA:HB3  | 1.97        | 0.64     |
| 2:F:504:3CS:O43  | 2:F:504:3CS:H23  | 1.98        | 0.64     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:120:LEU:CD2  | 2:D:505:3CS:H322 | 2.27        | 0.64     |
| 1:E:14:ILE:O     | 1:E:18:ILE:HD12  | 1.98        | 0.64     |
| 1:A:30:VAL:HG22  | 1:A:53:VAL:HG12  | 1.78        | 0.64     |
| 1:D:11:LEU:H     | 1:D:11:LEU:CD2   | 2.07        | 0.64     |
| 1:D:23:ASN:OD1   | 1:D:94:ARG:NH2   | 2.31        | 0.64     |
| 1:E:19:SER:HB3   | 1:E:91:LEU:HD11  | 1.78        | 0.64     |
| 2:B:502:3CS:H182 | 2:B:502:3CS:O42  | 1.97        | 0.64     |
| 1:F:119:ILE:CD1  | 2:F:504:3CS:H12  | 2.16        | 0.64     |
| 1:A:26:PHE:HA    | 1:A:98:PHE:HE2   | 1.60        | 0.64     |
| 1:A:42:PHE:N     | 1:A:42:PHE:CD1   | 2.65        | 0.64     |
| 1:F:142:ASP:C    | 1:F:144:GLU:H    | 2.00        | 0.64     |
| 1:A:74:ALA:HB2   | 1:A:122:LEU:O    | 1.98        | 0.63     |
| 1:A:40:ARG:HB2   | 1:C:52:ARG:HH12  | 1.63        | 0.63     |
| 1:A:64:TYR:CZ    | 1:A:68:LEU:HD21  | 2.33        | 0.63     |
| 1:B:11:LEU:HD23  | 1:B:80:GLN:OE1   | 1.98        | 0.63     |
| 1:B:6:VAL:O      | 1:B:10:VAL:HG23  | 1.99        | 0.63     |
| 1:A:10:VAL:HG21  | 1:C:133:TYR:CD2  | 2.33        | 0.63     |
| 1:D:33:GLU:HB3   | 1:D:50:PHE:HB2   | 1.80        | 0.63     |
| 1:B:10:VAL:HG12  | 1:B:11:LEU:HD13  | 1.79        | 0.63     |
| 2:E:506:3CS:H341 | 1:F:21:VAL:CG2   | 2.29        | 0.63     |
| 1:E:52:ARG:HG3   | 1:E:52:ARG:HH11  | 1.64        | 0.63     |
| 1:D:40:ARG:HB3   | 1:F:105:ARG:HH11 | 1.62        | 0.63     |
| 1:D:62:ASP:HB2   | 2:D:505:3CS:H2   | 1.81        | 0.63     |
| 1:E:97:TYR:HE2   | 1:E:114:PHE:CE1  | 2.17        | 0.63     |
| 1:D:10:VAL:HG21  | 1:F:133:TYR:CD2  | 2.33        | 0.63     |
| 1:A:42:PHE:CD1   | 1:C:112:TYR:HE1  | 2.16        | 0.63     |
| 1:C:11:LEU:H     | 1:C:11:LEU:CD2   | 1.96        | 0.63     |
| 1:C:125:MSE:O    | 1:C:128:ALA:HB3  | 1.97        | 0.63     |
| 1:D:133:TYR:HA   | 1:D:136:ILE:HD12 | 1.79        | 0.63     |
| 1:A:120:LEU:HD13 | 1:A:124:LEU:HD21 | 1.81        | 0.62     |
| 1:E:120:LEU:O    | 1:E:124:LEU:HD22 | 1.98        | 0.62     |
| 1:F:97:TYR:C     | 1:F:97:TYR:HD1   | 2.02        | 0.62     |
| 1:D:56:ALA:HA    | 1:D:101:TYR:CD2  | 2.34        | 0.62     |
| 1:E:10:VAL:HG13  | 1:E:14:ILE:CD1   | 2.28        | 0.62     |
| 1:E:116:LYS:HA   | 1:E:119:ILE:HD13 | 1.79        | 0.62     |
| 1:A:42:PHE:CD2   | 1:A:50:PHE:HZ    | 2.11        | 0.62     |
| 1:E:37:GLN:HE21  | 1:E:37:GLN:CA    | 2.11        | 0.62     |
| 1:D:116:LYS:HZ1  | 2:D:505:3CS:C12  | 2.12        | 0.62     |
| 1:F:97:TYR:CD1   | 1:F:97:TYR:C     | 2.72        | 0.62     |
| 1:B:120:LEU:O    | 1:B:124:LEU:HD22 | 1.99        | 0.62     |
| 1:A:123:PHE:HD1  | 1:A:124:LEU:CD1  | 2.12        | 0.62     |
| 1:A:94:ARG:HA    | 1:A:114:PHE:HE2  | 1.63        | 0.62     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:E:506:3CS:C4   | 1:F:27:ALA:HB2   | 2.30        | 0.62     |
| 1:E:26:PHE:HA    | 1:E:98:PHE:HE2   | 1.64        | 0.62     |
| 1:D:120:LEU:HD13 | 1:D:124:LEU:CD2  | 2.29        | 0.62     |
| 1:E:26:PHE:HA    | 1:E:98:PHE:CE2   | 2.34        | 0.62     |
| 1:D:72:TRP:O     | 1:D:76:LEU:HD22  | 1.99        | 0.62     |
| 1:F:11:LEU:N     | 1:F:11:LEU:HD22  | 2.04        | 0.62     |
| 1:E:89:MSE:O     | 1:E:93:VAL:HG23  | 2.00        | 0.62     |
| 1:B:120:LEU:HD13 | 1:B:124:LEU:CD2  | 2.30        | 0.62     |
| 1:A:116:LYS:HE3  | 2:A:503:3CS:C39  | 2.29        | 0.62     |
| 1:C:126:SER:O    | 1:C:130:ILE:HB   | 2.00        | 0.62     |
| 1:F:67:PHE:HB2   | 1:F:90:TYR:HE2   | 1.65        | 0.62     |
| 1:E:11:LEU:HD23  | 1:E:80:GLN:CD    | 2.21        | 0.62     |
| 1:D:42:PHE:N     | 1:D:42:PHE:CD1   | 2.67        | 0.62     |
| 1:A:110:PRO:HB3  | 1:B:42:PHE:N     | 2.14        | 0.61     |
| 1:D:103:GLY:O    | 1:D:104:GLU:HG3  | 2.00        | 0.61     |
| 1:A:111:GLY:HA2  | 1:B:31:GLU:OE2   | 2.00        | 0.61     |
| 1:D:120:LEU:HD13 | 1:D:124:LEU:HD22 | 1.81        | 0.61     |
| 1:D:24:GLY:C     | 2:F:504:3CS:H20  | 2.21        | 0.61     |
| 1:C:106:THR:HG22 | 1:C:107:GLN:N    | 2.14        | 0.61     |
| 1:C:30:VAL:HA    | 1:C:53:VAL:HG11  | 1.83        | 0.61     |
| 1:F:67:PHE:CG    | 1:F:90:TYR:CE2   | 2.89        | 0.61     |
| 1:A:116:LYS:CE   | 2:A:503:3CS:H391 | 2.30        | 0.61     |
| 1:C:119:ILE:CD1  | 2:C:501:3CS:H12  | 2.31        | 0.61     |
| 1:C:81:VAL:HB    | 1:C:82:PRO:HD3   | 1.83        | 0.61     |
| 2:C:501:3CS:H371 | 2:C:501:3CS:C19  | 2.30        | 0.61     |
| 1:E:114:PHE:CD1  | 1:E:114:PHE:N    | 2.64        | 0.61     |
| 1:B:142:ASP:O    | 1:B:144:GLU:N    | 2.33        | 0.61     |
| 1:C:78:CYS:O     | 1:C:125:MSE:HE3  | 2.00        | 0.61     |
| 1:F:121:PHE:CE1  | 1:F:125:MSE:HG3  | 2.36        | 0.61     |
| 1:F:95:GLN:HA    | 1:F:95:GLN:OE1   | 2.01        | 0.61     |
| 1:B:123:PHE:CE2  | 1:C:21:VAL:HG23  | 2.35        | 0.60     |
| 1:E:11:LEU:HD23  | 1:E:80:GLN:OE1   | 2.01        | 0.60     |
| 1:B:90:TYR:CA    | 1:B:118:ILE:HD13 | 2.32        | 0.60     |
| 1:C:10:VAL:O     | 1:C:14:ILE:HD12  | 2.01        | 0.60     |
| 1:F:40:ARG:HG3   | 1:F:40:ARG:O     | 2.01        | 0.60     |
| 1:D:96:LYS:HD2   | 1:D:96:LYS:H     | 1.67        | 0.60     |
| 1:B:120:LEU:HD13 | 1:B:124:LEU:HD22 | 1.82        | 0.60     |
| 1:F:89:MSE:O     | 1:F:93:VAL:HG23  | 2.01        | 0.60     |
| 1:B:145:ASN:O    | 1:B:147:ILE:N    | 2.29        | 0.60     |
| 1:E:45:THR:HG22  | 1:F:43:GLN:HG3   | 1.83        | 0.60     |
| 1:B:136:ILE:HA   | 1:B:140:GLY:HA3  | 1.82        | 0.60     |
| 1:A:97:TYR:HD2   | 1:A:114:PHE:CD2  | 2.19        | 0.60     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:D:505:3CS:H20  | 1:E:24:GLY:C     | 2.22        | 0.60     |
| 1:C:30:VAL:HG22  | 1:C:53:VAL:CG1   | 2.30        | 0.60     |
| 1:B:23:ASN:OD1   | 1:B:94:ARG:NH2   | 2.34        | 0.60     |
| 1:E:126:SER:O    | 1:E:130:ILE:HB   | 2.02        | 0.60     |
| 1:B:11:LEU:O     | 1:B:15:VAL:HG12  | 2.02        | 0.60     |
| 1:C:120:LEU:HD13 | 1:C:124:LEU:HD22 | 1.82        | 0.60     |
| 1:F:133:TYR:C    | 1:F:133:TYR:CD1  | 2.74        | 0.60     |
| 1:A:94:ARG:HA    | 1:A:114:PHE:CE2  | 2.37        | 0.60     |
| 1:D:40:ARG:HB3   | 1:F:105:ARG:NH1  | 2.16        | 0.60     |
| 1:B:95:GLN:OE1   | 1:B:95:GLN:HA    | 2.00        | 0.60     |
| 1:C:120:LEU:HD23 | 2:C:501:3CS:O35  | 2.01        | 0.60     |
| 1:E:120:LEU:HD13 | 1:E:124:LEU:HD22 | 1.82        | 0.60     |
| 1:D:81:VAL:HG23  | 1:D:82:PRO:CD    | 2.27        | 0.60     |
| 1:B:145:ASN:ND2  | 1:B:145:ASN:N    | 2.39        | 0.60     |
| 1:B:109:THR:N    | 1:B:110:PRO:HD3  | 2.17        | 0.60     |
| 1:B:11:LEU:HD23  | 1:B:80:GLN:CD    | 2.22        | 0.60     |
| 1:D:95:GLN:HA    | 1:D:95:GLN:OE1   | 2.01        | 0.60     |
| 1:F:140:GLY:C    | 1:F:142:ASP:H    | 2.05        | 0.60     |
| 2:B:502:3CS:C23  | 2:B:502:3CS:H371 | 2.32        | 0.60     |
| 1:A:10:VAL:HG12  | 1:A:11:LEU:HD13  | 1.82        | 0.60     |
| 1:A:119:ILE:CD1  | 2:A:503:3CS:H12  | 2.20        | 0.60     |
| 1:F:8:ASN:N      | 1:F:8:ASN:HD22   | 1.98        | 0.60     |
| 1:F:67:PHE:O     | 1:F:70:VAL:HG22  | 2.02        | 0.59     |
| 1:F:39:GLY:C     | 1:F:41:SER:H     | 2.05        | 0.59     |
| 1:D:14:ILE:O     | 1:D:18:ILE:HD12  | 2.02        | 0.59     |
| 1:E:90:TYR:HB2   | 1:E:118:ILE:HG21 | 1.83        | 0.59     |
| 1:F:37:GLN:HG3   | 1:F:47:THR:OG1   | 2.02        | 0.59     |
| 2:D:505:3CS:H341 | 1:E:21:VAL:HA    | 1.85        | 0.59     |
| 1:E:48:LEU:HD11  | 1:E:52:ARG:CD    | 2.31        | 0.59     |
| 1:B:11:LEU:H     | 1:B:11:LEU:CD2   | 2.01        | 0.59     |
| 1:B:52:ARG:NE    | 1:B:103:GLY:HA2  | 2.17        | 0.59     |
| 1:D:126:SER:O    | 1:D:130:ILE:HB   | 2.01        | 0.59     |
| 1:D:44:ARG:NH1   | 1:F:55:THR:OG1   | 2.36        | 0.59     |
| 1:B:64:TYR:CZ    | 1:B:68:LEU:HD21  | 2.37        | 0.59     |
| 1:B:30:VAL:CG2   | 1:B:53:VAL:HG12  | 2.32        | 0.59     |
| 1:A:113:ILE:HD12 | 1:B:31:GLU:HG2   | 1.84        | 0.59     |
| 1:C:33:GLU:HG3   | 1:C:50:PHE:HA    | 1.85        | 0.59     |
| 2:A:503:3CS:H371 | 2:A:503:3CS:C19  | 2.32        | 0.59     |
| 1:C:114:PHE:HD1  | 1:C:115:GLY:N    | 2.01        | 0.59     |
| 1:F:21:VAL:HG12  | 1:F:22:GLN:N     | 2.16        | 0.59     |
| 1:E:85:PHE:HZ    | 1:E:89:MSE:HE2   | 1.66        | 0.59     |
| 1:E:132:ASN:HD21 | 1:E:136:ILE:HD11 | 1.68        | 0.59     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:F:120:LEU:CD2  | 2:F:504:3CS:H313 | 2.33        | 0.59     |
| 1:D:35:ARG:NH2   | 1:D:39:GLY:HA2   | 2.18        | 0.59     |
| 1:E:97:TYR:OH    | 1:E:111:GLY:HA2  | 2.03        | 0.59     |
| 1:D:41:SER:HA    | 1:F:110:PRO:HD2  | 1.83        | 0.59     |
| 1:F:56:ALA:HA    | 1:F:101:TYR:CD2  | 2.36        | 0.59     |
| 1:A:54:TYR:HD2   | 1:B:44:ARG:HH12  | 1.47        | 0.59     |
| 2:D:505:3CS:H371 | 2:D:505:3CS:C19  | 2.33        | 0.59     |
| 1:E:11:LEU:HD23  | 1:E:80:GLN:NE2   | 2.18        | 0.59     |
| 1:E:85:PHE:CZ    | 1:E:89:MSE:HE2   | 2.38        | 0.59     |
| 1:E:139:PHE:CD1  | 1:E:139:PHE:N    | 2.69        | 0.59     |
| 1:D:94:ARG:HA    | 1:D:114:PHE:CE1  | 2.38        | 0.59     |
| 1:D:39:GLY:O     | 1:F:109:THR:HB   | 2.01        | 0.59     |
| 1:B:52:ARG:HG3   | 1:B:52:ARG:HH11  | 1.68        | 0.59     |
| 1:F:10:VAL:HG13  | 1:F:14:ILE:CD1   | 2.33        | 0.59     |
| 1:B:13:ALA:O     | 1:B:17:LEU:HD23  | 2.03        | 0.59     |
| 1:D:43:GLN:HA    | 1:D:44:ARG:NH2   | 2.14        | 0.58     |
| 1:B:44:ARG:CZ    | 1:C:44:ARG:HH22  | 2.15        | 0.58     |
| 1:E:42:PHE:N     | 1:E:42:PHE:CD1   | 2.71        | 0.58     |
| 1:C:85:PHE:CE1   | 1:C:89:MSE:HG2   | 2.38        | 0.58     |
| 1:B:121:PHE:CE1  | 1:B:125:MSE:HG3  | 2.38        | 0.58     |
| 1:A:10:VAL:HG21  | 1:C:133:TYR:CE2  | 2.38        | 0.58     |
| 1:D:108:SER:HA   | 1:E:40:ARG:CD    | 2.25        | 0.58     |
| 1:C:56:ALA:HA    | 1:C:101:TYR:HD2  | 1.66        | 0.58     |
| 1:D:44:ARG:HD2   | 1:F:51:GLU:HG3   | 1.84        | 0.58     |
| 1:D:10:VAL:HG21  | 1:F:133:TYR:CE2  | 2.38        | 0.58     |
| 1:F:56:ALA:HA    | 1:F:101:TYR:HD2  | 1.67        | 0.58     |
| 1:D:97:TYR:HD2   | 1:D:114:PHE:CE1  | 2.20        | 0.58     |
| 1:D:48:LEU:HD22  | 1:D:48:LEU:N     | 2.19        | 0.58     |
| 1:C:123:PHE:HD1  | 1:C:124:LEU:HD13 | 1.68        | 0.58     |
| 2:C:501:3CS:O35  | 2:C:501:3CS:H382 | 2.04        | 0.58     |
| 1:D:45:THR:OG1   | 1:F:44:ARG:HB2   | 2.03        | 0.58     |
| 1:A:132:ASN:ND2  | 1:A:136:ILE:HD11 | 2.19        | 0.58     |
| 1:E:120:LEU:HD23 | 2:E:506:3CS:C30  | 2.34        | 0.58     |
| 1:C:139:PHE:N    | 1:C:139:PHE:CD1  | 2.71        | 0.58     |
| 1:B:44:ARG:NH2   | 1:C:44:ARG:HH22  | 2.01        | 0.58     |
| 1:B:135:LEU:N    | 1:B:135:LEU:HD23 | 2.18        | 0.58     |
| 1:E:6:VAL:O      | 1:E:10:VAL:HG23  | 2.04        | 0.57     |
| 1:A:81:VAL:HB    | 1:A:82:PRO:CD    | 2.34        | 0.57     |
| 1:D:116:LYS:HZ2  | 1:D:116:LYS:HB3  | 1.70        | 0.57     |
| 1:B:144:GLU:HA   | 1:B:144:GLU:OE1  | 2.02        | 0.57     |
| 1:B:77:LEU:O     | 1:B:78:CYS:HB3   | 2.03        | 0.57     |
| 1:B:97:TYR:HD2   | 1:B:114:PHE:CD2  | 2.22        | 0.57     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:8:ASN:HA     | 1:A:80:GLN:OE1   | 2.03        | 0.57     |
| 1:B:144:GLU:HG3  | 1:B:146:TYR:CE1  | 2.40        | 0.57     |
| 1:E:123:PHE:HD1  | 1:E:124:LEU:HD13 | 1.70        | 0.57     |
| 1:E:119:ILE:HD11 | 2:E:506:3CS:C12  | 2.35        | 0.57     |
| 1:C:90:TYR:HA    | 1:C:118:ILE:HD12 | 1.87        | 0.57     |
| 1:B:145:ASN:O    | 1:B:147:ILE:HG13 | 2.04        | 0.57     |
| 1:E:30:VAL:CG2   | 1:E:53:VAL:HG12  | 2.32        | 0.57     |
| 1:A:33:GLU:HB3   | 1:A:50:PHE:HB2   | 1.86        | 0.57     |
| 1:A:125:MSE:O    | 1:A:128:ALA:HB3  | 2.04        | 0.57     |
| 1:D:30:VAL:HG11  | 1:F:112:TYR:CD2  | 2.39        | 0.57     |
| 1:C:56:ALA:HA    | 1:C:101:TYR:CD2  | 2.40        | 0.57     |
| 1:C:89:MSE:O     | 1:C:93:VAL:HG23  | 2.05        | 0.57     |
| 1:D:18:ILE:CG2   | 1:D:91:LEU:HD23  | 2.35        | 0.57     |
| 1:E:14:ILE:HG22  | 1:E:15:VAL:N     | 2.19        | 0.57     |
| 1:B:133:TYR:CD1  | 1:B:134:TYR:CD1  | 2.93        | 0.57     |
| 1:B:14:ILE:HG22  | 1:B:15:VAL:N     | 2.19        | 0.57     |
| 1:D:120:LEU:CD2  | 2:D:505:3CS:H301 | 2.31        | 0.57     |
| 1:E:97:TYR:HD2   | 1:E:114:PHE:CE2  | 2.22        | 0.57     |
| 1:A:43:GLN:NE2   | 1:C:51:GLU:O     | 2.38        | 0.57     |
| 1:D:136:ILE:O    | 1:D:140:GLY:HA3  | 2.04        | 0.57     |
