



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:53 PM UTC

PDB ID : 2Q7R / pdb\_00002q7r  
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 X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

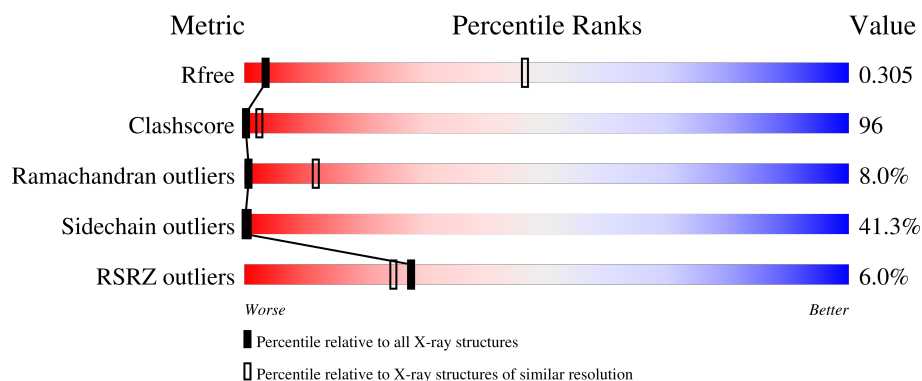
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1082 (4.20-3.80)                                      |
| Clashscore            | 190562                      | 1129 (4.20-3.80)                                      |
| Ramachandran outliers | 187476                      | 1064 (4.20-3.80)                                      |
| Sidechain outliers    | 187428                      | 1055 (4.20-3.80)                                      |
| RSRZ outliers         | 180081                      | 1082 (4.20-3.80)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                    |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------|
| 1   | A     | 161    | <div> <div>4%</div> <div>16%</div> <div>42%</div> <div>28%</div> <div>13%</div> </div>              |
| 1   | B     | 161    | <div> <div>4%</div> <div>11%</div> <div>43%</div> <div>30%</div> <div>8%</div> <div>8%</div> </div> |
| 1   | C     | 161    | <div> <div>7%</div> <div>21%</div> <div>42%</div> <div>27%</div> <div>7%</div> </div>               |
| 1   | D     | 161    | <div> <div>2%</div> <div>15%</div> <div>43%</div> <div>32%</div> <div>8%</div> </div>               |
| 1   | E     | 161    | <div> <div>5%</div> <div>14%</div> <div>40%</div> <div>30%</div> <div>13%</div> </div>              |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 161    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | 3CS  | A     | 503 | -         | -        | X       | -                |
| 2   | 3CS  | C     | 501 | -         | -        | X       | -                |
| 2   | 3CS  | D     | 505 | -         | -        | X       | -                |
| 2   | 3CS  | E     | 506 | -         | -        | X       | -                |
| 2   | 3CS  | F     | 504 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 7254 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Arachidonate 5-lipoxygenase-activating protein.

| 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:

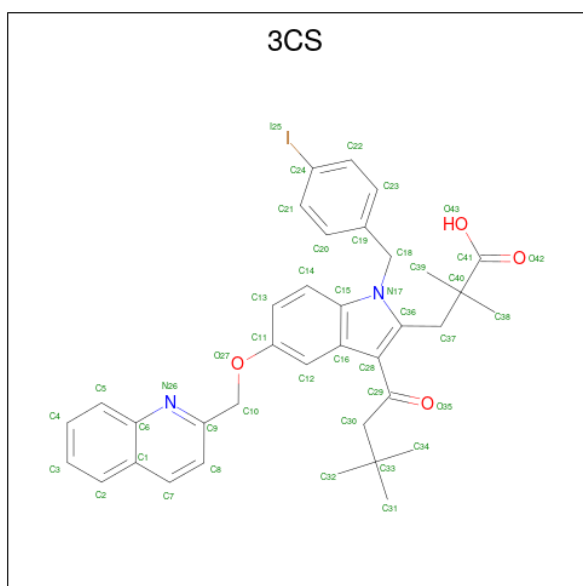
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 1       | MSE      | MET    | modified residue    | UNP P20292 |
| A     | 89      | MSE      | MET    | modified residue    | UNP P20292 |
| A     | 125     | MSE      | MET    | modified residue    | UNP P20292 |
| A     | 148     | ALA      | LYS    | engineered mutation | 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 mutation | 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 mutation | 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 mutation | 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 mutation | 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 mutation | UNP P20292 |