| 1:D:101:TYR:HD1  | 1:D:109:THR:CG2  | 2.16        | 0.56     |
| 1:B:47:THR:HA    | 1:B:51:GLU:CD    | 2.24        | 0.56     |
| 1:D:52:ARG:HH11  | 1:D:52:ARG:HG3   | 1.70        | 0.56     |
| 1:C:63:ALA:C     | 1:C:65:PRO:HD2   | 2.25        | 0.56     |
| 1:D:42:PHE:HD1   | 1:D:42:PHE:N     | 2.03        | 0.56     |
| 2:F:504:3CS:H371 | 2:F:504:3CS:C23  | 2.35        | 0.56     |
| 2:D:505:3CS:H341 | 1:E:21:VAL:HG22  | 1.86        | 0.56     |
| 2:E:506:3CS:I25  | 1:F:25:PHE:HB2   | 2.74        | 0.56     |
| 1:F:56:ALA:HB2   | 1:F:101:TYR:CD2  | 2.40        | 0.56     |
| 1:A:42:PHE:CD1   | 1:C:112:TYR:CE1  | 2.93        | 0.56     |
| 1:D:14:ILE:HG22  | 1:D:15:VAL:N     | 2.19        | 0.56     |
| 1:E:53:VAL:HG23  | 1:E:102:LEU:HD23 | 1.87        | 0.56     |
| 1:A:21:VAL:HG12  | 1:A:22:GLN:N     | 2.20        | 0.56     |
| 1:D:11:LEU:HD23  | 1:D:80:GLN:HE22  | 1.70        | 0.56     |
| 2:B:502:3CS:H20  | 1:C:24:GLY:C     | 2.26        | 0.56     |
| 1:A:120:LEU:CD1  | 1:A:124:LEU:HD21 | 2.36        | 0.56     |
| 1:D:35:ARG:HH21  | 1:D:39:GLY:HA2   | 1.71        | 0.56     |
| 1:A:42:PHE:HB2   | 1:C:112:TYR:OH   | 2.05        | 0.56     |
| 1:D:123:PHE:CD2  | 2:D:505:3CS:H311 | 2.40        | 0.56     |
| 1:E:79:SER:OG    | 1:E:82:PRO:HD2   | 2.05        | 0.56     |
| 1:B:44:ARG:HG3   | 1:B:44:ARG:O     | 2.05        | 0.56     |
| 1:A:13:ALA:O     | 1:A:17:LEU:HD23  | 2.05        | 0.56     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:E:135:LEU:HD23 | 1:E:135:LEU:N    | 2.20        | 0.56     |
| 1:E:95:GLN:HA    | 1:E:95:GLN:OE1   | 2.04        | 0.56     |
| 1:F:120:LEU:HA   | 2:F:504:3CS:H313 | 1.87        | 0.56     |
| 1:C:14:ILE:HG22  | 1:C:15:VAL:N     | 2.21        | 0.56     |
| 1:D:30:VAL:HG11  | 1:F:112:TYR:CE2  | 2.41        | 0.56     |
| 1:E:30:VAL:HA    | 1:E:53:VAL:HG11  | 1.88        | 0.56     |
| 1:B:18:ILE:CG2   | 1:B:91:LEU:HD23  | 2.36        | 0.56     |
| 1:D:11:LEU:CD2   | 1:D:80:GLN:HE22  | 2.18        | 0.56     |
| 1:D:44:ARG:HD3   | 1:F:55:THR:OG1   | 2.05        | 0.56     |
| 1:A:34:SER:HG    | 1:A:42:PHE:HE2   | 1.54        | 0.56     |
| 1:B:35:ARG:HE    | 1:B:35:ARG:HA    | 1.70        | 0.56     |
| 1:F:31:GLU:O     | 1:F:35:ARG:HG2   | 2.06        | 0.56     |
| 1:E:72:TRP:O     | 1:E:76:LEU:HD22  | 2.05        | 0.56     |
| 1:C:120:LEU:HD13 | 1:C:124:LEU:HD21 | 1.87        | 0.55     |
| 1:E:22:GLN:OE1   | 1:E:94:ARG:NE    | 2.39        | 0.55     |
| 1:B:142:ASP:O    | 1:B:143:PHE:HD1  | 1.89        | 0.55     |
| 1:D:11:LEU:HD23  | 1:D:80:GLN:CD    | 2.26        | 0.55     |
| 1:E:54:TYR:HD2   | 1:F:42:PHE:HE2   | 1.54        | 0.55     |
| 1:A:63:ALA:CB    | 1:A:114:PHE:HE1  | 2.19        | 0.55     |
| 1:A:121:PHE:CE1  | 1:A:125:MSE:HG3  | 2.41        | 0.55     |
| 1:B:137:PHE:CE2  | 1:B:138:PHE:HE1  | 2.24        | 0.55     |
| 1:B:99:VAL:HG12  | 1:B:100:GLY:N    | 2.21        | 0.55     |
| 1:B:97:TYR:HD1   | 1:B:109:THR:HG21 | 1.70        | 0.55     |
| 1:B:21:VAL:HG12  | 1:B:22:GLN:N     | 2.21        | 0.55     |
| 1:C:11:LEU:HD23  | 1:C:80:GLN:HG3   | 1.88        | 0.55     |
| 1:E:60:CYS:HB3   | 1:E:94:ARG:HD3   | 1.88        | 0.55     |
| 1:F:37:GLN:HA    | 1:F:37:GLN:OE1   | 2.07        | 0.55     |
| 1:E:112:TYR:O    | 1:E:113:ILE:HB   | 2.07        | 0.55     |
| 1:B:118:ILE:HG22 | 1:B:119:ILE:N    | 2.22        | 0.55     |
| 1:B:74:ALA:CB    | 1:B:125:MSE:HE2  | 2.29        | 0.55     |
| 1:A:120:LEU:HD13 | 1:A:124:LEU:HD22 | 1.89        | 0.55     |
| 1:A:20:VAL:HG22  | 1:C:66:THR:CG2   | 2.32        | 0.55     |
| 1:E:47:THR:HG23  | 1:E:50:PHE:HB3   | 1.89        | 0.55     |
| 1:D:141:SER:C    | 1:D:143:PHE:H    | 2.09        | 0.55     |
| 1:B:113:ILE:HG12 | 1:B:114:PHE:N    | 2.20        | 0.55     |
| 1:B:12:LEU:HG    | 1:B:80:GLN:HE21  | 1.72        | 0.55     |
| 1:E:111:GLY:O    | 1:E:112:TYR:O    | 2.25        | 0.55     |
| 1:E:81:VAL:HG22  | 1:E:82:PRO:HD3   | 1.88        | 0.55     |
| 1:B:133:TYR:CE1  | 1:B:134:TYR:CD1  | 2.95        | 0.55     |
| 1:A:58:GLN:O     | 1:A:58:GLN:HG3   | 2.07        | 0.55     |
| 1:B:105:ARG:HH11 | 1:B:105:ARG:HB3  | 1.72        | 0.55     |
| 1:B:120:LEU:HB2  | 2:B:502:3CS:O35  | 2.07        | 0.55     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:A:503:3CS:C4   | 1:B:27:ALA:HB2   | 2.37        | 0.55     |
| 1:B:130:ILE:HD11 | 1:C:14:ILE:HD12  | 1.89        | 0.55     |
| 1:E:33:GLU:HB3   | 1:E:50:PHE:HB2   | 1.88        | 0.55     |
| 1:E:64:TYR:CZ    | 1:E:68:LEU:HD21  | 2.41        | 0.55     |
| 1:B:10:VAL:HG13  | 1:B:14:ILE:HD12  | 1.88        | 0.55     |
| 1:A:31:GLU:OE1   | 1:A:31:GLU:HA    | 2.07        | 0.55     |
| 1:C:18:ILE:HG22  | 1:C:91:LEU:HD23  | 1.88        | 0.55     |
| 1:E:120:LEU:HD23 | 2:E:506:3CS:H322 | 1.89        | 0.55     |
| 1:D:11:LEU:HD23  | 1:D:80:GLN:OE1   | 2.07        | 0.55     |
| 1:D:30:VAL:CG2   | 1:D:53:VAL:HG12  | 2.37        | 0.55     |
| 1:A:34:SER:O     | 1:A:37:GLN:O     | 2.24        | 0.55     |
| 1:A:14:ILE:CD1   | 1:C:130:ILE:HD11 | 2.37        | 0.54     |
| 1:C:120:LEU:CD1  | 1:C:124:LEU:HD21 | 2.37        | 0.54     |
| 2:D:505:3CS:O35  | 2:D:505:3CS:H382 | 2.07        | 0.54     |
| 1:D:30:VAL:HA    | 1:D:53:VAL:HG11  | 1.88        | 0.54     |
| 1:B:104:GLU:O    | 1:B:105:ARG:HB2  | 2.07        | 0.54     |
| 1:A:43:GLN:HA    | 1:C:44:ARG:HH21  | 1.72        | 0.54     |
| 1:F:88:LEU:C     | 1:F:88:LEU:HD13  | 2.28        | 0.54     |
| 1:E:67:PHE:CD1   | 1:E:90:TYR:HD2   | 2.24        | 0.54     |
| 1:A:24:GLY:C     | 2:C:501:3CS:H20  | 2.28        | 0.54     |
| 1:F:30:VAL:HG22  | 1:F:53:VAL:HG12  | 1.89        | 0.54     |
| 1:E:66:THR:CG2   | 1:F:20:VAL:HG22  | 2.37        | 0.54     |
| 1:B:114:PHE:N    | 1:B:114:PHE:CD1  | 2.76        | 0.54     |
| 1:E:120:LEU:HD13 | 1:E:124:LEU:HD21 | 1.90        | 0.54     |
| 1:F:64:TYR:N     | 1:F:65:PRO:HD2   | 2.22        | 0.54     |
| 1:D:18:ILE:HG21  | 1:D:91:LEU:HD23  | 1.90        | 0.54     |
| 1:D:8:ASN:N      | 1:D:8:ASN:HD22   | 2.05        | 0.54     |
| 1:E:132:ASN:ND2  | 1:E:136:ILE:HD11 | 2.22        | 0.54     |
| 1:A:67:PHE:HB2   | 1:A:90:TYR:CE2   | 2.39        | 0.54     |
| 1:A:67:PHE:CG    | 1:A:90:TYR:CE2   | 2.96        | 0.54     |
| 1:F:94:ARG:HG2   | 1:F:114:PHE:CE2  | 2.42        | 0.54     |
| 1:E:130:ILE:HD11 | 1:F:14:ILE:CD1   | 2.38        | 0.54     |
| 2:B:502:3CS:C19  | 2:B:502:3CS:H371 | 2.38        | 0.54     |
| 1:C:21:VAL:HG12  | 1:C:22:GLN:N     | 2.22        | 0.54     |
| 1:A:18:ILE:CG2   | 1:A:91:LEU:HD23  | 2.37        | 0.54     |
| 1:C:119:ILE:CG1  | 2:C:501:3CS:H12  | 2.38        | 0.54     |
| 1:F:131:PHE:CD1  | 1:F:132:ASN:N    | 2.75        | 0.54     |
| 1:D:113:ILE:HG12 | 1:D:114:PHE:N    | 2.23        | 0.54     |
| 1:E:67:PHE:CD1   | 1:E:90:TYR:CD2   | 2.95        | 0.54     |
| 1:E:120:LEU:HD23 | 2:E:506:3CS:H301 | 1.89        | 0.54     |
| 2:E:506:3CS:H20  | 1:F:24:GLY:HA3   | 1.90        | 0.54     |
| 1:B:44:ARG:NE    | 1:C:44:ARG:HH12  | 2.05        | 0.54     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:C:106:THR:HG22 | 1:C:107:GLN:H    | 1.72        | 0.54     |
| 1:E:120:LEU:CD1  | 1:E:124:LEU:HD21 | 2.38        | 0.54     |
| 1:A:139:PHE:N    | 1:A:139:PHE:CD1  | 2.74        | 0.54     |
| 1:E:88:LEU:HD13  | 1:E:88:LEU:C     | 2.28        | 0.54     |
| 1:B:139:PHE:CD1  | 1:B:139:PHE:N    | 2.76        | 0.54     |
| 2:D:505:3CS:H341 | 1:E:21:VAL:CG2   | 2.38        | 0.54     |
| 1:D:42:PHE:CD1   | 1:F:101:TYR:CZ   | 2.96        | 0.54     |
| 1:D:94:ARG:CD    | 1:D:114:PHE:HZ   | 2.21        | 0.54     |
| 1:F:79:SER:HB2   | 1:F:82:PRO:HD2   | 1.89        | 0.53     |
| 1:C:18:ILE:HG21  | 1:C:91:LEU:HD23  | 1.89        | 0.53     |
| 1:D:62:ASP:N     | 1:D:62:ASP:OD1   | 2.39        | 0.53     |
| 1:E:120:LEU:HD23 | 2:E:506:3CS:O35  | 2.08        | 0.53     |
| 1:F:19:SER:CB    | 1:F:91:LEU:HD11  | 2.33        | 0.53     |
| 1:F:143:PHE:C    | 1:F:143:PHE:CD1  | 2.81        | 0.53     |
| 1:F:143:PHE:HD1  | 1:F:143:PHE:C    | 2.10        | 0.53     |
| 1:E:97:TYR:CE2   | 1:E:114:PHE:CE1  | 2.95        | 0.53     |
| 1:C:101:TYR:O    | 1:C:102:LEU:HD23 | 2.08        | 0.53     |
| 1:D:7:GLY:HA2    | 1:F:133:TYR:CE2  | 2.44        | 0.53     |
| 1:A:67:PHE:CD1   | 1:A:90:TYR:CD2   | 2.96        | 0.53     |
| 1:A:89:MSE:O     | 1:A:93:VAL:HG23  | 2.08        | 0.53     |
| 1:B:79:SER:HB3   | 1:B:82:PRO:CD    | 2.38        | 0.53     |
| 1:D:44:ARG:HD2   | 1:F:51:GLU:CG    | 2.38        | 0.53     |
| 1:C:95:GLN:HA    | 1:C:95:GLN:OE1   | 2.07        | 0.53     |
| 1:B:96:LYS:HD2   | 1:B:96:LYS:H     | 1.73        | 0.53     |
| 1:F:76:LEU:N     | 1:F:76:LEU:HD13  | 2.23        | 0.53     |
| 1:B:66:THR:CG2   | 1:C:20:VAL:HG22  | 2.38        | 0.53     |
| 1:D:143:PHE:CD1  | 1:D:143:PHE:N    | 2.75        | 0.53     |
| 1:D:110:PRO:CG   | 1:E:40:ARG:HD3   | 2.38        | 0.53     |
| 1:D:45:THR:CG2   | 1:D:46:GLY:H     | 2.21        | 0.53     |
| 1:F:143:PHE:O    | 1:F:144:GLU:O    | 2.27        | 0.53     |
| 1:F:121:PHE:C    | 1:F:121:PHE:CD1  | 2.80        | 0.53     |
| 2:C:501:3CS:H13  | 2:C:501:3CS:C8   | 2.39        | 0.53     |
| 1:A:43:GLN:OE1   | 1:C:44:ARG:O     | 2.26        | 0.53     |
| 1:B:114:PHE:N    | 1:B:114:PHE:HD1  | 2.05        | 0.53     |
| 1:A:15:VAL:HG13  | 1:A:16:THR:N     | 2.23        | 0.53     |
| 1:A:113:ILE:CD1  | 1:B:31:GLU:HG2   | 2.38        | 0.53     |
| 1:F:5:THR:O      | 1:F:9:VAL:HG13   | 2.08        | 0.53     |
| 1:F:120:LEU:HD22 | 2:F:504:3CS:H313 | 1.91        | 0.53     |
| 1:D:42:PHE:HE1   | 1:F:110:PRO:HG2  | 1.73        | 0.53     |
| 1:D:22:GLN:HG3   | 1:D:23:ASN:N     | 2.24        | 0.53     |
| 1:F:33:GLU:OE1   | 1:F:33:GLU:HA    | 2.09        | 0.53     |
| 1:F:116:LYS:O    | 1:F:119:ILE:HD13 | 2.09        | 0.53     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:14:ILE:HD12  | 1:C:130:ILE:HD11 | 1.90        | 0.53     |
| 1:D:120:LEU:CD1  | 1:D:124:LEU:HD21 | 2.39        | 0.53     |
| 1:E:97:TYR:CD2   | 1:E:114:PHE:CE2  | 2.97        | 0.53     |
| 1:F:34:SER:O     | 1:F:38:ASN:OD1   | 2.27        | 0.53     |
| 2:E:506:3CS:C5   | 1:F:27:ALA:HB2   | 2.39        | 0.53     |
| 1:F:60:CYS:HG    | 1:F:114:PHE:HE1  | 1.57        | 0.53     |
| 1:D:40:ARG:O     | 1:D:41:SER:HB2   | 2.09        | 0.53     |
| 1:B:81:VAL:CG1   | 1:B:82:PRO:HD3   | 2.34        | 0.52     |
| 1:D:44:ARG:HB3   | 1:E:44:ARG:HH22  | 1.72        | 0.52     |
| 1:E:133:TYR:CD1  | 1:E:134:TYR:CD1  | 2.97        | 0.52     |
| 1:B:102:LEU:HD13 | 1:B:104:GLU:OE2  | 2.09        | 0.52     |
| 1:C:22:GLN:HG3   | 1:C:23:ASN:N     | 2.24        | 0.52     |
| 1:C:25:PHE:C     | 1:C:25:PHE:CD1   | 2.82        | 0.52     |
| 1:A:3:GLN:NE2    | 1:C:133:TYR:CE1  | 2.77        | 0.52     |
| 1:A:88:LEU:C     | 1:A:88:LEU:HD13  | 2.29        | 0.52     |
| 1:A:63:ALA:C     | 1:A:65:PRO:HD2   | 2.29        | 0.52     |
| 1:D:139:PHE:N    | 1:D:139:PHE:CD1  | 2.76        | 0.52     |
| 1:B:119:ILE:HD13 | 1:B:119:ILE:H    | 1.75        | 0.52     |
| 1:F:25:PHE:CD1   | 1:F:25:PHE:C     | 2.82        | 0.52     |
| 1:B:137:PHE:CD2  | 1:B:138:PHE:CE1  | 2.98        | 0.52     |
| 1:E:58:GLN:O     | 1:E:58:GLN:HG3   | 2.10        | 0.52     |
| 1:C:13:ALA:O     | 1:C:17:LEU:HD23  | 2.09        | 0.52     |
| 1:D:94:ARG:HG2   | 1:D:114:PHE:CE1  | 2.45        | 0.52     |
| 1:A:96:LYS:HD2   | 1:A:96:LYS:H     | 1.71        | 0.52     |
| 1:B:31:GLU:OE1   | 1:B:31:GLU:HA    | 2.09        | 0.52     |
| 1:A:25:PHE:CD1   | 1:A:25:PHE:C     | 2.81        | 0.52     |
| 1:A:64:TYR:N     | 1:A:65:PRO:HD2   | 2.25        | 0.52     |
| 1:D:124:LEU:N    | 1:D:124:LEU:HD13 | 2.25        | 0.52     |
| 1:F:75:GLY:C     | 1:F:76:LEU:HD13  | 2.30        | 0.52     |
| 1:B:30:VAL:HA    | 1:B:53:VAL:HG11  | 1.91        | 0.52     |
| 1:B:48:LEU:O     | 1:B:50:PHE:N     | 2.42        | 0.52     |
| 1:E:64:TYR:CE1   | 1:E:68:LEU:HD22  | 2.45        | 0.52     |
| 1:F:133:TYR:HD1  | 1:F:133:TYR:C    | 2.12        | 0.52     |
| 1:C:8:ASN:N      | 1:C:8:ASN:HD22   | 2.07        | 0.52     |
| 1:B:131:PHE:CD1  | 1:B:132:ASN:N    | 2.78        | 0.52     |
| 1:A:23:ASN:OD1   | 1:A:94:ARG:NH2   | 2.42        | 0.52     |
| 1:F:97:TYR:O     | 1:F:97:TYR:HD1   | 1.92        | 0.52     |
| 1:B:79:SER:HB3   | 1:B:82:PRO:HD2   | 1.91        | 0.52     |
| 1:C:71:LEU:O     | 1:C:71:LEU:HD22  | 2.10        | 0.52     |
| 1:C:136:ILE:HA   | 1:C:140:GLY:HA3  | 1.92        | 0.52     |
| 1:B:19:SER:O     | 1:B:23:ASN:HB2   | 2.10        | 0.52     |
| 1:A:26:PHE:HB3   | 1:A:57:ASN:HD22  | 1.74        | 0.52     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:42:PHE:O     | 1:D:43:GLN:HG3   | 2.10        | 0.52     |
| 1:F:135:LEU:N    | 1:F:135:LEU:HD23 | 2.25        | 0.52     |
| 1:A:42:PHE:HD1   | 1:A:42:PHE:N     | 2.08        | 0.52     |
| 1:F:58:GLN:HG3   | 1:F:58:GLN:O     | 2.08        | 0.52     |
| 1:D:52:ARG:HH11  | 1:D:52:ARG:CG    | 2.23        | 0.51     |
| 1:F:120:LEU:C    | 1:F:120:LEU:HD13 | 2.30        | 0.51     |
| 1:B:126:SER:O    | 1:B:130:ILE:HB   | 2.10        | 0.51     |
| 1:E:21:VAL:HG12  | 1:E:22:GLN:N     | 2.24        | 0.51     |
| 1:F:94:ARG:HG2   | 1:F:114:PHE:CZ   | 2.45        | 0.51     |
| 1:A:104:GLU:O    | 1:A:105:ARG:HB2  | 2.10        | 0.51     |
| 1:F:81:VAL:HG22  | 1:F:82:PRO:N     | 2.24        | 0.51     |
| 1:D:133:TYR:CD1  | 1:D:134:TYR:CD1  | 2.98        | 0.51     |
| 1:F:119:ILE:HG12 | 1:F:120:LEU:N    | 2.24        | 0.51     |
| 1:A:97:TYR:HD2   | 1:A:114:PHE:CG   | 2.27        | 0.51     |
| 1:C:116:LYS:HA   | 1:C:119:ILE:CD1  | 2.41        | 0.51     |
| 1:C:63:ALA:CB    | 1:C:114:PHE:CE2  | 2.93        | 0.51     |
| 2:D:505:3CS:H21  | 1:E:25:PHE:HB2   | 1.91        | 0.51     |
| 1:D:110:PRO:HG3  | 1:E:40:ARG:O     | 2.10        | 0.51     |
| 1:F:10:VAL:O     | 1:F:14:ILE:HD12  | 2.10        | 0.51     |
| 1:F:14:ILE:HG22  | 1:F:15:VAL:N     | 2.23        | 0.51     |
| 1:E:131:PHE:CD1  | 1:E:132:ASN:N    | 2.78        | 0.51     |
| 1:D:71:LEU:O     | 1:D:71:LEU:HD22  | 2.10        | 0.51     |
| 1:D:31:GLU:OE1   | 1:D:31:GLU:HA    | 2.11        | 0.51     |
| 1:F:79:SER:CB    | 1:F:82:PRO:HD2   | 2.40        | 0.51     |
| 1:D:83:ALA:HB2   | 1:D:125:MSE:CE   | 2.35        | 0.51     |
| 1:F:13:ALA:O     | 1:F:17:LEU:HD23  | 2.11        | 0.51     |
| 1:A:10:VAL:O     | 1:A:14:ILE:HD12  | 2.11        | 0.51     |
| 1:E:11:LEU:CD2   | 1:E:80:GLN:HE22  | 2.24        | 0.51     |
| 1:E:67:PHE:CG    | 1:E:90:TYR:CE2   | 2.99        | 0.51     |
| 1:C:139:PHE:N    | 1:C:139:PHE:HD1  | 2.09        | 0.51     |
| 1:E:120:LEU:CD2  | 2:E:506:3CS:H322 | 2.41        | 0.51     |
| 1:D:18:ILE:HG22  | 1:D:19:SER:N     | 2.26        | 0.51     |
| 1:D:90:TYR:HA    | 1:D:118:ILE:HD12 | 1.92        | 0.51     |
| 1:D:90:TYR:CE1   | 1:D:94:ARG:HG3   | 2.46        | 0.51     |
| 1:A:17:LEU:O     | 1:A:20:VAL:HG12  | 2.11        | 0.51     |
| 1:B:14:ILE:O     | 1:B:18:ILE:HD12  | 2.10        | 0.51     |
| 2:F:504:3CS:H301 | 2:F:504:3CS:C37  | 2.27        | 0.51     |
| 1:B:125:MSE:O    | 1:B:128:ALA:HB3  | 2.11        | 0.51     |
| 1:C:116:LYS:O    | 1:C:119:ILE:HD13 | 2.10        | 0.51     |
| 1:D:3:GLN:NE2    | 1:F:133:TYR:CD1  | 2.79        | 0.51     |
| 1:D:131:PHE:CD1  | 1:D:132:ASN:N    | 2.79        | 0.51     |
| 1:D:25:PHE:HE2   | 1:D:95:GLN:HE22  | 1.59        | 0.50     |

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| Atom-1          | Atom-2           | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:C:114:PHE:CD1 | 1:C:115:GLY:N    | 2.78        | 0.50     |
| 1:D:116:LYS:HZ3 | 1:D:116:LYS:CA   | 2.22        | 0.50     |
| 1:D:97:TYR:HD2  | 1:D:114:PHE:CD1  | 2.29        | 0.50     |
| 1:E:8:ASN:N     | 1:E:8:ASN:HD22   | 2.07        | 0.50     |
| 1:E:47:THR:HG23 | 1:E:50:PHE:CB    | 2.41        | 0.50     |
| 1:F:26:PHE:CD2  | 1:F:98:PHE:CD2   | 2.99        | 0.50     |
| 2:A:503:3CS:C21 | 1:B:25:PHE:HB2   | 2.40        | 0.50     |
| 1:A:42:PHE:HD1  | 1:A:42:PHE:H     | 1.60        | 0.50     |
| 1:B:33:GLU:OE1  | 1:B:33:GLU:HA    | 2.11        | 0.50     |
| 1:E:64:TYR:N    | 1:E:65:PRO:HD2   | 2.25        | 0.50     |
| 1:A:22:GLN:HG3  | 1:A:23:ASN:N     | 2.26        | 0.50     |
| 1:A:14:ILE:HD11 | 1:C:130:ILE:CD1  | 2.41        | 0.50     |
| 1:D:64:TYR:CZ   | 1:D:68:LEU:HD21  | 2.46        | 0.50     |
| 1:E:79:SER:OG   | 1:E:80:GLN:N     | 2.44        | 0.50     |
| 1:B:133:TYR:CD1 | 1:B:134:TYR:HD1  | 2.29        | 0.50     |
| 1:D:116:LYS:NZ  | 1:D:116:LYS:HA   | 2.21        | 0.50     |
| 1:D:79:SER:HB3  | 1:D:82:PRO:CD    | 2.42        | 0.50     |
| 1:A:43:GLN:NE2  | 1:C:54:TYR:HB3   | 2.23        | 0.50     |
| 1:A:135:LEU:N   | 1:A:135:LEU:HD23 | 2.27        | 0.50     |
| 1:D:58:GLN:HG3  | 1:D:58:GLN:O     | 2.11        | 0.50     |
| 1:B:72:TRP:O    | 1:B:76:LEU:HD22  | 2.12        | 0.50     |
| 1:C:18:ILE:HG22 | 1:C:19:SER:N     | 2.26        | 0.50     |
| 1:B:64:TYR:N    | 1:B:65:PRO:HD2   | 2.26        | 0.50     |
| 1:D:143:PHE:N   | 1:D:143:PHE:HD1  | 2.09        | 0.50     |
| 1:C:96:LYS:H    | 1:C:96:LYS:HD2   | 1.72        | 0.50     |
| 1:F:14:ILE:O    | 1:F:18:ILE:HD12  | 2.12        | 0.50     |
| 1:B:116:LYS:HE2 | 2:B:502:3CS:H383 | 1.93        | 0.50     |
| 1:B:97:TYR:CD1  | 1:B:109:THR:HG21 | 2.46        | 0.50     |
| 1:F:79:SER:HB2  | 1:F:82:PRO:CD    | 2.42        | 0.50     |
| 1:C:74:ALA:CB   | 1:C:125:MSE:HE2  | 2.34        | 0.50     |
| 1:E:74:ALA:HB2  | 1:E:122:LEU:O    | 2.12        | 0.50     |
| 1:A:95:GLN:HA   | 1:A:95:GLN:OE1   | 2.11        | 0.50     |
| 1:D:105:ARG:O   | 1:D:107:GLN:HG3  | 2.12        | 0.50     |
| 1:B:64:TYR:CZ   | 1:B:68:LEU:CD2   | 2.95        | 0.50     |
| 1:B:133:TYR:HE1 | 1:B:134:TYR:CE1  | 2.30        | 0.50     |
| 1:E:119:ILE:CD1 | 2:E:506:3CS:H12  | 2.42        | 0.49     |
| 1:E:45:THR:HB   | 1:F:43:GLN:NE2   | 2.27        | 0.49     |
| 1:E:10:VAL:HG13 | 1:E:14:ILE:HD12  | 1.92        | 0.49     |
| 1:D:141:SER:O   | 1:D:142:ASP:OD1  | 2.29        | 0.49     |
| 1:B:119:ILE:CG1 | 2:B:502:3CS:H12  | 2.42        | 0.49     |
| 1:F:64:TYR:CZ   | 1:F:68:LEU:HD21  | 2.47        | 0.49     |
| 1:D:21:VAL:HG12 | 1:D:22:GLN:N     | 2.26        | 0.49     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:120:LEU:C    | 1:B:120:LEU:HD13 | 2.31        | 0.49     |
| 1:D:74:ALA:HB2   | 1:D:122:LEU:O    | 2.12        | 0.49     |
| 1:D:109:THR:N    | 1:D:110:PRO:HD3  | 2.26        | 0.49     |
| 1:E:54:TYR:CD2   | 1:F:42:PHE:HE2   | 2.29        | 0.49     |
| 1:B:112:TYR:HD2  | 1:C:30:VAL:CG1   | 2.24        | 0.49     |
| 1:E:130:ILE:HD11 | 1:F:14:ILE:HD12  | 1.95        | 0.49     |
| 1:B:123:PHE:HD1  | 1:B:124:LEU:HD13 | 1.76        | 0.49     |
| 1:E:112:TYR:CD2  | 1:F:30:VAL:HG11  | 2.48        | 0.49     |
| 1:E:105:ARG:O    | 1:E:106:THR:HB   | 2.12        | 0.49     |
| 1:A:30:VAL:HA    | 1:A:53:VAL:HG11  | 1.95        | 0.49     |
| 1:D:7:GLY:HA2    | 1:F:133:TYR:OH   | 2.13        | 0.49     |
| 1:E:62:ASP:OD1   | 1:E:62:ASP:N     | 2.42        | 0.49     |
| 1:F:124:LEU:O    | 1:F:127:VAL:HG12 | 2.11        | 0.49     |
| 1:A:25:PHE:N     | 2:C:501:3CS:H21  | 2.28        | 0.49     |
| 2:A:503:3CS:H301 | 2:A:503:3CS:H372 | 1.94        | 0.49     |
| 1:B:130:ILE:HD12 | 1:C:14:ILE:HD11  | 1.94        | 0.49     |
| 1:D:101:TYR:CD1  | 1:D:109:THR:CG2  | 2.92        | 0.49     |
| 1:F:34:SER:HB2   | 1:F:50:PHE:HE1   | 1.77        | 0.49     |
| 1:A:26:PHE:CD1   | 1:A:26:PHE:N     | 2.81        | 0.49     |
| 1:C:33:GLU:HG3   | 1:C:50:PHE:CA    | 2.42        | 0.49     |
| 2:A:503:3CS:H371 | 2:A:503:3CS:C23  | 2.42        | 0.49     |
| 1:F:97:TYR:CD2   | 1:F:114:PHE:CE1  | 3.01        | 0.49     |
| 1:E:52:ARG:HD3   | 1:E:104:GLU:OE1  | 2.13        | 0.49     |
| 1:C:77:LEU:CD1   | 1:C:77:LEU:N     | 2.75        | 0.49     |
| 1:B:120:LEU:HA   | 2:B:502:3CS:C31  | 2.39        | 0.48     |
| 2:A:503:3CS:H13  | 2:A:503:3CS:N26  | 2.28        | 0.48     |
| 1:A:57:ASN:C     | 1:A:59:ASN:H     | 2.15        | 0.48     |
| 1:E:78:CYS:HB3   | 1:E:125:MSE:HE3  | 1.95        | 0.48     |
| 1:A:124:LEU:O    | 1:A:127:VAL:HG12 | 2.13        | 0.48     |
| 1:D:116:LYS:NZ   | 1:D:116:LYS:CB   | 2.77        | 0.48     |
| 1:D:41:SER:OG    | 1:F:110:PRO:HD2  | 2.13        | 0.48     |
| 1:A:26:PHE:HD1   | 1:A:26:PHE:H     | 1.61        | 0.48     |
| 1:A:75:GLY:HA2   | 1:A:83:ALA:CB    | 2.43        | 0.48     |
| 1:C:11:LEU:O     | 1:C:15:VAL:HG12  | 2.13        | 0.48     |
| 1:D:119:ILE:HG12 | 1:D:120:LEU:N    | 2.27        | 0.48     |
| 1:D:116:LYS:NZ   | 2:D:505:3CS:C12  | 2.76        | 0.48     |
| 1:F:63:ALA:C     | 1:F:65:PRO:HD2   | 2.34        | 0.48     |
| 1:C:77:LEU:O     | 1:C:129:GLY:HA3  | 2.12        | 0.48     |
| 1:A:94:ARG:HG2   | 1:A:114:PHE:CZ   | 2.48        | 0.48     |
| 1:B:130:ILE:HD11 | 1:C:14:ILE:CD1   | 2.43        | 0.48     |
| 1:B:26:PHE:CD2   | 1:B:98:PHE:CD2   | 3.02        | 0.48     |
| 1:E:7:GLY:C      | 1:E:9:VAL:H      | 2.16        | 0.48     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:112:TYR:OH   | 1:B:27:ALA:HA    | 2.13        | 0.48     |
| 1:F:99:VAL:HG12  | 1:F:100:GLY:N    | 2.29        | 0.48     |
| 1:B:18:ILE:HG22  | 1:B:19:SER:N     | 2.28        | 0.48     |
| 1:A:26:PHE:N     | 1:A:26:PHE:HD1   | 2.12        | 0.48     |
| 1:F:12:LEU:HB3   | 1:F:72:TRP:CH2   | 2.48        | 0.48     |
| 1:D:136:ILE:HA   | 1:D:140:GLY:CA   | 2.44        | 0.48     |
| 1:B:47:THR:HA    | 1:B:51:GLU:CG    | 2.44        | 0.48     |
| 2:F:504:3CS:H371 | 2:F:504:3CS:C19  | 2.44        | 0.48     |
| 1:C:90:TYR:HD1   | 1:C:118:ILE:HG21 | 1.79        | 0.48     |
| 1:A:30:VAL:HG23  | 1:A:53:VAL:HG12  | 1.94        | 0.48     |
| 1:B:88:LEU:C     | 1:B:88:LEU:HD13  | 2.34        | 0.48     |
| 1:A:97:TYR:CD2   | 1:A:114:PHE:CG   | 3.02        | 0.48     |
| 1:B:44:ARG:CZ    | 1:C:44:ARG:HH12  | 2.27        | 0.48     |
| 1:E:96:LYS:H     | 1:E:96:LYS:HD2   | 1.74        | 0.48     |
| 1:B:133:TYR:CE1  | 1:B:134:TYR:HD1  | 2.31        | 0.48     |
| 1:C:133:TYR:CE1  | 1:C:137:PHE:HB2  | 2.49        | 0.48     |
| 1:C:114:PHE:CZ   | 2:C:501:3CS:C8   | 2.97        | 0.48     |
| 1:F:133:TYR:HA   | 1:F:136:ILE:HD12 | 1.96        | 0.48     |
| 1:E:51:GLU:OE2   | 1:F:43:GLN:NE2   | 2.47        | 0.48     |
| 1:E:99:VAL:HG12  | 1:E:100:GLY:N    | 2.29        | 0.48     |
| 1:B:18:ILE:HG21  | 1:B:91:LEU:HD23  | 1.96        | 0.48     |
| 1:B:60:CYS:HB3   | 1:B:94:ARG:HD3   | 1.94        | 0.48     |
| 1:F:42:PHE:HD1   | 1:F:43:GLN:H     | 1.60        | 0.48     |
| 1:E:90:TYR:N     | 1:E:118:ILE:CD1  | 2.77        | 0.48     |
| 1:D:26:PHE:CE2   | 1:D:98:PHE:HB2   | 2.49        | 0.48     |
| 1:B:97:TYR:CD2   | 1:B:114:PHE:CD2  | 3.00        | 0.47     |
| 1:A:85:PHE:O     | 1:A:88:LEU:HB3   | 2.14        | 0.47     |
| 1:A:26:PHE:CD2   | 1:A:98:PHE:CD2   | 3.02        | 0.47     |
| 1:D:10:VAL:O     | 1:D:14:ILE:HD12  | 2.14        | 0.47     |
| 1:A:11:LEU:HD23  | 1:A:80:GLN:CG    | 2.40        | 0.47     |
| 2:A:503:3CS:H393 | 2:A:503:3CS:N17  | 2.28        | 0.47     |
| 1:A:81:VAL:HB    | 1:A:82:PRO:HD3   | 1.96        | 0.47     |
| 1:B:141:SER:O    | 1:B:143:PHE:N    | 2.47        | 0.47     |
| 1:D:63:ALA:C     | 1:D:65:PRO:HD2   | 2.34        | 0.47     |
| 1:F:56:ALA:CB    | 1:F:101:TYR:CD2  | 2.97        | 0.47     |
| 1:C:26:PHE:N     | 1:C:26:PHE:CD1   | 2.82        | 0.47     |
| 1:F:120:LEU:HD13 | 1:F:124:LEU:CD2  | 2.43        | 0.47     |
| 2:A:503:3CS:C20  | 1:B:25:PHE:N     | 2.76        | 0.47     |
| 1:C:25:PHE:O     | 1:C:25:PHE:HD1   | 1.97        | 0.47     |
| 1:F:121:PHE:HE1  | 1:F:125:MSE:HG3  | 1.79        | 0.47     |
| 1:A:5:THR:O      | 1:A:9:VAL:HG13   | 2.13        | 0.47     |
| 1:B:130:ILE:CD1  | 1:C:14:ILE:HD11  | 2.44        | 0.47     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:124:LEU:O    | 1:D:127:VAL:HG12 | 2.14        | 0.47     |
| 1:C:29:LYS:HA    | 1:C:29:LYS:HD2   | 1.61        | 0.47     |
| 1:A:118:ILE:HG22 | 1:A:119:ILE:N    | 2.30        | 0.47     |
| 1:A:19:SER:O     | 1:A:23:ASN:HB2   | 2.15        | 0.47     |
| 1:B:25:PHE:HE1   | 1:B:29:LYS:HG2   | 1.77        | 0.47     |
| 1:D:119:ILE:HD11 | 2:D:505:3CS:C12  | 2.45        | 0.47     |
| 1:E:120:LEU:HA   | 2:E:506:3CS:H301 | 1.97        | 0.47     |
| 1:F:64:TYR:CZ    | 1:F:68:LEU:CD2   | 2.98        | 0.47     |
| 1:D:101:TYR:HD1  | 1:D:109:THR:HG22 | 1.75        | 0.47     |
| 1:D:30:VAL:CG1   | 1:F:112:TYR:CD2  | 2.96        | 0.47     |
| 1:D:90:TYR:N     | 1:D:118:ILE:CD1  | 2.78        | 0.47     |
| 1:B:132:ASN:O    | 1:B:136:ILE:HD12 | 2.14        | 0.47     |
| 1:B:71:LEU:C     | 1:B:71:LEU:HD22  | 2.34        | 0.47     |
| 1:C:58:GLN:O     | 1:C:58:GLN:HG3   | 2.15        | 0.47     |
| 1:A:29:LYS:HD2   | 1:A:29:LYS:HA    | 1.62        | 0.47     |
| 1:B:74:ALA:HB2   | 1:B:122:LEU:O    | 2.13        | 0.47     |
| 1:A:90:TYR:HD1   | 1:A:90:TYR:O     | 1.98        | 0.47     |
| 1:D:3:GLN:HE22   | 1:F:133:TYR:HD1  | 1.62        | 0.47     |
| 1:D:90:TYR:HE1   | 1:D:94:ARG:HG3   | 1.79        | 0.47     |
| 1:B:64:TYR:CE1   | 1:B:68:LEU:HD22  | 2.49        | 0.47     |
| 1:B:91:LEU:HA    | 1:B:91:LEU:HD12  | 1.72        | 0.47     |