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

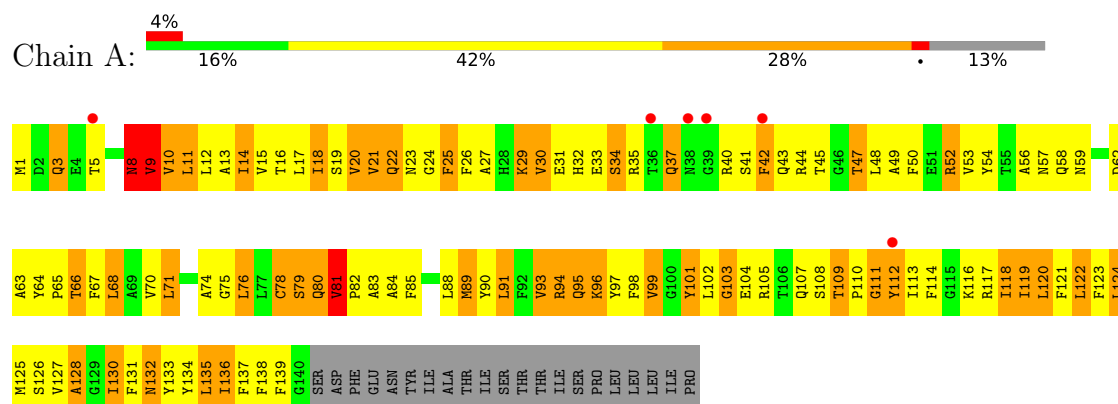


| Mol | Chain | Residues | Atoms       |         |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|---------|---------|
| 2   | A     | 1        | Total<br>43 | C<br>36 | I<br>1 | N<br>2 | O<br>4 | 0       | 0       |
| 2   |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

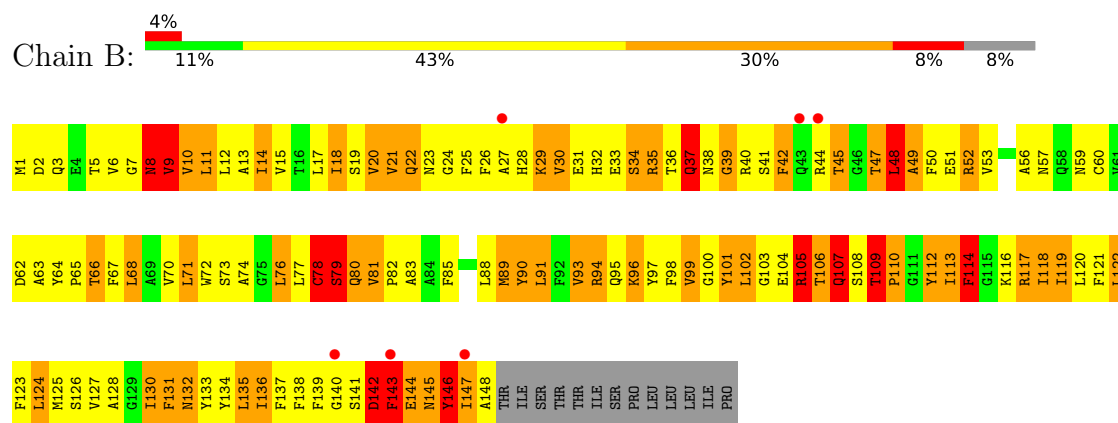
### 3 Residue-property plots

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

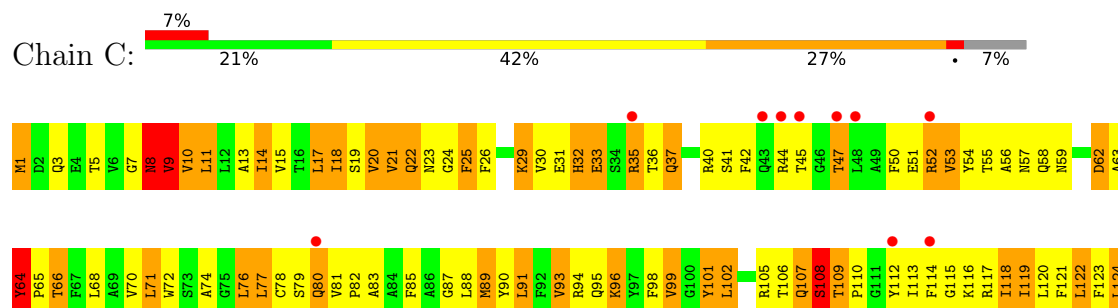
- Molecule 1: Arachidonate 5-lipoxygenase-activating protein

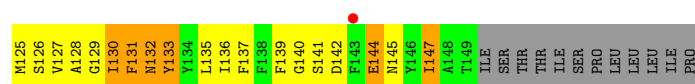


- Molecule 1: Arachidonate 5-lipoxygenase-activating protein

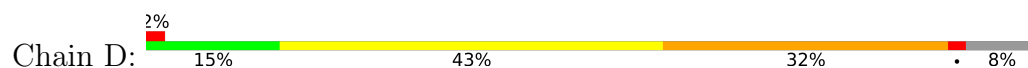


- Molecule 1: Arachidonate 5-lipoxygenase-activating protein

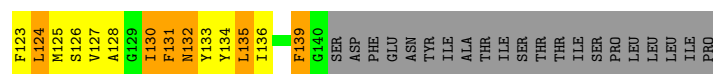
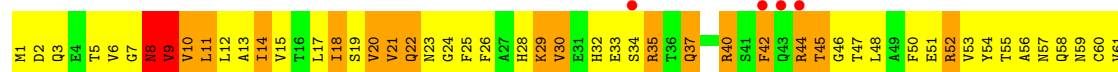




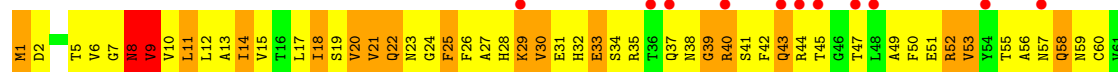
- Molecule 1: Arachidonate 5-lipoxygenase-activating protein



- Molecule 1: Arachidonate 5-lipoxygenase-activating protein



- Molecule 1: Arachidonate 5-lipoxygenase-activating protein



## 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>20.00 – 4.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.5 (20.00-4.00)<br>98.7 (20.00-4.00)                      | 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 1.9.3                                            | Depositor        |
| R, $R_{free}$                                                           | 0.268 , 0.281<br>0.282 , 0.305                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1021 reflections (5.10%)                                    | wwPDB-VP         |
| 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> ) | 0.29 , 80.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | 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.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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     | 0.45         | 0/1146      | 1.11        | 7/1550 (0.5%)  |
| 1   | B     | 0.40         | 0/1215      | 0.85        | 6/1644 (0.4%)  |
| 1   | C     | 0.47         | 0/1222      | 1.02        | 8/1654 (0.5%)  |
| 1   | D     | 0.44         | 0/1215      | 0.84        | 4/1644 (0.2%)  |
| 1   | E     | 0.41         | 0/1146      | 1.00        | 6/1550 (0.4%)  |
| 1   | F     | 0.46         | 0/1222      | 0.94        | 3/1654 (0.2%)  |
| All | All   | 0.44         | 0/7166      | 0.96        | 34/9696 (0.4%) |

There are no bond length outliers.

All (34) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 109 | THR  | CA-C-N | 13.88 | 137.18      | 119.84   |
| 1   | A     | 109 | THR  | C-N-CA | 13.88 | 137.18      | 119.84   |
| 1   | C     | 109 | THR  | N-CA-C | 10.18 | 132.30      | 109.81   |
| 1   | A     | 79  | SER  | N-CA-C | 9.34  | 124.05      | 110.42   |
| 1   | E     | 105 | ARG  | N-CA-C | -9.08 | 101.17      | 112.88   |
| 1   | C     | 145 | ASN  | N-CA-C | -8.84 | 102.04      | 112.92   |
| 1   | E     | 109 | THR  | CA-C-N | 8.65  | 130.65      | 119.84   |
| 1   | E     | 109 | THR  | C-N-CA | 8.65  | 130.65      | 119.84   |
| 1   | F     | 140 | GLY  | N-CA-C | -8.64 | 101.99      | 115.73   |
| 1   | C     | 108 | SER  | N-CA-C | -8.55 | 92.60       | 110.80   |
| 1   | A     | 81  | VAL  | CA-C-N | 7.34  | 126.87      | 119.24   |
| 1   | A     | 81  | VAL  | C-N-CA | 7.34  | 126.87      | 119.24   |
| 1   | F     | 147 | ILE  | N-CA-C | -7.04 | 105.95      | 112.43   |
| 1   | C     | 107 | GLN  | N-CA-C | 6.74  | 120.78      | 111.55   |
| 1   | E     | 104 | GLU  | N-CA-C | 6.63  | 124.92      | 110.80   |
| 1   | C     | 147 | ILE  | N-CA-C | -6.51 | 104.84      | 112.98   |
| 1   | A     | 107 | GLN  | N-CA-C | -6.09 | 100.38      | 109.15   |
| 1   | B     | 112 | TYR  | N-CA-C | -5.89 | 104.44      | 111.69   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | F     | 139 | PHE  | N-CA-C  | 5.86  | 120.25      | 111.81   |
| 1   | B     | 48  | LEU  | CB-CA-C | -5.73 | 109.95      | 116.54   |
| 1   | A     | 120 | LEU  | N-CA-C  | -5.70 | 104.99      | 111.14   |
| 1   | B     | 109 | THR  | CA-C-N  | 5.67  | 126.93      | 119.84   |
| 1   | B     | 109 | THR  | C-N-CA  | 5.67  | 126.93      | 119.84   |
| 1   | E     | 79  | SER  | CB-CA-C | -5.58 | 108.33      | 116.53   |
| 1   | D     | 141 | SER  | N-CA-C  | -5.46 | 103.49      | 110.53   |
| 1   | C     | 109 | THR  | CA-C-N  | -5.42 | 113.06      | 119.84   |
| 1   | C     | 109 | THR  | C-N-CA  | -5.42 | 113.06      | 119.84   |
| 1   | D     | 140 | GLY  | N-CA-C  | -5.38 | 106.26      | 112.50   |
| 1   | D     | 111 | GLY  | N-CA-C  | 5.24  | 119.56      | 111.08   |
| 1   | C     | 144 | GLU  | N-CA-C  | 5.21  | 117.21      | 110.65   |
| 1   | D     | 103 | GLY  | N-CA-C  | -5.19 | 100.89      | 113.18   |
| 1   | B     | 34  | SER  | N-CA-C  | -5.14 | 105.67      | 111.28   |
| 1   | B     | 79  | SER  | N-CA-C  | 5.11  | 121.68      | 110.80   |
| 1   | E     | 46  | GLY  | N-CA-C  | 5.02  | 117.20      | 110.43   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1119  | 0        | 1116     | 239     | 0            |
| 1   | B     | 1186  | 0        | 1171     | 265     | 0            |
| 1   | C     | 1193  | 0        | 1178     | 218     | 0            |
| 1   | D     | 1186  | 0        | 1171     | 269     | 0            |
| 1   | E     | 1119  | 0        | 1116     | 228     | 0            |
| 1   | F     | 1193  | 0        | 1178     | 265     | 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     | 1377    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 96.