| 1:A:121:PHE:C    | 1:A:121:PHE:CD1  | 2.86        | 0.47     |
| 1:C:115:GLY:O    | 1:C:119:ILE:HD12 | 2.14        | 0.47     |
| 1:D:123:PHE:HD1  | 1:D:124:LEU:CD1  | 2.27        | 0.47     |
| 1:F:12:LEU:O     | 1:F:15:VAL:HG12  | 2.14        | 0.47     |
| 1:F:57:ASN:C     | 1:F:59:ASN:H     | 2.17        | 0.47     |
| 1:F:31:GLU:HA    | 1:F:31:GLU:OE1   | 2.14        | 0.47     |
| 1:E:63:ALA:C     | 1:E:65:PRO:HD2   | 2.35        | 0.47     |
| 1:C:26:PHE:HA    | 1:C:98:PHE:CE2   | 2.49        | 0.47     |
| 1:C:31:GLU:OE1   | 1:C:31:GLU:HA    | 2.15        | 0.47     |
| 1:D:37:GLN:O     | 1:D:38:ASN:HB2   | 2.14        | 0.47     |
| 2:A:503:3CS:H20  | 1:B:24:GLY:C     | 2.35        | 0.47     |
| 1:B:39:GLY:O     | 1:B:42:PHE:N     | 2.48        | 0.47     |
| 1:D:116:LYS:O    | 1:D:119:ILE:HD13 | 2.14        | 0.47     |
| 1:D:116:LYS:HE3  | 2:D:505:3CS:C16  | 2.44        | 0.47     |
| 1:E:75:GLY:O     | 1:E:79:SER:O     | 2.33        | 0.47     |
| 1:B:102:LEU:HD22 | 1:B:102:LEU:C    | 2.35        | 0.47     |
| 1:F:62:ASP:OD1   | 1:F:62:ASP:N     | 2.47        | 0.47     |
| 1:A:64:TYR:CZ    | 1:A:68:LEU:CD2   | 2.98        | 0.47     |
| 1:B:142:ASP:OD2  | 1:F:117:ARG:NH1  | 2.35        | 0.47     |
| 2:E:506:3CS:C32  | 2:E:506:3CS:H372 | 2.33        | 0.47     |
| 1:E:45:THR:HA    | 1:F:43:GLN:NE2   | 2.29        | 0.47     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:119:ILE:HD11 | 2:D:505:3CS:H12  | 1.96        | 0.47     |
| 1:E:11:LEU:HB2   | 1:E:80:GLN:NE2   | 2.29        | 0.47     |
| 1:E:11:LEU:CD2   | 1:E:80:GLN:NE2   | 2.78        | 0.47     |
| 1:C:76:LEU:HA    | 1:C:76:LEU:HD12  | 1.78        | 0.47     |
| 1:A:94:ARG:CG    | 1:A:114:PHE:HE2  | 2.13        | 0.46     |
| 1:C:90:TYR:HD1   | 1:C:118:ILE:CG2  | 2.28        | 0.46     |
| 1:A:120:LEU:CD2  | 2:A:503:3CS:H313 | 2.45        | 0.46     |
| 1:C:18:ILE:HG22  | 1:C:91:LEU:CD2   | 2.45        | 0.46     |
| 1:F:12:LEU:HD13  | 1:F:72:TRP:CE3   | 2.50        | 0.46     |
| 1:D:106:THR:O    | 1:D:107:GLN:HB2  | 2.16        | 0.46     |
| 1:A:133:TYR:CD1  | 1:A:134:TYR:CD1  | 3.02        | 0.46     |
| 1:A:133:TYR:CE1  | 1:A:134:TYR:CD1  | 3.03        | 0.46     |
| 1:D:48:LEU:H     | 1:D:48:LEU:HD22  | 1.81        | 0.46     |
| 1:E:64:TYR:CZ    | 1:E:68:LEU:CD2   | 2.98        | 0.46     |
| 1:B:120:LEU:CD2  | 2:B:502:3CS:H313 | 2.46        | 0.46     |
| 1:F:120:LEU:HD23 | 2:F:504:3CS:H313 | 1.97        | 0.46     |
| 1:F:120:LEU:HB2  | 2:F:504:3CS:O35  | 2.14        | 0.46     |
| 1:A:18:ILE:HG22  | 1:A:19:SER:N     | 2.30        | 0.46     |
| 1:C:124:LEU:O    | 1:C:127:VAL:HG12 | 2.15        | 0.46     |
| 1:B:105:ARG:O    | 1:B:106:THR:O    | 2.33        | 0.46     |
| 1:B:21:VAL:CG1   | 1:B:22:GLN:N     | 2.79        | 0.46     |
| 1:D:29:LYS:HD2   | 1:D:29:LYS:HA    | 1.48        | 0.46     |
| 1:A:124:LEU:O    | 1:A:128:ALA:N    | 2.49        | 0.46     |
| 1:B:52:ARG:HH11  | 1:B:52:ARG:CG    | 2.26        | 0.46     |
| 1:F:142:ASP:C    | 1:F:144:GLU:N    | 2.67        | 0.46     |
| 1:B:73:SER:O     | 1:B:77:LEU:HB2   | 2.15        | 0.46     |
| 2:F:504:3CS:C29  | 2:F:504:3CS:H382 | 2.45        | 0.46     |
| 1:A:116:LYS:O    | 1:A:120:LEU:HB2  | 2.14        | 0.46     |
| 1:A:52:ARG:NH1   | 1:A:52:ARG:HG3   | 2.25        | 0.46     |
| 1:B:146:TYR:O    | 1:B:148:ALA:N    | 2.48        | 0.46     |
| 1:F:56:ALA:CA    | 1:F:101:TYR:CD2  | 2.97        | 0.46     |
| 1:D:31:GLU:CG    | 1:F:113:ILE:HD11 | 2.37        | 0.46     |
| 1:E:8:ASN:O      | 1:E:9:VAL:HG12   | 2.16        | 0.46     |
| 1:C:37:GLN:HG3   | 1:C:47:THR:OG1   | 2.15        | 0.46     |
| 1:B:22:GLN:HG3   | 1:B:23:ASN:N     | 2.29        | 0.46     |
| 1:A:90:TYR:N     | 1:A:118:ILE:CD1  | 2.78        | 0.46     |
| 1:A:9:VAL:N      | 1:A:80:GLN:NE2   | 2.63        | 0.46     |
| 1:F:1:MSE:HB3    | 1:F:6:VAL:CG2    | 2.46        | 0.46     |
| 1:E:95:GLN:O     | 1:E:99:VAL:HB    | 2.16        | 0.46     |
| 1:B:109:THR:N    | 1:B:110:PRO:CD   | 2.78        | 0.46     |
| 1:A:56:ALA:O     | 1:A:59:ASN:HB2   | 2.15        | 0.46     |
| 1:E:77:LEU:CD1   | 1:E:77:LEU:N     | 2.78        | 0.46     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:C:5:THR:O      | 1:C:9:VAL:HG13   | 2.15        | 0.46     |
| 1:B:113:ILE:O    | 1:B:114:PHE:HB3  | 2.16        | 0.46     |
| 1:A:27:ALA:HB2   | 2:C:501:3CS:C3   | 2.46        | 0.46     |
| 1:A:78:CYS:HB2   | 1:A:125:MSE:O    | 2.16        | 0.46     |
| 1:F:25:PHE:O     | 1:F:28:HIS:HB3   | 2.16        | 0.46     |
| 1:F:10:VAL:HG13  | 1:F:14:ILE:HD12  | 1.96        | 0.46     |
| 1:D:135:LEU:N    | 1:D:135:LEU:HD23 | 2.30        | 0.46     |
| 1:C:35:ARG:HA    | 1:C:35:ARG:NE    | 2.28        | 0.46     |
| 1:F:77:LEU:O     | 1:F:78:CYS:HB3   | 2.16        | 0.46     |
| 1:A:91:LEU:HA    | 1:A:91:LEU:HD12  | 1.78        | 0.46     |
| 1:E:67:PHE:CB    | 1:E:90:TYR:HE2   | 2.25        | 0.46     |
| 1:E:18:ILE:CG2   | 1:E:91:LEU:HD23  | 2.46        | 0.46     |
| 1:D:27:ALA:HB2   | 2:F:504:3CS:C3   | 2.46        | 0.46     |
| 1:D:116:LYS:CA   | 1:D:116:LYS:NZ   | 2.79        | 0.46     |
| 1:E:91:LEU:HA    | 1:E:91:LEU:HD12  | 1.74        | 0.46     |
| 1:D:136:ILE:HA   | 1:D:140:GLY:HA3  | 1.98        | 0.46     |
| 1:F:77:LEU:N     | 1:F:77:LEU:CD1   | 2.79        | 0.45     |
| 1:B:25:PHE:CE1   | 1:B:29:LYS:HG2   | 2.51        | 0.45     |
| 1:E:22:GLN:HG3   | 1:E:23:ASN:N     | 2.28        | 0.45     |
| 1:E:11:LEU:CD2   | 1:E:11:LEU:H     | 2.18        | 0.45     |
| 1:D:44:ARG:HB3   | 1:E:44:ARG:HH21  | 1.79        | 0.45     |
| 1:B:35:ARG:HA    | 1:B:35:ARG:NE    | 2.30        | 0.45     |
| 1:B:137:PHE:CD2  | 1:B:138:PHE:HE1  | 2.34        | 0.45     |
| 1:B:10:VAL:HG13  | 1:B:14:ILE:CD1   | 2.45        | 0.45     |
| 1:D:10:VAL:CG2   | 1:F:133:TYR:CD2  | 2.98        | 0.45     |
| 1:D:91:LEU:HA    | 1:D:91:LEU:HD12  | 1.75        | 0.45     |
| 1:E:90:TYR:HA    | 1:E:118:ILE:HD12 | 1.97        | 0.45     |
| 1:E:26:PHE:CD2   | 1:E:98:PHE:CD2   | 3.04        | 0.45     |
| 1:C:120:LEU:HD23 | 2:C:501:3CS:H323 | 1.99        | 0.45     |
| 1:E:111:GLY:HA3  | 1:F:40:ARG:NH2   | 2.31        | 0.45     |
| 1:E:123:PHE:CE2  | 1:F:21:VAL:HG23  | 2.52        | 0.45     |
| 1:E:18:ILE:HG22  | 1:E:19:SER:N     | 2.31        | 0.45     |
| 1:D:133:TYR:CE1  | 1:D:134:TYR:CD1  | 3.05        | 0.45     |
| 1:A:74:ALA:O     | 1:A:78:CYS:O     | 2.33        | 0.45     |
| 1:B:142:ASP:C    | 1:B:143:PHE:HD1  | 2.20        | 0.45     |
| 1:C:52:ARG:CG    | 1:C:52:ARG:HH11  | 2.30        | 0.45     |
| 1:E:83:ALA:CB    | 1:E:125:MSE:HE1  | 2.37        | 0.45     |
| 1:C:26:PHE:N     | 1:C:26:PHE:HD1   | 2.14        | 0.45     |
| 1:B:18:ILE:HG22  | 1:B:91:LEU:CD2   | 2.47        | 0.45     |
| 1:F:90:TYR:C     | 1:F:90:TYR:CD1   | 2.89        | 0.45     |
| 1:D:12:LEU:HG    | 1:D:80:GLN:HE21  | 1.81        | 0.45     |
| 1:D:90:TYR:HE1   | 1:D:94:ARG:CG    | 2.30        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:112:TYR:HD2  | 1:C:30:VAL:HG11  | 1.81        | 0.45     |
| 1:D:132:ASN:O    | 1:D:135:LEU:HB2  | 2.17        | 0.45     |
| 1:C:26:PHE:CD2   | 1:C:98:PHE:CD2   | 3.05        | 0.45     |
| 1:D:79:SER:HB3   | 1:D:82:PRO:HD2   | 1.97        | 0.45     |
| 1:D:12:LEU:O     | 1:D:15:VAL:HG12  | 2.17        | 0.45     |
| 1:D:67:PHE:HB2   | 1:D:90:TYR:CE2   | 2.52        | 0.45     |
| 1:A:37:GLN:OE1   | 1:A:47:THR:HG21  | 2.16        | 0.45     |
| 1:A:42:PHE:CZ    | 1:C:112:TYR:HE1  | 2.34        | 0.45     |
| 1:A:132:ASN:HD21 | 1:A:136:ILE:HD11 | 1.81        | 0.45     |
| 1:B:116:LYS:N    | 1:B:119:ILE:CD1  | 2.80        | 0.45     |
| 1:B:90:TYR:N     | 1:B:118:ILE:HD13 | 2.32        | 0.45     |
| 1:A:81:VAL:O     | 1:A:84:ALA:HB3   | 2.17        | 0.45     |
| 2:C:501:3CS:C41  | 2:C:501:3CS:H182 | 2.47        | 0.45     |
| 1:F:102:LEU:HA   | 1:F:102:LEU:HD22 | 1.69        | 0.45     |
| 1:C:106:THR:CG2  | 1:C:107:GLN:H    | 2.30        | 0.45     |
| 1:C:106:THR:CG2  | 1:C:107:GLN:N    | 2.78        | 0.45     |
| 1:E:25:PHE:O     | 1:E:28:HIS:HB3   | 2.17        | 0.45     |
| 1:F:67:PHE:CD1   | 1:F:67:PHE:C     | 2.89        | 0.45     |
| 1:F:70:VAL:HG23  | 1:F:71:LEU:N     | 2.31        | 0.45     |
| 1:D:81:VAL:N     | 1:D:82:PRO:CD    | 2.80        | 0.45     |
| 1:D:79:SER:C     | 1:D:82:PRO:HD2   | 2.37        | 0.45     |
| 1:E:121:PHE:CE1  | 1:E:125:MSE:HG3  | 2.51        | 0.45     |
| 1:B:63:ALA:C     | 1:B:65:PRO:HD2   | 2.37        | 0.45     |
| 1:F:106:THR:O    | 1:F:107:GLN:HB2  | 2.16        | 0.45     |
| 1:A:124:LEU:N    | 1:A:124:LEU:HD13 | 2.31        | 0.45     |
| 1:A:3:GLN:NE2    | 1:C:133:TYR:CD1  | 2.85        | 0.45     |
| 1:A:90:TYR:HE1   | 1:A:114:PHE:CE2  | 2.35        | 0.45     |
| 1:A:18:ILE:HG21  | 1:A:91:LEU:HD23  | 1.98        | 0.45     |
| 1:A:42:PHE:CG    | 1:C:112:TYR:CE1  | 3.05        | 0.45     |
| 1:A:95:GLN:O     | 1:A:99:VAL:HB    | 2.17        | 0.45     |
| 1:B:106:THR:O    | 1:B:108:SER:N    | 2.50        | 0.45     |
| 1:B:139:PHE:CD2  | 1:F:121:PHE:HB2  | 2.52        | 0.45     |
| 1:A:56:ALA:HA    | 1:A:101:TYR:HD2  | 1.81        | 0.45     |
| 2:A:503:3CS:C9   | 2:A:503:3CS:H13  | 2.47        | 0.45     |
| 2:A:503:3CS:C23  | 2:A:503:3CS:H382 | 2.44        | 0.45     |
| 2:A:503:3CS:I25  | 1:B:25:PHE:HB2   | 2.87        | 0.45     |
| 1:E:22:GLN:CG    | 1:E:23:ASN:N     | 2.80        | 0.45     |
| 2:E:506:3CS:H23  | 2:E:506:3CS:O42  | 2.16        | 0.45     |
| 1:D:64:TYR:N     | 1:D:65:PRO:HD2   | 2.32        | 0.45     |
| 1:E:130:ILE:CD1  | 1:F:14:ILE:HD11  | 2.47        | 0.45     |
| 1:E:109:THR:N    | 1:E:110:PRO:HD3  | 2.32        | 0.45     |
| 1:C:116:LYS:HA   | 1:C:119:ILE:HD11 | 1.99        | 0.44     |

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| Atom-1          | Atom-2           | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:C:11:LEU:CD2  | 1:C:80:GLN:NE2   | 2.69        | 0.44     |
| 1:D:123:PHE:HB2 | 2:D:505:3CS:H313 | 1.98        | 0.44     |
| 1:E:59:ASN:ND2  | 1:E:112:TYR:H    | 2.15        | 0.44     |
| 1:E:56:ALA:HA   | 1:E:101:TYR:CD2  | 2.52        | 0.44     |
| 1:B:2:ASP:OD1   | 1:B:5:THR:HG23   | 2.17        | 0.44     |
| 1:A:76:LEU:HD12 | 1:A:76:LEU:HA    | 1.81        | 0.44     |
| 1:F:11:LEU:HD22 | 1:F:80:GLN:HE22  | 1.82        | 0.44     |
| 1:D:79:SER:O    | 1:D:82:PRO:HD2   | 2.18        | 0.44     |
| 1:D:18:ILE:HG22 | 1:D:91:LEU:CD2   | 2.47        | 0.44     |
| 1:D:42:PHE:CE2  | 1:F:112:TYR:CA   | 3.01        | 0.44     |
| 1:A:22:GLN:OE1  | 1:A:94:ARG:NE    | 2.49        | 0.44     |
| 1:D:99:VAL:HG12 | 1:D:100:GLY:N    | 2.32        | 0.44     |
| 1:E:44:ARG:HH11 | 1:E:44:ARG:HB2   | 1.82        | 0.44     |
| 1:D:94:ARG:CG   | 1:D:114:PHE:CZ   | 2.93        | 0.44     |
| 1:D:94:ARG:HD3  | 1:D:114:PHE:HZ   | 1.82        | 0.44     |
| 1:B:77:LEU:N    | 1:B:77:LEU:CD1   | 2.80        | 0.44     |
| 1:A:137:PHE:CE2 | 1:A:138:PHE:HE1  | 2.36        | 0.44     |
| 1:D:2:ASP:OD2   | 1:D:5:THR:HG23   | 2.17        | 0.44     |
| 1:B:74:ALA:CB   | 1:B:122:LEU:HD12 | 2.48        | 0.44     |
| 1:C:133:TYR:C   | 1:C:133:TYR:CD1  | 2.90        | 0.44     |
| 2:B:502:3CS:H21 | 1:C:25:PHE:N     | 2.32        | 0.44     |
| 1:F:78:CYS:O    | 1:F:79:SER:CB    | 2.65        | 0.44     |
| 1:C:64:TYR:N    | 1:C:65:PRO:HD2   | 2.33        | 0.44     |
| 1:D:15:VAL:O    | 1:D:18:ILE:HB    | 2.18        | 0.44     |
| 1:D:6:VAL:HG12  | 1:F:133:TYR:CD2  | 2.52        | 0.44     |
| 1:F:55:THR:HG21 | 1:F:101:TYR:OH   | 2.18        | 0.44     |
| 1:A:102:LEU:CG  | 1:A:103:GLY:H    | 2.15        | 0.44     |
| 1:E:12:LEU:HD13 | 1:E:72:TRP:CE3   | 2.52        | 0.44     |
| 1:D:143:PHE:CE2 | 1:D:144:GLU:HG2  | 2.53        | 0.44     |
| 1:D:89:MSE:O    | 1:D:93:VAL:HG23  | 2.16        | 0.44     |
| 1:C:26:PHE:HD1  | 1:C:26:PHE:H     | 1.65        | 0.44     |
| 1:B:90:TYR:N    | 1:B:118:ILE:CD1  | 2.81        | 0.44     |
| 1:A:14:ILE:HD11 | 1:C:130:ILE:HD12 | 1.99        | 0.44     |
| 1:C:120:LEU:CD2 | 2:C:501:3CS:H323 | 2.47        | 0.44     |
| 1:C:90:TYR:CD1  | 1:C:118:ILE:HG21 | 2.53        | 0.44     |
| 1:D:66:THR:CG2  | 1:E:20:VAL:HG22  | 2.44        | 0.44     |
| 1:B:90:TYR:C    | 1:B:90:TYR:CD1   | 2.91        | 0.44     |
| 1:F:121:PHE:HE1 | 1:F:125:MSE:CG   | 2.30        | 0.44     |
| 1:A:63:ALA:HB2  | 1:A:114:PHE:HE1  | 1.82        | 0.44     |
| 1:A:97:TYR:CD2  | 1:A:114:PHE:CB   | 3.01        | 0.44     |
| 1:E:119:ILE:CG1 | 2:E:506:3CS:H12  | 2.48        | 0.44     |
| 1:F:52:ARG:HG3  | 1:F:52:ARG:NH1   | 2.29        | 0.44     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:F:140:GLY:C    | 1:F:142:ASP:N    | 2.71        | 0.44     |