All (1377) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B: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:H     | 1:C:11:LEU:HD22  | 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:C:83:ALA:HB2   | 1:C:125:MSE:HE1  | 1.35                     | 1.02              |
| 1:F:11:LEU:HD22  | 1:F:11:LEU:H     | 1.22                     | 1.02              |
| 2:F:504:3CS:H301 | 2:F:504:3CS:H372 | 1.40                     | 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              |
| 1:C:52:ARG:HB3   | 1:C:102:LEU:HB2  | 1.41                     | 0.97              |
| 1:E:81:VAL:HG13  | 1:E:82:PRO:HD3   | 1.47                     | 0.96              |
| 2:E:506:3CS:H323 | 2:E:506:3CS:H372 | 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:B:145:ASN:ND2  | 1:B:145:ASN:H    | 1.64                     | 0.95              |
| 1:C:74:ALA:HB1   | 1:C:125:MSE:HE2  | 1.48                     | 0.95              |
| 1:D:11:LEU:HD22  | 1:D:11:LEU:H     | 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              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 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:89:MSE:HB3   | 1:D:118:ILE:HD11 | 1.54                     | 0.90              |
| 1:D:120:LEU:HD23 | 2:D:505:3CS:H301 | 1.51                     | 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:D:116:LYS:HA   | 1:D:116:LYS:HZ3  | 1.36                     | 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:31:GLU:HG2   | 1:F:113:ILE:HD11 | 1.55                     | 0.88              |
| 1:D:101:TYR:HA   | 1:D:109:THR:CG2  | 2.04                     | 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:D:35:ARG:HE    | 1:D:35:ARG:HA    | 1.38                     | 0.87              |
| 1:E:35:ARG:HA    | 1:E:35:ARG:HE    | 1.40                     | 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              |
| 1:B:8:ASN:H      | 1:B:8:ASN:ND2    | 1.70                     | 0.86              |
| 1:E:89:MSE:HB3   | 1:E:118:ILE:HD11 | 1.57                     | 0.85              |
| 1:F:96:LYS:N     | 1:F:96:LYS:HD2   | 1.90                     | 0.85              |
| 1:C:52:ARG:HB3   | 1:C:102:LEU:CB   | 2.05                     | 0.85              |
| 1:F:120:LEU:HD23 | 2:F:504:3CS:C30  | 2.04                     | 0.85              |
| 1:F:89:MSE:HB3   | 1:F:118:ILE:HD11 | 1.59                     | 0.85              |
| 1:A:8:ASN:H      | 1:A:8:ASN:ND2    | 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:H     | 1:E:11:LEU:HD22  | 1.40                     | 0.85              |
| 1:E:53:VAL:CG2   | 1:E:102:LEU:HD23 | 2.07                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 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:HD2   | 1:C:96:LYS:N     | 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:ND2    | 1:B:8:ASN:N      | 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:31:GLU:HG2   | 1:C:113:ILE:HD11 | 1.63                     | 0.80              |
| 1:A:123:PHE:HD1  | 1:A:124:LEU:HD13 | 1.46                     | 0.80              |
| 1:B:101:TYR:OH   | 1:C:42:PHE:HB3   | 1.81                     | 0.80              |
| 1:E:116:LYS:HA   | 1:E:119:ILE:CD1  | 2.10                     | 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              |
| 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:E:101:TYR:OH   | 1:F:40:ARG:HG2   | 1.83                     | 0.78              |
| 1:F:83:ALA:HB2   | 1:F:125:MSE:CE   | 2.11                     | 0.78              |
| 1:E:96:LYS:HD2   | 1:E:96:LYS:N     | 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              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:124:LEU:HA   | 1:C:127:VAL:CG1  | 2.14                     | 0.77              |
| 1:B:145:ASN:H    | 1:B:145:ASN:HD22 | 1.27                     | 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:H      | 1:F:8:ASN:ND2    | 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:43:GLN:O     | 1:F:45:THR:HG23  | 1.86                     | 0.76              |
| 1:F:74:ALA:HB1   | 1:F:125:MSE:CE   | 2.10                     | 0.76              |
| 1:D:66:THR:HG22  | 1:E:20:VAL:HG22  | 1.67                     | 0.76              |
| 1:E:124:LEU:HA   | 1:E:127:VAL:CG1  | 2.15                     | 0.76              |
| 1:C:119:ILE:HD11 | 2:C:501:3CS:H12  | 1.66                     | 0.76              |
| 1:D:116:LYS:HZ1  | 2:D:505:3CS:C12  | 1.98                     | 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:34:SER:HB2   | 1:A:42:PHE:HE2   | 1.50                     | 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: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              |
| 1:A:19:SER:HB3   | 1:A:91:LEU:HD11  | 1.69                     | 0.74              |