| 1:D:47:THR:HG22  | 1:D:49:ALA:H     | 1.83        | 0.44     |
| 1:B:110:PRO:HB3  | 1:C:35:ARG:HH22  | 1.83        | 0.44     |
| 1:A:110:PRO:CB   | 1:B:42:PHE:HB2   | 2.48        | 0.44     |
| 1:A:90:TYR:HB2   | 1:A:118:ILE:HG21 | 1.99        | 0.44     |
| 1:A:35:ARG:NH2   | 1:C:113:ILE:CD1  | 2.81        | 0.44     |
| 1:B:144:GLU:CB   | 1:B:146:TYR:CE1  | 2.99        | 0.44     |
| 1:E:126:SER:HB2  | 1:F:17:LEU:HD11  | 2.00        | 0.44     |
| 1:A:90:TYR:HA    | 1:A:118:ILE:HD12 | 2.00        | 0.43     |
| 1:D:10:VAL:HG12  | 1:D:11:LEU:N     | 2.32        | 0.43     |
| 1:D:44:ARG:CA    | 1:D:44:ARG:HE    | 2.31        | 0.43     |
| 1:A:25:PHE:HD1   | 1:A:25:PHE:O     | 2.01        | 0.43     |
| 1:C:119:ILE:H    | 1:C:119:ILE:HD13 | 1.82        | 0.43     |
| 1:F:97:TYR:HB3   | 1:F:114:PHE:CZ   | 2.53        | 0.43     |
| 1:E:80:GLN:H     | 1:E:82:PRO:HD2   | 1.83        | 0.43     |
| 1:B:145:ASN:HD22 | 1:B:145:ASN:N    | 2.01        | 0.43     |
| 1:D:44:ARG:HH11  | 1:F:51:GLU:HG2   | 1.81        | 0.43     |
| 1:E:133:TYR:CD1  | 1:E:134:TYR:HD1  | 2.34        | 0.43     |
| 1:A:67:PHE:CD1   | 1:A:90:TYR:HD2   | 2.36        | 0.43     |
| 1:B:130:ILE:CD1  | 1:C:14:ILE:CD1   | 2.96        | 0.43     |
| 1:D:116:LYS:HZ3  | 1:D:119:ILE:HD11 | 1.83        | 0.43     |
| 1:F:64:TYR:CE1   | 1:F:68:LEU:HD22  | 2.53        | 0.43     |
| 1:C:87:GLY:O     | 1:C:90:TYR:HB3   | 2.19        | 0.43     |
| 1:E:90:TYR:HB2   | 1:E:118:ILE:HD13 | 2.00        | 0.43     |
| 1:E:133:TYR:CE1  | 1:E:134:TYR:CD1  | 3.07        | 0.43     |
| 1:D:52:ARG:NH1   | 1:D:52:ARG:CG    | 2.81        | 0.43     |
| 1:D:85:PHE:O     | 1:D:88:LEU:HB3   | 2.18        | 0.43     |
| 2:B:502:3CS:C21  | 1:C:25:PHE:N     | 2.81        | 0.43     |
| 1:F:104:GLU:HA   | 1:F:104:GLU:OE1  | 2.17        | 0.43     |
| 1:A:111:GLY:HA2  | 1:B:31:GLU:CD    | 2.38        | 0.43     |
| 1:C:33:GLU:CG    | 1:C:50:PHE:HA    | 2.48        | 0.43     |
| 1:C:7:GLY:C      | 1:C:9:VAL:H      | 2.22        | 0.43     |
| 1:D:57:ASN:C     | 1:D:59:ASN:H     | 2.21        | 0.43     |
| 1:C:22:GLN:HB2   | 1:C:22:GLN:HE21  | 1.67        | 0.43     |
| 1:A:74:ALA:CB    | 1:A:122:LEU:HD12 | 2.49        | 0.43     |
| 1:D:21:VAL:HG23  | 1:F:123:PHE:CE2  | 2.53        | 0.43     |
| 1:E:10:VAL:O     | 1:E:14:ILE:HD12  | 2.19        | 0.43     |
| 1:D:133:TYR:HD1  | 1:D:134:TYR:CD1  | 2.37        | 0.43     |
| 1:C:81:VAL:N     | 1:C:82:PRO:CD    | 2.81        | 0.43     |
| 1:E:29:LYS:HD2   | 1:E:29:LYS:HA    | 1.55        | 0.43     |
| 1:C:144:GLU:OE1  | 1:C:147:ILE:HD11 | 2.19        | 0.43     |
| 1:F:79:SER:HB2   | 1:F:82:PRO:HG2   | 2.01        | 0.43     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:F:29:LYS:HA    | 1:F:29:LYS:HD2   | 1.51        | 0.43     |
| 1:F:1:MSE:HB3    | 1:F:6:VAL:HG22   | 1.99        | 0.43     |
| 1:A:30:VAL:HG23  | 1:A:53:VAL:CG1   | 2.48        | 0.43     |
| 1:F:22:GLN:HG3   | 1:F:23:ASN:N     | 2.33        | 0.43     |
| 1:D:10:VAL:CG2   | 1:F:133:TYR:CE2  | 3.00        | 0.43     |
| 1:E:74:ALA:HB1   | 1:E:125:MSE:HE2  | 2.00        | 0.43     |
| 1:B:124:LEU:N    | 1:B:124:LEU:HD13 | 2.34        | 0.43     |
| 1:B:90:TYR:HA    | 1:B:118:ILE:HD13 | 1.99        | 0.43     |
| 2:E:506:3CS:H371 | 2:E:506:3CS:C19  | 2.49        | 0.43     |
| 1:F:90:TYR:N     | 1:F:118:ILE:CD1  | 2.81        | 0.43     |
| 1:F:12:LEU:HD11  | 1:F:75:GLY:HA3   | 1.99        | 0.43     |
| 1:B:26:PHE:CG    | 1:B:98:PHE:CD2   | 3.06        | 0.43     |
| 1:D:26:PHE:CD1   | 1:D:26:PHE:N     | 2.87        | 0.43     |
| 1:B:67:PHE:HB2   | 1:B:90:TYR:CE2   | 2.53        | 0.43     |
| 1:F:90:TYR:HD1   | 1:F:90:TYR:O     | 2.01        | 0.43     |
| 1:C:90:TYR:CB    | 1:C:118:ILE:HG21 | 2.46        | 0.43     |
| 1:A:43:GLN:HB2   | 1:C:51:GLU:OE1   | 2.19        | 0.43     |
| 1:B:56:ALA:HA    | 1:B:101:TYR:CD2  | 2.54        | 0.43     |
| 1:F:26:PHE:HB3   | 1:F:57:ASN:HD22  | 1.84        | 0.43     |
| 1:E:47:THR:CG2   | 1:E:50:PHE:HB3   | 2.48        | 0.43     |
| 1:B:120:LEU:CD1  | 1:B:124:LEU:HD21 | 2.48        | 0.43     |
| 2:B:502:3CS:I25  | 1:C:25:PHE:HB2   | 2.88        | 0.43     |
| 1:A:67:PHE:CD1   | 1:A:67:PHE:C     | 2.92        | 0.43     |
| 1:A:9:VAL:O      | 1:A:9:VAL:HG23   | 2.18        | 0.43     |
| 1:D:120:LEU:HD23 | 2:D:505:3CS:C29  | 2.48        | 0.43     |
| 1:E:23:ASN:OD1   | 1:E:94:ARG:NH2   | 2.51        | 0.43     |
| 1:F:132:ASN:HD21 | 1:F:136:ILE:HD11 | 1.83        | 0.43     |
| 1:D:133:TYR:CD1  | 1:D:134:TYR:HD1  | 2.36        | 0.43     |
| 1:A:81:VAL:N     | 1:A:82:PRO:HD2   | 2.33        | 0.42     |
| 1:C:63:ALA:CB    | 1:C:114:PHE:CZ   | 3.02        | 0.42     |
| 1:C:63:ALA:HB1   | 1:C:114:PHE:CZ   | 2.53        | 0.42     |
| 1:D:124:LEU:HD12 | 1:D:124:LEU:HA   | 1.82        | 0.42     |
| 1:E:60:CYS:HG    | 1:E:114:PHE:HE2  | 1.63        | 0.42     |
| 1:D:2:ASP:N      | 1:D:2:ASP:OD1    | 2.51        | 0.42     |
| 1:C:131:PHE:CD1  | 1:C:132:ASN:N    | 2.87        | 0.42     |
| 1:A:90:TYR:CD1   | 1:A:90:TYR:C     | 2.93        | 0.42     |
| 1:B:144:GLU:O    | 1:F:89:MSE:HE3   | 2.19        | 0.42     |
| 1:C:55:THR:HG22  | 1:C:101:TYR:CE2  | 2.54        | 0.42     |
| 1:D:42:PHE:CE2   | 1:F:111:GLY:C    | 2.93        | 0.42     |
| 1:E:133:TYR:HD1  | 1:E:134:TYR:CD1  | 2.36        | 0.42     |
| 1:B:30:VAL:CG2   | 1:B:53:VAL:CG1   | 2.97        | 0.42     |
| 1:C:1:MSE:HE3    | 1:C:5:THR:OG1    | 2.19        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:D:505:3CS:C21  | 1:E:25:PHE:HB2   | 2.49        | 0.42     |
| 1:C:83:ALA:HB2   | 1:C:125:MSE:CE   | 2.25        | 0.42     |
| 1:F:132:ASN:ND2  | 1:F:136:ILE:HD11 | 2.34        | 0.42     |
| 1:B:116:LYS:CA   | 1:B:119:ILE:HD11 | 2.50        | 0.42     |
| 1:B:48:LEU:O     | 1:B:51:GLU:N     | 2.52        | 0.42     |
| 1:B:102:LEU:HD23 | 1:B:102:LEU:HA   | 1.87        | 0.42     |
| 1:B:18:ILE:HG22  | 1:B:91:LEU:HD23  | 2.00        | 0.42     |
| 1:A:11:LEU:HD13  | 1:A:11:LEU:N     | 2.34        | 0.42     |
| 2:A:503:3CS:C23  | 2:A:503:3CS:C38  | 2.96        | 0.42     |
| 1:C:135:LEU:HA   | 1:C:135:LEU:HD23 | 1.78        | 0.42     |
| 1:E:7:GLY:O      | 1:E:9:VAL:N      | 2.52        | 0.42     |
| 1:B:135:LEU:C    | 1:B:137:PHE:H    | 2.22        | 0.42     |
| 1:E:33:GLU:OE1   | 1:E:33:GLU:HA    | 2.20        | 0.42     |
| 2:B:502:3CS:O42  | 2:B:502:3CS:H23  | 2.19        | 0.42     |
| 1:C:22:GLN:CG    | 1:C:23:ASN:N     | 2.82        | 0.42     |
| 1:B:144:GLU:CG   | 1:B:146:TYR:CE1  | 3.02        | 0.42     |
| 1:E:52:ARG:HH11  | 1:E:52:ARG:CG    | 2.29        | 0.42     |
| 1:E:77:LEU:HD21  | 1:F:13:ALA:HB1   | 2.01        | 0.42     |
| 1:D:47:THR:HB    | 1:D:50:PHE:HB3   | 2.02        | 0.42     |
| 1:B:133:TYR:CE1  | 1:B:134:TYR:CE1  | 3.08        | 0.42     |
| 1:B:118:ILE:CG2  | 1:B:119:ILE:N    | 2.82        | 0.42     |
| 1:F:74:ALA:HB2   | 1:F:122:LEU:O    | 2.18        | 0.42     |
| 1:F:124:LEU:HD12 | 1:F:124:LEU:HA   | 1.78        | 0.42     |
| 2:A:503:3CS:H393 | 2:A:503:3CS:H182 | 2.02        | 0.42     |
| 1:B:57:ASN:C     | 1:B:59:ASN:H     | 2.21        | 0.42     |
| 1:A:48:LEU:HA    | 1:A:48:LEU:HD23  | 1.80        | 0.42     |
| 2:B:502:3CS:C21  | 1:C:25:PHE:CA    | 2.98        | 0.42     |
| 2:A:503:3CS:H181 | 1:B:28:HIS:HB2   | 2.02        | 0.42     |
| 1:E:81:VAL:CB    | 1:E:82:PRO:HD3   | 2.50        | 0.42     |
| 1:C:53:VAL:HG12  | 1:C:54:TYR:N     | 2.35        | 0.42     |
| 1:B:90:TYR:HD1   | 1:B:90:TYR:C     | 2.24        | 0.42     |
| 1:F:124:LEU:C    | 1:F:127:VAL:HG12 | 2.40        | 0.42     |
| 1:D:90:TYR:CD1   | 1:D:90:TYR:C     | 2.94        | 0.42     |
| 1:E:85:PHE:CZ    | 1:E:89:MSE:CE    | 3.03        | 0.42     |
| 1:E:133:TYR:CE1  | 1:F:10:VAL:HG21  | 2.55        | 0.42     |
| 1:B:138:PHE:CD1  | 1:B:138:PHE:N    | 2.87        | 0.42     |
| 1:B:133:TYR:HD1  | 1:B:134:TYR:CD1  | 2.38        | 0.42     |
| 1:F:35:ARG:HA    | 1:F:38:ASN:OD1   | 2.19        | 0.42     |
| 1:F:7:GLY:C      | 1:F:9:VAL:H      | 2.23        | 0.42     |
| 1:A:126:SER:O    | 1:A:130:ILE:HB   | 2.19        | 0.42     |
| 1:A:124:LEU:HA   | 1:A:124:LEU:HD12 | 1.87        | 0.42     |
| 1:A:15:VAL:CG1   | 1:A:16:THR:N     | 2.83        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:11:LEU:CD2   | 1:A:80:GLN:NE2   | 2.80        | 0.42     |
| 1:B:29:LYS:HD2   | 1:B:29:LYS:HA    | 1.57        | 0.42     |
| 1:E:114:PHE:O    | 1:E:115:GLY:C    | 2.58        | 0.42     |
| 1:C:74:ALA:HB2   | 1:C:122:LEU:O    | 2.20        | 0.42     |
| 1:F:139:PHE:C    | 1:F:141:SER:H    | 2.20        | 0.42     |
| 1:C:72:TRP:O     | 1:C:76:LEU:HD22  | 2.20        | 0.42     |
| 1:C:124:LEU:C    | 1:C:127:VAL:HG12 | 2.40        | 0.41     |
| 1:D:123:PHE:HD1  | 1:D:124:LEU:HD13 | 1.85        | 0.41     |
| 1:D:56:ALA:HB2   | 1:D:101:TYR:HB3  | 2.02        | 0.41     |
| 1:D:22:GLN:CG    | 1:D:23:ASN:N     | 2.81        | 0.41     |
| 1:D:26:PHE:H     | 1:D:26:PHE:HD1   | 1.67        | 0.41     |
| 1:B:116:LYS:HA   | 1:B:119:ILE:HD11 | 2.01        | 0.41     |
| 1:A:25:PHE:CA    | 2:C:501:3CS:C21  | 2.98        | 0.41     |
| 1:C:113:ILE:O    | 1:C:114:PHE:CG   | 2.73        | 0.41     |
| 1:C:62:ASP:OD1   | 1:C:62:ASP:N     | 2.53        | 0.41     |
| 1:B:85:PHE:HZ    | 1:B:89:MSE:HE2   | 1.85        | 0.41     |
| 1:D:120:LEU:O    | 1:D:124:LEU:HD22 | 2.20        | 0.41     |
| 1:D:108:SER:C    | 1:E:40:ARG:HD2   | 2.38        | 0.41     |
| 1:E:48:LEU:HD13  | 1:E:48:LEU:C     | 2.40        | 0.41     |
| 1:C:85:PHE:O     | 1:C:88:LEU:HB3   | 2.20        | 0.41     |
| 1:D:67:PHE:C     | 1:D:67:PHE:CD1   | 2.91        | 0.41     |
| 1:D:112:TYR:CE2  | 1:E:30:VAL:CG1   | 2.99        | 0.41     |
| 1:A:42:PHE:CD2   | 1:A:50:PHE:CZ    | 2.96        | 0.41     |
| 1:C:135:LEU:O    | 1:C:139:PHE:N    | 2.53        | 0.41     |
| 1:E:15:VAL:O     | 1:E:18:ILE:HB    | 2.20        | 0.41     |
| 1:B:50:PHE:HD1   | 1:B:50:PHE:O     | 2.03        | 0.41     |
| 1:D:88:LEU:C     | 1:D:88:LEU:HD13  | 2.40        | 0.41     |
| 1:C:113:ILE:HG22 | 1:C:114:PHE:O    | 2.20        | 0.41     |
| 1:F:64:TYR:O     | 1:F:67:PHE:HB3   | 2.20        | 0.41     |
| 1:D:33:GLU:HA    | 1:D:33:GLU:OE1   | 2.21        | 0.41     |
| 1:B:107:GLN:CG   | 1:C:40:ARG:HD2   | 2.50        | 0.41     |
| 1:A:12:LEU:O     | 1:A:15:VAL:HG12  | 2.21        | 0.41     |
| 1:D:116:LYS:NZ   | 2:D:505:3CS:C16  | 2.78        | 0.41     |
| 1:F:26:PHE:CE2   | 1:F:98:PHE:CD2   | 3.08        | 0.41     |
| 1:B:11:LEU:HD13  | 1:B:11:LEU:N     | 2.35        | 0.41     |
| 1:F:79:SER:OG    | 1:F:82:PRO:HD2   | 2.20        | 0.41     |
| 1:D:25:PHE:O     | 1:D:28:HIS:HB3   | 2.21        | 0.41     |
| 1:D:124:LEU:N    | 1:D:124:LEU:CD1  | 2.83        | 0.41     |
| 1:E:44:ARG:HG2   | 1:E:44:ARG:H     | 1.44        | 0.41     |
| 1:E:68:LEU:HD12  | 1:E:68:LEU:HA    | 1.80        | 0.41     |
| 1:F:2:ASP:N      | 1:F:2:ASP:OD1    | 2.54        | 0.41     |
| 1:E:2:ASP:OD1    | 1:E:5:THR:HG23   | 2.21        | 0.41     |

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| Atom-1          | Atom-2           | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:B:120:LEU:CD1 | 1:B:124:LEU:CD2  | 2.97        | 0.41     |
| 1:A:64:TYR:CE1  | 1:A:68:LEU:HD22  | 2.55        | 0.41     |
| 1:E:113:ILE:C   | 1:E:114:PHE:HD1  | 2.23        | 0.41     |
| 2:D:505:3CS:C21 | 1:E:25:PHE:CA    | 2.99        | 0.41     |
| 1:B:26:PHE:CD1  | 1:B:26:PHE:N     | 2.89        | 0.41     |
| 1:B:135:LEU:C   | 1:B:137:PHE:N    | 2.72        | 0.41     |
| 1:C:26:PHE:CE2  | 1:C:98:PHE:CD2   | 3.09        | 0.41     |
| 1:A:71:LEU:HD22 | 1:A:71:LEU:O     | 2.20        | 0.41     |
| 1:D:138:PHE:N   | 1:D:138:PHE:CD1  | 2.88        | 0.41     |
| 1:F:121:PHE:HD1 | 1:F:121:PHE:O    | 2.04        | 0.41     |
| 1:A:22:GLN:CG   | 1:A:23:ASN:N     | 2.83        | 0.41     |
| 1:D:124:LEU:C   | 1:D:127:VAL:HG12 | 2.41        | 0.41     |
| 1:E:55:THR:OG1  | 1:F:42:PHE:HD2   | 2.02        | 0.41     |
| 1:F:91:LEU:HA   | 1:F:91:LEU:HD12  | 1.78        | 0.41     |
| 1:F:10:VAL:CG1  | 1:F:14:ILE:CD1   | 2.98        | 0.41     |
| 1:B:65:PRO:HG2  | 1:B:66:THR:H     | 1.84        | 0.41     |
| 1:F:79:SER:O    | 1:F:80:GLN:CB    | 2.69        | 0.41     |
| 1:A:56:ALA:HA   | 1:A:101:TYR:CD2  | 2.56        | 0.41     |
| 1:A:8:ASN:C     | 1:A:9:VAL:HG12   | 2.41        | 0.41     |
| 1:A:25:PHE:N    | 2:C:501:3CS:C21  | 2.83        | 0.41     |
| 1:C:10:VAL:HG13 | 1:C:14:ILE:HD13  | 2.00        | 0.41     |