| 1:A:83:ALA:HB2   | 1:A:125:MSE:CE   | 2.16                     | 0.74              |
| 1:D:105:ARG:O    | 1:D:107:GLN:N    | 2.21                     | 0.74              |
| 1:F:74:ALA:CB    | 1:F:125:MSE:HE2  | 2.11                     | 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:66:THR:HG22  | 1:F:20:VAL:HG22  | 1.67                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:70:VAL:HB    | 1:E:122:LEU:HB3  | 1.69                     | 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: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:11:LEU:HD23  | 1:B:80:GLN:HE22  | 1.53                     | 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:A:44:ARG:NE    | 1:C:45:THR:HG21  | 2.04                     | 0.73              |
| 1:D:19:SER:HB3   | 1:D:91:LEU:HD11  | 1.70                     | 0.73              |
| 1:C:10:VAL:HG13  | 1:C:14:ILE:CD1   | 2.19                     | 0.72              |
| 1:A:44:ARG:HE    | 1:C:45:THR:CG2   | 2.01                     | 0.72              |
| 1:C:8:ASN:ND2    | 1:C:8:ASN:H      | 1.86                     | 0.72              |
| 1:D:20:VAL:HG22  | 1:F:66:THR:CG2   | 2.19                     | 0.72              |
| 1:A:43:GLN:HE22  | 1:C:54:TYR:HB3   | 1.55                     | 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: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              |
| 1:A:66:THR:HG22  | 1:B:20:VAL:HG22  | 1.72                     | 0.72              |
| 1:B:26:PHE:HA    | 1:B:98:PHE:CE2   | 2.25                     | 0.72              |
| 1:D:100:GLY:O    | 1:D:109:THR:HG23 | 1.90                     | 0.72              |
| 1:D:43:GLN:CA    | 1:D:44:ARG:HH21  | 2.01                     | 0.71              |
| 1:A:52:ARG:HG3   | 1:A:52:ARG:HH11  | 1.54                     | 0.71              |
| 1:B:124:LEU:CA   | 1:B:127:VAL:HG12 | 2.18                     | 0.71              |
| 1:E:97:TYR:HD2   | 1:E:114:PHE:CD2  | 2.08                     | 0.71              |
| 1:D:116:LYS:HZ3  | 1:D:116:LYS:CA   | 2.02                     | 0.71              |
| 1:B:66:THR:HG22  | 1:C:20:VAL:HG22  | 1.72                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 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:C:14:ILE:O     | 1:C:18:ILE:HD12  | 1.89                     | 0.71              |
| 1:D:27:ALA:HB2   | 2:F:504:3CS:C4   | 2.20                     | 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:HE    | 1:C:35:ARG:HA    | 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:A:67:PHE:HB2   | 1:A:90:TYR:HE2   | 1.57                     | 0.70              |
| 1:F:11:LEU:H     | 1:F:11:LEU:CD2   | 2.01                     | 0.70              |
| 1:D:8:ASN:N      | 1:D:8:ASN:ND2    | 2.38                     | 0.69              |
| 1:D:10:VAL:HG13  | 1:D:14:ILE:HD12  | 1.74                     | 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:79:SER:HB3   | 1:B:82:PRO:CG    | 2.21                     | 0.69              |
| 1:B:90:TYR:CE1   | 1:B:94:ARG:HG3   | 2.26                     | 0.69              |
| 1:B:38:ASN:O     | 1:B:40:ARG:N     | 2.25                     | 0.69              |
| 1:C:83:ALA:CB    | 1:C:125:MSE:HE1  | 2.18                     | 0.69              |
| 1:F:11:LEU:CD2   | 1:F:80:GLN:HE22  | 2.04                     | 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:37:GLN:HA    | 1:C:37:GLN:OE1   | 1.91                     | 0.69              |
| 1:C:52:ARG:NH2   | 1:C:105:ARG:HA   | 2.07                     | 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              |
| 1:E:13:ALA:O     | 1:E:17:LEU:HD23  | 1.92                     | 0.69              |
| 1:F:142:ASP:C    | 1:F:144:GLU:H    | 2.00                     | 0.69              |
| 1:D:8:ASN:ND2    | 1:D:8:ASN:H      | 1.89                     | 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:C:119:ILE:HD11 | 2:C:501:3CS:C12  | 2.23                     | 0.68              |
| 1:A:30:VAL:CG2   | 1:A:53:VAL:HG12  | 2.24                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:120:LEU:HD13 | 1:E:124:LEU:CD2  | 2.23                     | 0.68              |
| 1:E:42:PHE:HD1   | 1:E:42:PHE:H     | 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:D:11:LEU:HD22  | 1:D:11:LEU:N     | 2.06                     | 0.67              |
| 1:E:114:PHE:HD1  | 1:E:114:PHE:N    | 1.92                     | 0.67              |
| 1:F:96:LYS:HD2   | 1:F:96:LYS:H     | 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:HD22 | 1:E:102:LEU:O    | 1.94                     | 0.67              |
| 1:F:97:TYR:C     | 1:F:97:TYR:HD1   | 2.02                     | 0.67              |
| 1:F:97:TYR:C     | 1:F:97:TYR:CD1   | 2.72                     | 0.67              |
| 1:A:26:PHE:HA    | 1:A:98:PHE:CE2   | 2.30                     | 0.67              |
| 1:A:133:TYR:HA   | 1:A:136:ILE:HD12 | 1.76                     | 0.67              |
| 1:D:10:VAL:HG13  | 1:D:14:ILE:CD1   | 2.25                     | 0.67              |
| 1:C:8:ASN:ND2    | 1:C:8:ASN:N      | 2.42                     | 0.67              |
| 1:C:120:LEU:O    | 1:C:124:LEU:HD22 | 1.95                     | 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:D:116:LYS:HZ1  | 2:D:505:3CS:C16  | 2.07                     | 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:B:71:LEU:HD22  | 1:B:71:LEU:O     | 1.95                     | 0.67              |
| 1:C:32:HIS:O     | 1:C:36:THR:HG23  | 1.95                     | 0.67              |
| 1:D:79:SER:CB    | 1:D:82:PRO:HG2   | 2.25                     | 0.67              |
| 1:F:23:ASN:OD1   | 1:F:94:ARG:NH2   | 2.27                     | 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:B:11:LEU:CD2   | 1:B:80:GLN:HE22  | 2.07                     | 0.67              |
| 1:B:17:LEU:O     | 1:B:20:VAL:HG12  | 1.95                     | 0.66              |
| 1:E:11:LEU:HD23  | 1:E:80:GLN:CD    | 2.21                     | 0.66              |
| 1:F:6:VAL:O      | 1:F:10:VAL:HG23  | 1.96                     | 0.66              |
| 1:F:25:PHE:CE1   | 1:F:29:LYS:HG2   | 2.26                     | 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              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:24:GLY:C     | 2:F:504:3CS:H20  | 2.21                     | 0.66              |
| 1:D:35:ARG:HA    | 1:D:35:ARG:NE    | 2.11                     | 0.66              |
| 1:B:117:ARG:HH12 | 1:F:141:SER:CB   | 2.08                     | 0.66              |
| 1:C:116:LYS:HG3  | 1:C:117:ARG:N    | 2.08                     | 0.66              |
| 1:F:104:GLU:O    | 1:F:105:ARG:HG2  | 1.94                     | 0.66              |
| 2:A:503:3CS:H382 | 2:A:503:3CS:H182 | 1.76                     | 0.66              |
| 1:B:35:ARG:O     | 1:B:37:GLN:N     | 2.28                     | 0.66              |
| 1:C:11:LEU:HD21  | 1:C:80:GLN:NE2   | 2.06                     | 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:A:34:SER:CB    | 1:A:42:PHE:HE2   | 2.09                     | 0.65              |
| 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:124:LEU:HA   | 1:A:127:VAL:CG1  | 2.24                     | 0.65              |
| 1:C:18:ILE:CG2   | 1:C:91:LEU:HD23  | 2.25                     | 0.65              |
| 1:C:25:PHE:HE1   | 1:C:29:LYS:HG2   | 1.62                     | 0.65              |
| 1:D:44:ARG:NH1   | 1:F:51:GLU:HG2   | 2.11                     | 0.65              |
| 1:D:110:PRO:HG3  | 1:E:40:ARG:HD3   | 1.78                     | 0.65              |
| 1:F:120:LEU:CD2  | 2:F:504:3CS:H302 | 2.08                     | 0.65              |
| 1:F:124:LEU:HA   | 1:F:127:VAL:CG1  | 2.25                     | 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:H23  | 2:A:503:3CS:C38  | 2.27                     | 0.65              |
| 1:B:44:ARG:O     | 1:B:45:THR:HB    | 1.95                     | 0.65              |
| 1:D:11:LEU:HD23  | 1:D:80:GLN:NE2   | 2.10                     | 0.65              |
| 1:E:81:VAL:CG1   | 1:E:82:PRO:HD3   | 2.24                     | 0.65              |
| 2:D:505:3CS:H20  | 1:E:24:GLY:C     | 2.22                     | 0.65              |
| 1:F:26:PHE:HA    | 1:F:98:PHE:HE2   | 1.60                     | 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:A:34:SER:HB2   | 1:A:42:PHE:CE2   | 2.29                     | 0.65              |
| 1:B:11:LEU:HD23  | 1:B:80:GLN:CD    | 2.22                     | 0.65              |
| 2:C:501:3CS:H371 | 2:C:501:3CS:C23  | 2.27                     | 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:F:133:TYR:CD1  | 1:F:133:TYR:C    | 2.74                     | 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              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:140:GLY:C    | 1:F:142:ASP:H    | 2.05                     | 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              |
| 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:F:39:GLY:C     | 1:F:41:SER:H     | 2.05                     | 0.64              |
| 2:F:504:3CS:H23  | 2:F:504:3CS:O43  | 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              |
| 1:A:26:PHE:HA    | 1:A:98:PHE:HE2   | 1.60                     | 0.64              |
| 1:A:42:PHE:CD1   | 1:A:42:PHE:N     | 2.65                     | 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:40:ARG:HB2   | 1:C:52:ARG:HH12  | 1.63                     | 0.63              |
| 1:A:74:ALA:HB2   | 1:A:122:LEU:O    | 1.98                     | 0.63              |
| 1:A:64:TYR:CZ    | 1:A:68:LEU:HD21  | 2.33                     | 0.63              |
| 1:A:10:VAL:HG21  | 1:C:133:TYR:CD2  | 2.33                     | 0.63              |