| 1:F:30:VAL:CG2  | 1:F:53:VAL:HG12  | 2.51        | 0.41     |
| 1:E:22:GLN:HB2  | 1:E:22:GLN:HE21  | 1.72        | 0.41     |
| 1:D:78:CYS:HB2  | 1:D:125:MSE:O    | 2.21        | 0.41     |
| 1:E:52:ARG:CG   | 1:E:52:ARG:NH1   | 2.83        | 0.41     |
| 1:D:19:SER:HB2  | 1:D:64:TYR:CE1   | 2.56        | 0.41     |
| 1:B:81:VAL:N    | 1:B:82:PRO:CD    | 2.84        | 0.41     |
| 1:A:33:GLU:OE2  | 1:A:49:ALA:HB1   | 2.20        | 0.41     |
| 1:B:112:TYR:CD2 | 1:C:30:VAL:CG1   | 2.97        | 0.41     |
| 1:B:26:PHE:CG   | 1:B:98:PHE:CE2   | 3.09        | 0.41     |
| 1:B:38:ASN:C    | 1:B:40:ARG:N     | 2.74        | 0.41     |
| 1:A:133:TYR:CD1 | 1:A:133:TYR:C    | 2.94        | 0.41     |
| 1:B:35:ARG:C    | 1:B:37:GLN:H     | 2.24        | 0.41     |
| 1:C:95:GLN:O    | 1:C:99:VAL:HB    | 2.20        | 0.41     |
| 1:B:10:VAL:HG12 | 1:B:11:LEU:N     | 2.34        | 0.41     |
| 1:D:25:PHE:CA   | 2:F:504:3CS:C21  | 2.99        | 0.41     |
| 1:A:10:VAL:HG13 | 1:A:14:ILE:HD13  | 2.01        | 0.41     |
| 1:A:64:TYR:CE1  | 1:A:68:LEU:CD2   | 3.03        | 0.41     |
| 1:D:74:ALA:CB   | 1:D:122:LEU:HD12 | 2.51        | 0.41     |
| 1:F:67:PHE:CG   | 1:F:90:TYR:HE2   | 2.37        | 0.41     |
| 1:E:90:TYR:CD1  | 1:E:90:TYR:C     | 2.91        | 0.41     |
| 1:B:56:ALA:HB2  | 1:B:101:TYR:HB3  | 2.03        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:E:135:LEU:CD2  | 1:E:135:LEU:N    | 2.84        | 0.41     |
| 1:D:5:THR:O      | 1:D:9:VAL:HG13   | 2.21        | 0.41     |
| 1:F:146:TYR:O    | 1:F:147:ILE:HD13 | 2.21        | 0.41     |
| 1:F:78:CYS:O     | 1:F:78:CYS:SG    | 2.79        | 0.40     |
| 1:A:97:TYR:CD2   | 1:A:114:PHE:HB3  | 2.56        | 0.40     |
| 1:B:25:PHE:CD1   | 1:B:25:PHE:C     | 2.94        | 0.40     |
| 1:D:116:LYS:CE   | 2:D:505:3CS:C16  | 3.00        | 0.40     |
| 1:E:64:TYR:CE1   | 1:E:68:LEU:CD2   | 3.03        | 0.40     |
| 1:F:33:GLU:OE2   | 1:F:49:ALA:HB1   | 2.21        | 0.40     |
| 1:D:121:PHE:C    | 1:D:121:PHE:CD1  | 2.94        | 0.40     |
| 1:A:10:VAL:HG21  | 1:C:133:TYR:HD2  | 1.80        | 0.40     |
| 2:E:506:3CS:C21  | 1:F:25:PHE:N     | 2.84        | 0.40     |
| 1:C:147:ILE:O    | 1:C:147:ILE:HG22 | 2.20        | 0.40     |
| 1:B:11:LEU:N     | 1:B:11:LEU:HD22  | 2.09        | 0.40     |
| 1:F:81:VAL:N     | 1:F:82:PRO:CD    | 2.84        | 0.40     |
| 1:D:25:PHE:CE1   | 1:D:29:LYS:HG2   | 2.57        | 0.40     |
| 1:A:40:ARG:HD3   | 1:C:52:ARG:HH22  | 1.86        | 0.40     |
| 1:C:52:ARG:NE    | 1:C:102:LEU:HA   | 2.36        | 0.40     |
| 1:D:64:TYR:CZ    | 1:D:68:LEU:CD2   | 3.04        | 0.40     |
| 1:D:113:ILE:HG12 | 1:D:114:PHE:O    | 2.20        | 0.40     |
| 1:A:33:GLU:OE1   | 1:A:33:GLU:HA    | 2.21        | 0.40     |
| 1:A:42:PHE:CG    | 1:C:112:TYR:HE1  | 2.40        | 0.40     |
| 1:D:132:ASN:ND2  | 1:D:136:ILE:HD11 | 2.37        | 0.40     |
| 1:A:137:PHE:O    | 1:A:137:PHE:CD1  | 2.74        | 0.40     |
| 1:A:22:GLN:NE2   | 1:A:26:PHE:CZ    | 2.89        | 0.40     |
| 1:D:11:LEU:HB2   | 1:D:80:GLN:NE2   | 2.36        | 0.40     |
| 1:E:45:THR:CB    | 1:F:43:GLN:NE2   | 2.85        | 0.40     |
| 1:E:8:ASN:C      | 1:E:9:VAL:CG1    | 2.89        | 0.40     |
| 1:D:133:TYR:CE1  | 1:D:134:TYR:HD1  | 2.40        | 0.40     |
| 1:B:85:PHE:C     | 1:B:85:PHE:CD1   | 2.94        | 0.40     |
| 1:A:11:LEU:HB3   | 1:A:84:ALA:CB    | 2.51        | 0.40     |
| 1:F:90:TYR:CE1   | 1:F:94:ARG:HG3   | 2.56        | 0.40     |
| 1:E:130:ILE:CD1  | 1:F:14:ILE:CD1   | 2.99        | 0.40     |
| 1:B:26:PHE:HD1   | 1:B:26:PHE:N     | 2.19        | 0.40     |
| 1:A:136:ILE:H    | 1:A:136:ILE:HG13 | 1.63        | 0.40     |
| 1:C:50:PHE:C     | 1:C:50:PHE:CD1   | 2.94        | 0.40     |
| 1:D:26:PHE:HD1   | 1:D:26:PHE:N     | 2.20        | 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     | 138/161 (86%) | 108 (78%) | 21 (15%)  | 9 (6%)   | 2           | 36 |
| 1   | B     | 146/161 (91%) | 98 (67%)  | 26 (18%)  | 22 (15%) | 0           | 8  |
| 1   | C     | 147/161 (91%) | 115 (78%) | 25 (17%)  | 7 (5%)   | 4           | 44 |
| 1   | D     | 146/161 (91%) | 109 (75%) | 31 (21%)  | 6 (4%)   | 4           | 49 |
| 1   | E     | 138/161 (86%) | 110 (80%) | 17 (12%)  | 11 (8%)  | 1           | 28 |
| 1   | F     | 147/161 (91%) | 107 (73%) | 26 (18%)  | 14 (10%) | 1           | 22 |
| All | All   | 862/966 (89%) | 647 (75%) | 146 (17%) | 69 (8%)  | 1           | 28 |

All (69) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 36  | THR  |
| 1   | B     | 39  | GLY  |
| 1   | B     | 42  | PHE  |
| 1   | B     | 45  | THR  |
| 1   | B     | 49  | ALA  |
| 1   | B     | 106 | THR  |
| 1   | B     | 143 | PHE  |
| 1   | C     | 41  | SER  |
| 1   | C     | 79  | SER  |
| 1   | C     | 109 | THR  |
| 1   | D     | 106 | THR  |
| 1   | E     | 104 | GLU  |
| 1   | E     | 112 | TYR  |
| 1   | E     | 115 | GLY  |
| 1   | F     | 40  | ARG  |
| 1   | F     | 79  | SER  |
| 1   | F     | 108 | SER  |
| 1   | F     | 144 | GLU  |
| 1   | A     | 103 | GLY  |
| 1   | B     | 37  | GLN  |
| 1   | B     | 41  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 107 | GLN  |
| 1   | B     | 114 | PHE  |
| 1   | B     | 146 | TYR  |
| 1   | E     | 8   | ASN  |
| 1   | E     | 106 | THR  |
| 1   | E     | 110 | PRO  |
| 1   | E     | 111 | GLY  |
| 1   | E     | 113 | ILE  |
| 1   | F     | 80  | GLN  |
| 1   | F     | 115 | GLY  |
| 1   | F     | 148 | ALA  |
| 1   | A     | 45  | THR  |
| 1   | A     | 80  | GLN  |
| 1   | B     | 8   | ASN  |
| 1   | B     | 79  | SER  |
| 1   | B     | 147 | ILE  |
| 1   | C     | 3   | GLN  |
| 1   | C     | 8   | ASN  |
| 1   | D     | 3   | GLN  |
| 1   | D     | 41  | SER  |
| 1   | D     | 104 | GLU  |
| 1   | D     | 143 | PHE  |
| 1   | E     | 80  | GLN  |
| 1   | F     | 134 | TYR  |
| 1   | A     | 8   | ASN  |
| 1   | A     | 128 | ALA  |
| 1   | B     | 47  | THR  |
| 1   | B     | 78  | CYS  |
| 1   | B     | 105 | ARG  |
| 1   | B     | 142 | ASP  |
| 1   | F     | 8   | ASN  |
| 1   | F     | 39  | GLY  |
| 1   | F     | 78  | CYS  |
| 1   | A     | 3   | GLN  |
| 1   | B     | 3   | GLN  |
| 1   | C     | 64  | TYR  |
| 1   | E     | 3   | GLN  |
| 1   | E     | 9   | VAL  |
| 1   | F     | 58  | GLN  |
| 1   | A     | 9   | VAL  |
| 1   | A     | 111 | GLY  |
| 1   | C     | 9   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 9   | VAL  |
| 1   | B     | 9   | VAL  |
| 1   | D     | 9   | VAL  |
| 1   | B     | 110 | PRO  |
| 1   | F     | 65  | PRO  |
| 1   | A     | 81  | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed      | Rotameric | Outliers  | Percentiles |   |
|-----|-------|---------------|-----------|-----------|-------------|---|
| 1   | A     | 117/134 (87%) | 67 (57%)  | 50 (43%)  | 0           | 1 |
| 1   | B     | 124/134 (92%) | 69 (56%)  | 55 (44%)  | 0           | 0 |
| 1   | C     | 125/134 (93%) | 83 (66%)  | 42 (34%)  | 0           | 3 |
| 1   | D     | 124/134 (92%) | 75 (60%)  | 49 (40%)  | 0           | 1 |
| 1   | E     | 117/134 (87%) | 67 (57%)  | 50 (43%)  | 0           | 1 |
| 1   | F     | 125/134 (93%) | 74 (59%)  | 51 (41%)  | 0           | 1 |
| All | All   | 732/804 (91%) | 435 (59%) | 297 (41%) | 0           | 1 |

All (297) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | MSE  |
| 1   | A     | 8   | ASN  |
| 1   | A     | 10  | VAL  |
| 1   | A     | 11  | LEU  |
| 1   | A     | 14  | ILE  |
| 1   | A     | 18  | ILE  |
| 1   | A     | 20  | VAL  |
| 1   | A     | 22  | GLN  |
| 1   | A     | 25  | PHE  |
| 1   | A     | 29  | LYS  |
| 1   | A     | 30  | VAL  |
| 1   | A     | 32  | HIS  |
| 1   | A     | 34  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 37  | GLN  |
| 1   | A     | 41  | SER  |
| 1   | A     | 42  | PHE  |
| 1   | A     | 47  | THR  |
| 1   | A     | 52  | ARG  |
| 1   | A     | 62  | ASP  |
| 1   | A     | 64  | TYR  |
| 1   | A     | 66  | THR  |
| 1   | A     | 67  | PHE  |
| 1   | A     | 68  | LEU  |
| 1   | A     | 71  | LEU  |
| 1   | A     | 76  | LEU  |
| 1   | A     | 78  | CYS  |
| 1   | A     | 79  | SER  |
| 1   | A     | 89  | MSE  |
| 1   | A     | 90  | TYR  |
| 1   | A     | 91  | LEU  |
| 1   | A     | 94  | ARG  |
| 1   | A     | 95  | GLN  |
| 1   | A     | 96  | LYS  |
| 1   | A     | 99  | VAL  |
| 1   | A     | 101 | TYR  |
| 1   | A     | 108 | SER  |
| 1   | A     | 109 | THR  |
| 1   | A     | 112 | TYR  |
| 1   | A     | 114 | PHE  |
| 1   | A     | 117 | ARG  |
| 1   | A     | 118 | ILE  |
| 1   | A     | 119 | ILE  |
| 1   | A     | 121 | PHE  |
| 1   | A     | 122 | LEU  |
| 1   | A     | 124 | LEU  |
| 1   | A     | 130 | ILE  |
| 1   | A     | 131 | PHE  |
| 1   | A     | 132 | ASN  |
| 1   | A     | 133 | TYR  |
| 1   | A     | 135 | LEU  |
| 1   | B     | 1   | MSE  |
| 1   | B     | 8   | ASN  |
| 1   | B     | 11  | LEU  |
| 1   | B     | 14  | ILE  |
| 1   | B     | 18  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 20  | VAL  |
| 1   | B     | 21  | VAL  |
| 1   | B     | 22  | GLN  |
| 1   | B     | 25  | PHE  |
| 1   | B     | 29  | LYS  |
| 1   | B     | 30  | VAL  |
| 1   | B     | 32  | HIS  |
| 1   | B     | 34  | SER  |
| 1   | B     | 35  | ARG  |
| 1   | B     | 37  | GLN  |
| 1   | B     | 50  | PHE  |
| 1   | B     | 52  | ARG  |
| 1   | B     | 62  | ASP  |
| 1   | B     | 66  | THR  |
| 1   | B     | 67  | PHE  |
| 1   | B     | 68  | LEU  |
| 1   | B     | 71  | LEU  |
| 1   | B     | 76  | LEU  |
| 1   | B     | 78  | CYS  |
| 1   | B     | 80  | GLN  |
| 1   | B     | 81  | VAL  |
| 1   | B     | 89  | MSE  |
| 1   | B     | 90  | TYR  |
| 1   | B     | 91  | LEU  |
| 1   | B     | 93  | VAL  |
| 1   | B     | 94  | ARG  |
| 1   | B     | 96  | LYS  |
| 1   | B     | 99  | VAL  |
| 1   | B     | 101 | TYR  |
| 1   | B     | 102 | LEU  |
| 1   | B     | 105 | ARG  |
| 1   | B     | 109 | THR  |
| 1   | B     | 113 | ILE  |
| 1   | B     | 114 | PHE  |
| 1   | B     | 117 | ARG  |
| 1   | B     | 118 | ILE  |
| 1   | B     | 119 | ILE  |
| 1   | B     | 121 | PHE  |
| 1   | B     | 122 | LEU  |
| 1   | B     | 124 | LEU  |
| 1   | B     | 130 | ILE  |
| 1   | B     | 131 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 132 | ASN  |
| 1   | B     | 133 | TYR  |
| 1   | B     | 135 | LEU  |
| 1   | B     | 142 | ASP  |
| 1   | B     | 143 | PHE  |
| 1   | B     | 144 | GLU  |
| 1   | B     | 145 | ASN  |
| 1   | B     | 146 | TYR  |
| 1   | C     | 1   | MSE  |
| 1   | C     | 8   | ASN  |
| 1   | C     | 10  | VAL  |
| 1   | C     | 11  | LEU  |
| 1   | C     | 14  | ILE  |
| 1   | C     | 18  | ILE  |
| 1   | C     | 20  | VAL  |
| 1   | C     | 21  | VAL  |
| 1   | C     | 22  | GLN  |
| 1   | C     | 23  | ASN  |
| 1   | C     | 25  | PHE  |
| 1   | C     | 29  | LYS  |
| 1   | C     | 32  | HIS  |
| 1   | C     | 33  | GLU  |
| 1   | C     | 35  | ARG  |
| 1   | C     | 37  | GLN  |
| 1   | C     | 47  | THR  |
| 1   | C     | 52  | ARG  |
| 1   | C     | 62  | ASP  |
| 1   | C     | 64  | TYR  |
| 1   | C     | 66  | THR  |
| 1   | C     | 68  | LEU  |
| 1   | C     | 71  | LEU  |
| 1   | C     | 76  | LEU  |
| 1   | C     | 80  | GLN  |
| 1   | C     | 89  | MSE  |
| 1   | C     | 91  | LEU  |
| 1   | C     | 93  | VAL  |
| 1   | C     | 94  | ARG  |
| 1   | C     | 96  | LYS  |
| 1   | C     | 101 | TYR  |
| 1   | C     | 102 | LEU  |
| 1   | C     | 108 | SER  |
| 1   | C     | 118 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 119 | ILE  |
| 1   | C     | 122 | LEU  |
| 1   | C     | 124 | LEU  |
| 1   | C     | 130 | ILE  |
| 1   | C     | 131 | PHE  |
| 1   | C     | 132 | ASN  |
| 1   | C     | 133 | TYR  |
| 1   | C     | 141 | SER  |
| 1   | D     | 1   | MSE  |
| 1   | D     | 8   | ASN  |
| 1   | D     | 10  | VAL  |
| 1   | D     | 11  | LEU  |
| 1   | D     | 14  | ILE  |
| 1   | D     | 18  | ILE  |
| 1   | D     | 20  | VAL  |
| 1   | D     | 21  | VAL  |
| 1   | D     | 22  | GLN  |
| 1   | D     | 29  | LYS  |
| 1   | D     | 30  | VAL  |
| 1   | D     | 32  | HIS  |
| 1   | D     | 35  | ARG  |
| 1   | D     | 41  | SER  |
| 1   | D     | 42  | PHE  |
| 1   | D     | 44  | ARG  |
| 1   | D     | 51  | GLU  |
| 1   | D     | 52  | ARG  |
| 1   | D     | 62  | ASP  |
| 1   | D     | 66  | THR  |
| 1   | D     | 67  | PHE  |
| 1   | D     | 68  | LEU  |
| 1   | D     | 71  | LEU  |
| 1   | D     | 76  | LEU  |
| 1   | D     | 79  | SER  |
| 1   | D     | 89  | MSE  |
| 1   | D     | 90  | TYR  |
| 1   | D     | 91  | LEU  |
| 1   | D     | 93  | VAL  |
| 1   | D     | 94  | ARG  |
| 1   | D     | 95  | GLN  |
| 1   | D     | 96  | LYS  |
| 1   | D     | 101 | TYR  |