| 1:B:6:VAL:O      | 1:B:10:VAL:HG23  | 1.99                     | 0.63              |
| 1:B:11:LEU:HD23  | 1:B:80:GLN:OE1   | 1.98                     | 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              |
| 1:E:52:ARG:HG3   | 1:E:52:ARG:HH11  | 1.64                     | 0.63              |
| 2:E:506:3CS:H341 | 1:F:21:VAL:CG2   | 2.29                     | 0.63              |
| 1:D:40:ARG:HB3   | 1:F:105:ARG:HH11 | 1.62                     | 0.63              |
| 1:A:42:PHE:CD1   | 1:C:112:TYR:HE1  | 2.16                     | 0.63              |
| 1:D:10:VAL:HG21  | 1:F:133:TYR:CD2  | 2.33                     | 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: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: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:120:LEU:O    | 1:E:124:LEU:HD22 | 1.98                     | 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:E:116:LYS:HA   | 1:E:119:ILE:HD13 | 1.79                     | 0.62              |
| 1:A:94:ARG:HA    | 1:A:114:PHE:HE2  | 1.63                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:123:PHE:HD1  | 1:A:124:LEU:CD1  | 2.12                     | 0.62              |
| 1:B:120:LEU:O    | 1:B:124:LEU:HD22 | 1.99                     | 0.62              |
| 1:E:26:PHE:HA    | 1:E:98:PHE:HE2   | 1.64                     | 0.62              |
| 2:E:506:3CS:C4   | 1:F:27:ALA:HB2   | 2.30                     | 0.62              |
| 1:D:72:TRP:O     | 1:D:76:LEU:HD22  | 1.99                     | 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:F:11:LEU:HD22  | 1:F:11:LEU:N     | 2.04                     | 0.62              |
| 1:E:89:MSE:O     | 1:E:93:VAL:HG23  | 2.00                     | 0.62              |
| 1:A:116:LYS:HE3  | 2:A:503:3CS:C39  | 2.29                     | 0.62              |
| 1:B:120:LEU:HD13 | 1:B:124:LEU:CD2  | 2.30                     | 0.62              |
| 1:C:126:SER:O    | 1:C:130:ILE:HB   | 2.00                     | 0.62              |
| 1:D:42:PHE:N     | 1:D:42:PHE:CD1   | 2.67                     | 0.62              |
| 1:F:67:PHE:HB2   | 1:F:90:TYR:HE2   | 1.65                     | 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: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:B:47:THR:HA    | 1:B:51:GLU:CD    | 2.24                     | 0.61              |
| 1:C:63:ALA:C     | 1:C:65:PRO:HD2   | 2.25                     | 0.61              |
| 1:F:79:SER:OG    | 1:F:80:GLN:N     | 2.26                     | 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:81:VAL:HB    | 1:C:82:PRO:HD3   | 1.83                     | 0.61              |
| 1:C:119:ILE:CD1  | 2:C:501:3CS:H12  | 2.31                     | 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              |
| 2:C:501:3CS:H371 | 2:C:501:3CS:C19  | 2.30                     | 0.61              |
| 1:E:114:PHE:N    | 1:E:114:PHE:CD1  | 2.64                     | 0.61              |
| 1:F:95:GLN:OE1   | 1:F:95:GLN:HA    | 2.01                     | 0.61              |
| 1:F:121:PHE:CE1  | 1:F:125:MSE:HG3  | 2.36                     | 0.61              |
| 1:B:123:PHE:CE2  | 1:C:21:VAL:HG23  | 2.35                     | 0.60              |
| 2:B:502:3CS:H20  | 1:C:24:GLY:C     | 2.26                     | 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: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:B:136:ILE:HA   | 1:B:140:GLY:HA3  | 1.82                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 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:F:89:MSE:O     | 1:F:93:VAL:HG23  | 2.01                     | 0.60              |
| 1:A:97:TYR:HD2   | 1:A:114:PHE:CD2  | 2.19                     | 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:D:11:LEU:HD23  | 1:D:80:GLN:CD    | 2.26                     | 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:A:94:ARG:HA    | 1:A:114:PHE:CE2  | 2.37                     | 0.60              |
| 1:B:95:GLN:OE1   | 1:B:95:GLN:HA    | 2.00                     | 0.60              |
| 1:D:40:ARG:HB3   | 1:F:105:ARG:NH1  | 2.16                     | 0.60              |
| 1:B:145:ASN:ND2  | 1:B:145:ASN:N    | 2.39                     | 0.60              |
| 1:C:120:LEU:HD23 | 2:C:501:3CS:O35  | 2.01                     | 0.60              |
| 1:D:81:VAL:HG23  | 1:D:82:PRO:CD    | 2.27                     | 0.60              |
| 1:E:120:LEU:HD13 | 1:E:124:LEU:HD22 | 1.82                     | 0.60              |
| 1:B:109:THR:N    | 1:B:110:PRO:HD3  | 2.17                     | 0.60              |
| 1:D:95:GLN:OE1   | 1:D:95:GLN:HA    | 2.01                     | 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              |
| 2:B:502:3CS:C23  | 2:B:502:3CS:H371 | 2.32                     | 0.60              |