| 1   | D     | 102 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 108 | SER  |
| 1   | D     | 113 | ILE  |
| 1   | D     | 114 | PHE  |
| 1   | D     | 116 | LYS  |
| 1   | D     | 118 | ILE  |
| 1   | D     | 119 | ILE  |
| 1   | D     | 122 | LEU  |
| 1   | D     | 124 | LEU  |
| 1   | D     | 125 | MSE  |
| 1   | D     | 130 | ILE  |
| 1   | D     | 131 | PHE  |
| 1   | D     | 132 | ASN  |
| 1   | D     | 135 | LEU  |
| 1   | D     | 142 | ASP  |
| 1   | D     | 143 | PHE  |
| 1   | E     | 1   | MSE  |
| 1   | E     | 8   | ASN  |
| 1   | E     | 11  | LEU  |
| 1   | E     | 14  | ILE  |
| 1   | E     | 18  | ILE  |
| 1   | E     | 20  | VAL  |
| 1   | E     | 22  | GLN  |
| 1   | E     | 25  | PHE  |
| 1   | E     | 29  | LYS  |
| 1   | E     | 32  | HIS  |
| 1   | E     | 34  | SER  |
| 1   | E     | 35  | ARG  |
| 1   | E     | 37  | GLN  |
| 1   | E     | 40  | ARG  |
| 1   | E     | 42  | PHE  |
| 1   | E     | 44  | ARG  |
| 1   | E     | 45  | THR  |
| 1   | E     | 51  | GLU  |
| 1   | E     | 52  | ARG  |
| 1   | E     | 62  | ASP  |
| 1   | E     | 64  | TYR  |
| 1   | E     | 66  | THR  |
| 1   | E     | 67  | PHE  |
| 1   | E     | 68  | LEU  |
| 1   | E     | 71  | LEU  |
| 1   | E     | 76  | LEU  |
| 1   | E     | 80  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 81  | VAL  |
| 1   | E     | 89  | MSE  |
| 1   | E     | 90  | TYR  |
| 1   | E     | 91  | LEU  |
| 1   | E     | 94  | ARG  |
| 1   | E     | 96  | LYS  |
| 1   | E     | 99  | VAL  |
| 1   | E     | 101 | TYR  |
| 1   | E     | 102 | LEU  |
| 1   | E     | 112 | TYR  |
| 1   | E     | 114 | PHE  |
| 1   | E     | 116 | LYS  |
| 1   | E     | 117 | ARG  |
| 1   | E     | 118 | ILE  |
| 1   | E     | 119 | ILE  |
| 1   | E     | 121 | PHE  |
| 1   | E     | 122 | LEU  |
| 1   | E     | 124 | LEU  |
| 1   | E     | 130 | ILE  |
| 1   | E     | 131 | PHE  |
| 1   | E     | 132 | ASN  |
| 1   | E     | 135 | LEU  |
| 1   | E     | 139 | PHE  |
| 1   | F     | 1   | MSE  |
| 1   | F     | 8   | ASN  |
| 1   | F     | 11  | LEU  |
| 1   | F     | 14  | ILE  |
| 1   | F     | 18  | ILE  |
| 1   | F     | 20  | VAL  |
| 1   | F     | 21  | VAL  |
| 1   | F     | 22  | GLN  |
| 1   | F     | 25  | PHE  |
| 1   | F     | 29  | LYS  |
| 1   | F     | 32  | HIS  |
| 1   | F     | 42  | PHE  |
| 1   | F     | 43  | GLN  |
| 1   | F     | 52  | ARG  |
| 1   | F     | 62  | ASP  |
| 1   | F     | 64  | TYR  |
| 1   | F     | 66  | THR  |
| 1   | F     | 67  | PHE  |
| 1   | F     | 68  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 71  | LEU  |
| 1   | F     | 76  | LEU  |
| 1   | F     | 78  | CYS  |
| 1   | F     | 81  | VAL  |
| 1   | F     | 89  | MSE  |
| 1   | F     | 90  | TYR  |
| 1   | F     | 91  | LEU  |
| 1   | F     | 93  | VAL  |
| 1   | F     | 94  | ARG  |
| 1   | F     | 95  | GLN  |
| 1   | F     | 96  | LYS  |
| 1   | F     | 97  | TYR  |
| 1   | F     | 101 | TYR  |
| 1   | F     | 102 | LEU  |
| 1   | F     | 104 | GLU  |
| 1   | F     | 108 | SER  |
| 1   | F     | 109 | THR  |
| 1   | F     | 114 | PHE  |
| 1   | F     | 117 | ARG  |
| 1   | F     | 118 | ILE  |
| 1   | F     | 119 | ILE  |
| 1   | F     | 121 | PHE  |
| 1   | F     | 122 | LEU  |
| 1   | F     | 124 | LEU  |
| 1   | F     | 130 | ILE  |
| 1   | F     | 131 | PHE  |
| 1   | F     | 132 | ASN  |
| 1   | F     | 133 | TYR  |
| 1   | F     | 135 | LEU  |
| 1   | F     | 143 | PHE  |
| 1   | F     | 144 | GLU  |
| 1   | F     | 147 | ILE  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 8   | ASN  |
| 1   | A     | 57  | ASN  |
| 1   | B     | 8   | ASN  |
| 1   | B     | 38  | ASN  |
| 1   | B     | 80  | GLN  |
| 1   | B     | 132 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 145 | ASN  |
| 1   | C     | 8   | ASN  |
| 1   | C     | 57  | ASN  |
| 1   | C     | 58  | GLN  |
| 1   | C     | 80  | GLN  |
| 1   | D     | 3   | GLN  |
| 1   | D     | 8   | ASN  |
| 1   | D     | 58  | GLN  |
| 1   | D     | 80  | GLN  |
| 1   | D     | 95  | GLN  |
| 1   | E     | 8   | ASN  |
| 1   | E     | 37  | GLN  |
| 1   | E     | 59  | ASN  |
| 1   | E     | 80  | GLN  |
| 1   | E     | 132 | ASN  |
| 1   | F     | 8   | ASN  |
| 1   | F     | 43  | GLN  |
| 1   | F     | 80  | 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 ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | 3CS  | A     | 503 | -    | 47,47,47     | 2.88 | 19 (40%)    | 70,70,70    | 2.30 | 24 (34%)    |
| 2   | 3CS  | B     | 502 | -    | 47,47,47     | 2.19 | 18 (38%)    | 70,70,70    | 2.34 | 20 (28%)    |
| 2   | 3CS  | C     | 501 | -    | 47,47,47     | 2.33 | 13 (27%)    | 70,70,70    | 2.29 | 20 (28%)    |
| 2   | 3CS  | D     | 505 | -    | 47,47,47     | 2.35 | 17 (36%)    | 70,70,70    | 2.33 | 23 (32%)    |
| 2   | 3CS  | E     | 506 | -    | 47,47,47     | 1.97 | 14 (29%)    | 70,70,70    | 2.22 | 22 (31%)    |
| 2   | 3CS  | F     | 504 | -    | 47,47,47     | 2.40 | 19 (40%)    | 70,70,70    | 2.24 | 21 (30%)    |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | 3CS  | A     | 503 | -    | -       | 0/27/29/29 | 0/1/5/5 |
| 2   | 3CS  | B     | 502 | -    | -       | 0/27/29/29 | 0/1/5/5 |
| 2   | 3CS  | C     | 501 | -    | -       | 0/27/29/29 | 0/1/5/5 |
| 2   | 3CS  | D     | 505 | -    | -       | 0/27/29/29 | 0/1/5/5 |
| 2   | 3CS  | E     | 506 | -    | -       | 0/27/29/29 | 0/1/5/5 |
| 2   | 3CS  | F     | 504 | -    | -       | 0/27/29/29 | 0/1/5/5 |

All (100) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2   | A     | 503 | 3CS  | C40-C41 | -14.48 | 1.41        | 1.51     |
| 2   | F     | 504 | 3CS  | C40-C41 | -10.11 | 1.44        | 1.51     |
| 2   | C     | 501 | 3CS  | C40-C41 | -9.15  | 1.45        | 1.51     |
| 2   | D     | 505 | 3CS  | C40-C41 | -8.94  | 1.45        | 1.51     |
| 2   | B     | 502 | 3CS  | C40-C41 | -6.74  | 1.47        | 1.51     |
| 2   | C     | 501 | 3CS  | O27-C11 | -6.05  | 1.23        | 1.37     |
| 2   | F     | 504 | 3CS  | O27-C11 | -5.07  | 1.25        | 1.37     |
| 2   | E     | 506 | 3CS  | O27-C11 | -5.05  | 1.25        | 1.37     |
| 2   | A     | 503 | 3CS  | O27-C11 | -4.74  | 1.26        | 1.37     |
| 2   | D     | 505 | 3CS  | O27-C11 | -4.69  | 1.26        | 1.37     |
| 2   | B     | 502 | 3CS  | O27-C11 | -4.60  | 1.27        | 1.37     |
| 2   | C     | 501 | 3CS  | C30-C29 | -4.41  | 1.45        | 1.51     |
| 2   | B     | 502 | 3CS  | C28-C29 | -4.23  | 1.39        | 1.50     |
| 2   | D     | 505 | 3CS  | C30-C29 | -4.23  | 1.45        | 1.51     |
| 2   | A     | 503 | 3CS  | C28-C29 | -4.22  | 1.39        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | E     | 506 | 3CS  | C28-C29 | -4.19 | 1.40        | 1.50     |
| 2   | D     | 505 | 3CS  | C28-C29 | -3.95 | 1.40        | 1.50     |
| 2   | C     | 501 | 3CS  | C28-C29 | -3.89 | 1.40        | 1.50     |
| 2   | F     | 504 | 3CS  | C28-C29 | -3.84 | 1.40        | 1.50     |
| 2   | C     | 501 | 3CS  | O27-C10 | -3.78 | 1.31        | 1.43     |
| 2   | E     | 506 | 3CS  | C40-C41 | -3.72 | 1.49        | 1.51     |
| 2   | B     | 502 | 3CS  | C12-C11 | 3.68  | 1.43        | 1.37     |
| 2   | F     | 504 | 3CS  | C30-C29 | -3.57 | 1.46        | 1.51     |
| 2   | D     | 505 | 3CS  | C18-N17 | -3.49 | 1.42        | 1.48     |
| 2   | E     | 506 | 3CS  | C30-C29 | -3.46 | 1.46        | 1.51     |
| 2   | B     | 502 | 3CS  | C30-C29 | -3.35 | 1.46        | 1.51     |
| 2   | A     | 503 | 3CS  | C15-N17 | -3.30 | 1.34        | 1.38     |
| 2   | D     | 505 | 3CS  | C15-N17 | -3.27 | 1.34        | 1.38     |
| 2   | A     | 503 | 3CS  | C12-C11 | 3.25  | 1.42        | 1.37     |
| 2   | E     | 506 | 3CS  | C12-C11 | 3.18  | 1.42        | 1.37     |
| 2   | E     | 506 | 3CS  | O27-C10 | -3.17 | 1.33        | 1.43     |
| 2   | F     | 504 | 3CS  | C23-C22 | 3.15  | 1.44        | 1.38     |
| 2   | A     | 503 | 3CS  | C30-C29 | -3.06 | 1.47        | 1.51     |
| 2   | D     | 505 | 3CS  | O27-C10 | -3.04 | 1.34        | 1.43     |
| 2   | B     | 502 | 3CS  | C15-N17 | -3.03 | 1.35        | 1.38     |
| 2   | F     | 504 | 3CS  | C12-C11 | 2.91  | 1.42        | 1.37     |
| 2   | D     | 505 | 3CS  | C12-C11 | 2.90  | 1.42        | 1.37     |
| 2   | B     | 502 | 3CS  | O27-C10 | -2.90 | 1.34        | 1.43     |
| 2   | A     | 503 | 3CS  | O27-C10 | -2.88 | 1.34        | 1.43     |
| 2   | F     | 504 | 3CS  | O27-C10 | -2.87 | 1.34        | 1.43     |
| 2   | C     | 501 | 3CS  | C10-C9  | -2.87 | 1.43        | 1.50     |
| 2   | D     | 505 | 3CS  | C14-C13 | 2.85  | 1.42        | 1.36     |
| 2   | A     | 503 | 3CS  | C1-C6   | 2.84  | 1.46        | 1.42     |
| 2   | C     | 501 | 3CS  | C18-C19 | -2.81 | 1.44        | 1.51     |
| 2   | E     | 506 | 3CS  | C18-N17 | -2.80 | 1.43        | 1.48     |
| 2   | A     | 503 | 3CS  | C24-I25 | -2.76 | 2.02        | 2.10     |
| 2   | B     | 502 | 3CS  | C4-C5   | 2.75  | 1.43        | 1.36     |
| 2   | F     | 504 | 3CS  | C15-N17 | -2.75 | 1.35        | 1.38     |
| 2   | B     | 502 | 3CS  | C1-C6   | 2.74  | 1.46        | 1.42     |
| 2   | A     | 503 | 3CS  | C18-N17 | -2.72 | 1.43        | 1.48     |
| 2   | C     | 501 | 3CS  | C12-C11 | 2.68  | 1.41        | 1.37     |
| 2   | C     | 501 | 3CS  | C15-N17 | -2.65 | 1.35        | 1.38     |
| 2   | A     | 503 | 3CS  | C3-C2   | 2.62  | 1.42        | 1.36     |
| 2   | A     | 503 | 3CS  | C9-N26  | 2.61  | 1.38        | 1.32     |
| 2   | D     | 505 | 3CS  | C18-C19 | -2.59 | 1.44        | 1.51     |
| 2   | B     | 502 | 3CS  | C3-C2   | 2.57  | 1.42        | 1.36     |
| 2   | F     | 504 | 3CS  | C22-C24 | 2.57  | 1.45        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | E     | 506 | 3CS  | C4-C5   | 2.56  | 1.42        | 1.36     |
| 2   | A     | 503 | 3CS  | C4-C5   | 2.56  | 1.42        | 1.36     |
| 2   | D     | 505 | 3CS  | C10-C9  | -2.55 | 1.44        | 1.50     |
| 2   | B     | 502 | 3CS  | C18-N17 | -2.53 | 1.43        | 1.48     |
| 2   | E     | 506 | 3CS  | C1-C6   | 2.50  | 1.45        | 1.42     |
| 2   | C     | 501 | 3CS  | C18-N17 | -2.48 | 1.44        | 1.48     |
| 2   | E     | 506 | 3CS  | C15-N17 | -2.45 | 1.35        | 1.38     |
| 2   | F     | 504 | 3CS  | C4-C5   | 2.45  | 1.42        | 1.36     |
| 2   | E     | 506 | 3CS  | C10-C9  | -2.44 | 1.44        | 1.50     |
| 2   | E     | 506 | 3CS  | C3-C2   | 2.43  | 1.42        | 1.36     |
| 2   | B     | 502 | 3CS  | C14-C13 | 2.43  | 1.41        | 1.36     |
| 2   | B     | 502 | 3CS  | C18-C19 | -2.36 | 1.45        | 1.51     |
| 2   | C     | 501 | 3CS  | C4-C5   | 2.36  | 1.42        | 1.36     |
| 2   | D     | 505 | 3CS  | C4-C5   | 2.34  | 1.42        | 1.36     |
| 2   | A     | 503 | 3CS  | O43-C41 | -2.31 | 1.21        | 1.30     |
| 2   | A     | 503 | 3CS  | C37-C36 | -2.31 | 1.46        | 1.50     |
| 2   | D     | 505 | 3CS  | C3-C2   | 2.30  | 1.41        | 1.36     |
| 2   | A     | 503 | 3CS  | C14-C13 | 2.30  | 1.41        | 1.36     |
| 2   | A     | 503 | 3CS  | C7-C8   | 2.30  | 1.41        | 1.36     |
| 2   | F     | 504 | 3CS  | C3-C2   | 2.29  | 1.41        | 1.36     |
| 2   | C     | 501 | 3CS  | C3-C2   | 2.28  | 1.41        | 1.36     |
| 2   | A     | 503 | 3CS  | C10-C9  | -2.27 | 1.45        | 1.50     |
| 2   | D     | 505 | 3CS  | O43-C41 | -2.22 | 1.21        | 1.30     |
| 2   | B     | 502 | 3CS  | C7-C8   | 2.21  | 1.41        | 1.36     |
| 2   | E     | 506 | 3CS  | C13-C11 | 2.19  | 1.43        | 1.38     |
| 2   | A     | 503 | 3CS  | C18-C19 | -2.19 | 1.45        | 1.51     |
| 2   | D     | 505 | 3CS  | C9-N26  | 2.18  | 1.37        | 1.32     |
| 2   | B     | 502 | 3CS  | C10-C9  | -2.17 | 1.45        | 1.50     |
| 2   | E     | 506 | 3CS  | C14-C13 | 2.16  | 1.41        | 1.36     |
| 2   | B     | 502 | 3CS  | C9-N26  | 2.16  | 1.37        | 1.32     |
| 2   | B     | 502 | 3CS  | C13-C11 | 2.15  | 1.43        | 1.38     |
| 2   | D     | 505 | 3CS  | C7-C8   | 2.15  | 1.41        | 1.36     |
| 2   | F     | 504 | 3CS  | C18-N17 | -2.12 | 1.44        | 1.48     |
| 2   | F     | 504 | 3CS  | C21-C20 | 2.11  | 1.42        | 1.38     |
| 2   | F     | 504 | 3CS  | C14-C13 | 2.11  | 1.41        | 1.36     |
| 2   | C     | 501 | 3CS  | C24-I25 | -2.09 | 2.04        | 2.10     |
| 2   | F     | 504 | 3CS  | O43-C41 | -2.08 | 1.22        | 1.30     |
| 2   | F     | 504 | 3CS  | C18-C19 | -2.08 | 1.45        | 1.51     |
| 2   | F     | 504 | 3CS  | C9-N26  | 2.07  | 1.37        | 1.32     |
| 2   | F     | 504 | 3CS  | C21-C24 | 2.07  | 1.43        | 1.38     |
| 2   | F     | 504 | 3CS  | C10-C9  | -2.06 | 1.45        | 1.50     |
| 2   | B     | 502 | 3CS  | O43-C41 | -2.05 | 1.22        | 1.30     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | D     | 505 | 3CS  | C13-C11 | 2.00 | 1.42        | 1.38     |

All (130) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | D     | 505 | 3CS  | O35-C29-C30 | -7.64 | 110.88      | 120.67   |
| 2   | F     | 504 | 3CS  | C37-C36-C28 | -7.60 | 120.72      | 130.95   |
| 2   | C     | 501 | 3CS  | O35-C29-C30 | -7.59 | 110.95      | 120.67   |
| 2   | A     | 503 | 3CS  | C28-C36-N17 | 7.35  | 113.06      | 107.82   |
| 2   | B     | 502 | 3CS  | O35-C29-C30 | -6.90 | 111.83      | 120.67   |
| 2   | B     | 502 | 3CS  | C28-C36-N17 | 6.82  | 112.68      | 107.82   |
| 2   | F     | 504 | 3CS  | O35-C29-C30 | -6.78 | 111.99      | 120.67   |
| 2   | C     | 501 | 3CS  | C28-C36-N17 | 6.55  | 112.49      | 107.82   |
| 2   | B     | 502 | 3CS  | C37-C36-C28 | -6.52 | 122.17      | 130.95   |
| 2   | E     | 506 | 3CS  | O35-C29-C30 | -6.35 | 112.53      | 120.67   |
| 2   | A     | 503 | 3CS  | O35-C29-C30 | -6.28 | 112.62      | 120.67   |
| 2   | F     | 504 | 3CS  | C28-C36-N17 | 6.24  | 112.27      | 107.82   |
| 2   | A     | 503 | 3CS  | C36-C28-C16 | -6.24 | 102.59      | 109.00   |
| 2   | D     | 505 | 3CS  | C37-C36-C28 | -6.21 | 122.58      | 130.95   |
| 2   | C     | 501 | 3CS  | C36-C28-C16 | -6.15 | 102.69      | 109.00   |
| 2   | C     | 501 | 3CS  | C37-C36-C28 | -6.07 | 122.78      | 130.95   |
| 2   | D     | 505 | 3CS  | C36-C28-C16 | -6.02 | 102.82      | 109.00   |
| 2   | E     | 506 | 3CS  | C37-C36-C28 | -5.89 | 123.03      | 130.95   |
| 2   | D     | 505 | 3CS  | C28-C36-N17 | 5.85  | 111.99      | 107.82   |
| 2   | B     | 502 | 3CS  | C36-C28-C16 | -5.76 | 103.08      | 109.00   |
| 2   | F     | 504 | 3CS  | C36-C28-C16 | -5.44 | 103.42      | 109.00   |
| 2   | A     | 503 | 3CS  | C37-C36-C28 | -5.28 | 123.83      | 130.95   |
| 2   | E     | 506 | 3CS  | O43-C41-C40 | 4.88  | 126.32      | 115.18   |
| 2   | E     | 506 | 3CS  | O43-C41-O42 | -4.88 | 108.40      | 123.76   |
| 2   | E     | 506 | 3CS  | C36-C28-C16 | -4.87 | 104.00      | 109.00   |
| 2   | B     | 502 | 3CS  | O43-C41-O42 | -4.64 | 109.16      | 123.76   |
| 2   | B     | 502 | 3CS  | O43-C41-C40 | 4.58  | 125.64      | 115.18   |
| 2   | D     | 505 | 3CS  | O43-C41-C40 | 4.40  | 125.21      | 115.18   |
| 2   | E     | 506 | 3CS  | C28-C36-N17 | 4.29  | 110.88      | 107.82   |
| 2   | D     | 505 | 3CS  | O43-C41-O42 | -4.11 | 110.83      | 123.76   |
| 2   | B     | 502 | 3CS  | C33-C30-C29 | 4.10  | 123.71      | 115.69   |
| 2   | D     | 505 | 3CS  | C38-C40-C41 | -4.06 | 103.04      | 109.33   |
| 2   | C     | 501 | 3CS  | O43-C41-C40 | 4.06  | 124.43      | 115.18   |
| 2   | B     | 502 | 3CS  | C10-O27-C11 | 4.02  | 128.40      | 117.66   |
| 2   | F     | 504 | 3CS  | O43-C41-C40 | 3.93  | 124.15      | 115.18   |
| 2   | A     | 503 | 3CS  | C33-C30-C29 | 3.91  | 123.35      | 115.69   |
| 2   | D     | 505 | 3CS  | C30-C29-C28 | 3.89  | 126.12      | 119.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | C     | 501 | 3CS  | O43-C41-O42 | -3.82 | 111.73      | 123.76   |
| 2   | E     | 506 | 3CS  | C39-C40-C38 | -3.62 | 100.24      | 109.44   |
| 2   | F     | 504 | 3CS  | C33-C30-C29 | 3.59  | 122.71      | 115.69   |
| 2   | F     | 504 | 3CS  | O43-C41-O42 | -3.54 | 112.63      | 123.76   |
| 2   | A     | 503 | 3CS  | C10-O27-C11 | 3.53  | 127.09      | 117.66   |
| 2   | B     | 502 | 3CS  | C16-C28-C29 | 3.45  | 132.14      | 124.66   |
| 2   | C     | 501 | 3CS  | O27-C11-C12 | -3.41 | 112.64      | 123.95   |
| 2   | E     | 506 | 3CS  | C22-C24-I25 | -3.41 | 114.47      | 119.69   |
| 2   | D     | 505 | 3CS  | O27-C11-C12 | -3.41 | 112.65      | 123.95   |
| 2   | A     | 503 | 3CS  | C16-C28-C29 | 3.39  | 132.02      | 124.66   |
| 2   | F     | 504 | 3CS  | C16-C28-C29 | 3.36  | 131.94      | 124.66   |
| 2   | E     | 506 | 3CS  | O27-C11-C12 | -3.32 | 112.94      | 123.95   |
| 2   | B     | 502 | 3CS  | O27-C11-C12 | -3.27 | 113.10      | 123.95   |
| 2   | A     | 503 | 3CS  | O27-C11-C12 | -3.25 | 113.17      | 123.95   |
| 2   | A     | 503 | 3CS  | C40-C37-C36 | -3.24 | 111.12      | 115.55   |
| 2   | C     | 501 | 3CS  | C16-C28-C29 | 3.21  | 131.61      | 124.66   |
| 2   | A     | 503 | 3CS  | O43-C41-O42 | -3.19 | 113.71      | 123.76   |
| 2   | F     | 504 | 3CS  | O27-C11-C12 | -3.13 | 113.57      | 123.95   |
| 2   | E     | 506 | 3CS  | C33-C30-C29 | 3.10  | 121.75      | 115.69   |
| 2   | D     | 505 | 3CS  | C10-O27-C11 | 3.08  | 125.88      | 117.66   |
| 2   | E     | 506 | 3CS  | C5-C6-C1    | 3.05  | 122.36      | 119.09   |
| 2   | A     | 503 | 3CS  | C5-C6-C1    | 3.04  | 122.36      | 119.09   |
| 2   | A     | 503 | 3CS  | O43-C41-C40 | 3.02  | 122.06      | 115.18   |
| 2   | C     | 501 | 3CS  | C30-C29-C28 | 2.99  | 124.56      | 119.31   |
| 2   | C     | 501 | 3CS  | C5-C6-C1    | 2.99  | 122.30      | 119.09   |
| 2   | C     | 501 | 3CS  | C33-C30-C29 | 2.96  | 121.48      | 115.69   |
| 2   | E     | 506 | 3CS  | C30-C29-C28 | 2.96  | 124.50      | 119.31   |
| 2   | F     | 504 | 3CS  | C10-O27-C11 | 2.93  | 125.48      | 117.66   |
| 2   | D     | 505 | 3CS  | C33-C30-C29 | 2.92  | 121.39      | 115.69   |
| 2   | E     | 506 | 3CS  | C4-C5-C6    | -2.90 | 115.46      | 120.02   |
| 2   | F     | 504 | 3CS  | O27-C10-C9  | 2.89  | 117.25      | 109.48   |
| 2   | A     | 503 | 3CS  | C21-C24-I25 | -2.81 | 115.39      | 119.69   |
| 2   | D     | 505 | 3CS  | C5-C6-C1    | 2.77  | 122.06      | 119.09   |
| 2   | E     | 506 | 3CS  | C10-O27-C11 | 2.70  | 124.87      | 117.66   |
| 2   | B     | 502 | 3CS  | C30-C29-C28 | 2.69  | 124.03      | 119.31   |
| 2   | D     | 505 | 3CS  | C34-C33-C30 | 2.69  | 119.28      | 109.75   |
| 2   | A     | 503 | 3CS  | C38-C40-C37 | 2.68  | 115.28      | 110.03   |
| 2   | A     | 503 | 3CS  | C30-C29-C28 | 2.67  | 123.99      | 119.31   |
| 2   | D     | 505 | 3CS  | C16-C28-C29 | 2.63  | 130.36      | 124.66   |
| 2   | D     | 505 | 3CS  | C28-C16-C15 | 2.57  | 109.53      | 107.82   |
| 2   | D     | 505 | 3CS  | C1-C6-N26   | -2.54 | 117.35      | 122.20   |
| 2   | C     | 501 | 3CS  | C28-C16-C15 | 2.54  | 109.51      | 107.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | E     | 506 | 3CS  | C3-C2-C1    | -2.54 | 116.27      | 120.43   |
| 2   | F     | 504 | 3CS  | C39-C40-C38 | -2.53 | 103.01      | 109.44   |
| 2   | E     | 506 | 3CS  | C2-C1-C7    | -2.51 | 117.39      | 123.22   |
| 2   | B     | 502 | 3CS  | C4-C5-C6    | -2.50 | 116.08      | 120.02   |
| 2   | B     | 502 | 3CS  | C39-C40-C38 | -2.50 | 103.10      | 109.44   |
| 2   | C     | 501 | 3CS  | C1-C6-N26   | -2.48 | 117.47      | 122.20   |
| 2   | F     | 504 | 3CS  | C34-C33-C30 | 2.48  | 118.53      | 109.75   |
| 2   | A     | 503 | 3CS  | C22-C24-C21 | 2.47  | 124.67      | 120.65   |
| 2   | A     | 503 | 3CS  | C4-C5-C6    | -2.46 | 116.15      | 120.02   |
| 2   | C     | 501 | 3CS  | C38-C40-C41 | -2.46 | 105.51      | 109.33   |
| 2   | E     | 506 | 3CS  | C40-C37-C36 | 2.46  | 118.91      | 115.55   |
| 2   | D     | 505 | 3CS  | C16-C15-N17 | -2.46 | 106.48      | 108.91   |
| 2   | A     | 503 | 3CS  | C1-C6-N26   | -2.45 | 117.53      | 122.20   |
| 2   | D     | 505 | 3CS  | C4-C5-C6    | -2.43 | 116.19      | 120.02   |
| 2   | C     | 501 | 3CS  | C2-C1-C7    | -2.43 | 117.59      | 123.22   |
| 2   | B     | 502 | 3CS  | C3-C2-C1    | -2.43 | 116.45      | 120.43   |
| 2   | C     | 501 | 3CS  | C13-C11-C12 | 2.40  | 124.25      | 120.84   |
| 2   | E     | 506 | 3CS  | O27-C10-C9  | 2.40  | 115.93      | 109.48   |
| 2   | C     | 501 | 3CS  | C4-C5-C6    | -2.39 | 116.26      | 120.02   |
| 2   | E     | 506 | 3CS  | C34-C33-C30 | 2.39  | 118.23      | 109.75   |
| 2   | B     | 502 | 3CS  | C34-C33-C30 | 2.39  | 118.21      | 109.75   |
| 2   | B     | 502 | 3CS  | O27-C10-C9  | 2.32  | 115.73      | 109.48   |
| 2   | D     | 505 | 3CS  | C37-C40-C41 | 2.30  | 115.61      | 108.18   |
| 2   | F     | 504 | 3CS  | C2-C1-C7    | -2.27 | 117.95      | 123.22   |
| 2   | D     | 505 | 3CS  | C7-C8-C9    | -2.27 | 116.15      | 119.15   |
| 2   | B     | 502 | 3CS  | C2-C1-C7    | -2.26 | 117.98      | 123.22   |
| 2   | F     | 504 | 3CS  | C39-C40-C41 | 2.26  | 112.83      | 109.33   |
| 2   | A     | 503 | 3CS  | C18-N17-C15 | 2.24  | 129.42      | 124.96   |
| 2   | F     | 504 | 3CS  | C30-C29-C28 | 2.24  | 123.24      | 119.31   |
| 2   | F     | 504 | 3CS  | C22-C24-I25 | 2.24  | 123.12      | 119.69   |
| 2   | D     | 505 | 3CS  | C39-C40-C38 | -2.22 | 103.80      | 109.44   |
| 2   | E     | 506 | 3CS  | C11-C12-C16 | -2.22 | 116.38      | 119.99   |
| 2   | B     | 502 | 3CS  | C5-C6-C1    | 2.22  | 121.47      | 119.09   |
| 2   | E     | 506 | 3CS  | C21-C24-I25 | 2.21  | 123.07      | 119.69   |
| 2   | F     | 504 | 3CS  | O35-C29-C28 | 2.14  | 124.76      | 120.11   |
| 2   | A     | 503 | 3CS  | C2-C1-C7    | -2.13 | 118.28      | 123.22   |
| 2   | F     | 504 | 3CS  | C4-C5-C6    | -2.11 | 116.70      | 120.02   |
| 2   | F     | 504 | 3CS  | C5-C6-C1    | 2.10  | 121.34      | 119.09   |
| 2   | B     | 502 | 3CS  | C1-C6-N26   | -2.09 | 118.20      | 122.20   |
| 2   | A     | 503 | 3CS  | C16-C15-N17 | -2.09 | 106.84      | 108.91   |
| 2   | A     | 503 | 3CS  | C3-C2-C1    | -2.09 | 117.01      | 120.43   |
| 2   | D     | 505 | 3CS  | C3-C2-C1    | -2.08 | 117.02      | 120.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | C     | 501 | 3CS  | C16-C15-N17 | -2.08 | 106.85      | 108.91   |
| 2   | F     | 504 | 3CS  | C1-C6-N26   | -2.08 | 118.23      | 122.20   |
| 2   | E     | 506 | 3CS  | O42-C41-C40 | 2.06  | 125.28      | 122.71   |
| 2   | D     | 505 | 3CS  | C2-C1-C7    | -2.05 | 118.47      | 123.22   |
| 2   | B     | 502 | 3CS  | C16-C15-N17 | -2.04 | 106.89      | 108.91   |
| 2   | A     | 503 | 3CS  | C34-C33-C30 | 2.04  | 116.99      | 109.75   |
| 2   | C     | 501 | 3CS  | C18-N17-C15 | 2.02  | 128.97      | 124.96   |
| 2   | A     | 503 | 3CS  | C39-C40-C38 | -2.01 | 104.33      | 109.44   |
| 2   | C     | 501 | 3CS  | C22-C24-C21 | 2.01  | 123.92      | 120.65   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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     | 140/161 (86%) | 0.28   | 3 (2%) 60 47  | 78, 114, 163, 182     | 0     |
| 1   | B     | 148/161 (91%) | 0.11   | 0 100 100     | 75, 112, 162, 171     | 0     |
| 1   | C     | 149/161 (92%) | 0.20   | 6 (4%) 36 30  | 67, 104, 158, 173     | 0     |
| 1   | D     | 148/161 (91%) | 0.09   | 1 (0%) 84 73  | 74, 114, 163, 170     | 0     |
| 1   | E     | 140/161 (86%) | 0.25   | 3 (2%) 60 47  | 83, 117, 170, 188     | 0     |
| 1   | F     | 149/161 (92%) | 0.36   | 8 (5%) 25 22  | 80, 116, 172, 205     | 0     |
| All | All   | 874/966 (90%) | 0.22   | 21 (2%) 54 43 | 67, 114, 165, 205     | 0     |

All (21) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 43  | GLN  | 6.3  |
| 1   | F     | 44  | ARG  | 6.1  |
| 1   | E     | 107 | GLN  | 4.3  |
| 1   | C     | 146 | TYR  | 3.5  |
| 1   | E     | 140 | GLY  | 3.4  |
| 1   | F     | 36  | THR  | 2.9  |
| 1   | F     | 1   | MSE  | 2.8  |
| 1   | A     | 140 | GLY  | 2.8  |
| 1   | C     | 112 | TYR  | 2.7  |
| 1   | D     | 45  | THR  | 2.7  |
| 1   | E     | 1   | MSE  | 2.4  |
| 1   | F     | 35  | ARG  | 2.4  |
| 1   | C     | 104 | GLU  | 2.4  |
| 1   | F     | 149 | THR  | 2.3  |
| 1   | A     | 112 | TYR  | 2.2  |
| 1   | C     | 140 | GLY  | 2.2  |
| 1   | C     | 1   | MSE  | 2.1  |
| 1   | F     | 37  | GLN  | 2.1  |
| 1   | F     | 42  | PHE  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 147 | ILE  | 2.0  |
| 1   | A     | 89  | MSE  | 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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | 3CS  | B     | 502 | 43/43 | 0.48 | 2.73 | 152,152,152,152            | 0     |
| 2   | 3CS  | D     | 505 | 43/43 | 0.39 | 1.93 | 159,159,159,159            | 0     |
| 2   | 3CS  | F     | 504 | 43/43 | 0.38 | 1.30 | 155,155,155,155            | 0     |
| 2   | 3CS  | E     | 506 | 43/43 | 0.33 | 0.94 | 160,160,160,160            | 0     |
| 2   | 3CS  | C     | 501 | 43/43 | 0.37 | 0.67 | 155,155,155,155            | 0     |
| 2   | 3CS  | A     | 503 | 43/43 | 0.34 | 0.46 | 159,159,159,159            | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.