| 1:D:141:SER:C    | 1:D:143:PHE:H    | 2.09                     | 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: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:F:40:ARG:HG3   | 1:F:40:ARG:O     | 2.01                     | 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:A:113:ILE:HD12 | 1:B:31:GLU:HG2   | 1.84                     | 0.59              |
| 1:B:30:VAL:CG2   | 1:B:53:VAL:HG12  | 2.32                     | 0.59              |
| 1:B:64:TYR:CZ    | 1:B:68:LEU:HD21  | 2.37                     | 0.59              |
| 1:C:33:GLU:HG3   | 1:C:50:PHE:HA    | 1.85                     | 0.59              |
| 1:D:44:ARG:NH1   | 1:F:55:THR:OG1   | 2.36                     | 0.59              |
| 2:A:503:3CS:C19  | 2:A:503:3CS:H371 | 2.32                     | 0.59              |
| 1:C:114:PHE:HD1  | 1:C:115:GLY:N    | 2.01                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 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              |
| 1:F:21:VAL:HG12  | 1:F:22:GLN:N     | 2.16                     | 0.59              |
| 1:F:88:LEU:C     | 1:F:88:LEU:HD13  | 2.28                     | 0.59              |
| 1:D:35:ARG:NH2   | 1:D:39:GLY:HA2   | 2.18                     | 0.59              |
| 1:F:120:LEU:CD2  | 2:F:504:3CS:H313 | 2.33                     | 0.59              |
| 1:A:54:TYR:HD2   | 1:B:44:ARG:HH12  | 1.47                     | 0.59              |
| 1:D:41:SER:HA    | 1:F:110:PRO:HD2  | 1.83                     | 0.59              |
| 1:E:97:TYR:OH    | 1:E:111:GLY:HA2  | 2.03                     | 0.59              |
| 1:F:56:ALA:HA    | 1:F:101:TYR:CD2  | 2.36                     | 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:B:13:ALA:O     | 1:B:17:LEU:HD23  | 2.03                     | 0.59              |
| 1:B:52:ARG:HG3   | 1:B:52:ARG:HH11  | 1.68                     | 0.59              |
| 1:D:39:GLY:O     | 1:F:109:THR:HB   | 2.01                     | 0.59              |
| 1:D:94:ARG:HA    | 1:D:114:PHE:CE1  | 2.38                     | 0.59              |
| 1:F:10:VAL:HG13  | 1:F:14:ILE:CD1   | 2.33                     | 0.59              |
| 1:A:24:GLY:C     | 2:C:501:3CS:H20  | 2.28                     | 0.58              |
| 1:B:44:ARG:CZ    | 1:C:44:ARG:HH22  | 2.15                     | 0.58              |
| 1:D:43:GLN:HA    | 1:D:44:ARG:NH2   | 2.14                     | 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:A:10:VAL:HG21  | 1:C:133:TYR:CE2  | 2.38                     | 0.58              |
| 1:B:121:PHE:CE1  | 1:B:125:MSE:HG3  | 2.38                     | 0.58              |
| 1:C:56:ALA:HA    | 1:C:101:TYR:HD2  | 1.66                     | 0.58              |
| 1:D:108:SER:HA   | 1:E:40:ARG:CD    | 2.25                     | 0.58              |
| 1:E:88:LEU:HD13  | 1:E:88:LEU:C     | 2.28                     | 0.58              |
| 1:F:121:PHE:CD1  | 1:F:121:PHE:C    | 2.80                     | 0.58              |
| 1:F:143:PHE:C    | 1:F:143:PHE:HD1  | 2.10                     | 0.58              |
| 1:F:143:PHE:C    | 1:F:143:PHE:CD1  | 2.81                     | 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:D:48:LEU:N     | 1:D:48:LEU:HD22  | 2.19                     | 0.58              |
| 1:D:97:TYR:HD2   | 1:D:114:PHE:CE1  | 2.20                     | 0.58              |
| 1:F:56:ALA:HA    | 1:F:101:TYR:HD2  | 1.67                     | 0.58              |
| 1:A:132:ASN:ND2  | 1:A:136:ILE:HD11 | 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              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:139:PHE:CD1  | 1:C:139:PHE:N    | 2.71                     | 0.58              |
| 1:E:120:LEU:HD23 | 2:E:506:3CS:C30  | 2.34                     | 0.58              |
| 1:B:44:ARG:NH2   | 1:C:44:ARG:HH22  | 2.01                     | 0.58              |
| 1:B:135:LEU:HD23 | 1:B:135:LEU:N    | 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:B:77:LEU:O     | 1:B:78:CYS:HB3   | 2.03                     | 0.57              |
| 1:B:144:GLU:HA   | 1:B:144:GLU:OE1  | 2.02                     | 0.57              |
| 1:B:97:TYR:HD2   | 1:B:114:PHE:CD2  | 2.22                     | 0.57              |
| 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:B:145:ASN:O    | 1:B:147:ILE:HG13 | 2.04                     | 0.57              |
| 1:C:90:TYR:HA    | 1:C:118:ILE:HD12 | 1.87                     | 0.57              |
| 1:E:30:VAL:CG2   | 1:E:53:VAL:HG12  | 2.32                     | 0.57              |
| 1:E:119:ILE:HD11 | 2:E:506:3CS:C12  | 2.35                     | 0.57              |
| 1:E:123:PHE:HD1  | 1:E:124:LEU:HD13 | 1.70                     | 0.57              |
| 1:A:33:GLU:HB3   | 1:A:50:PHE:HB2   | 1.86                     | 0.57              |
| 1:A:88:LEU:C     | 1:A:88:LEU:HD13  | 2.29                     | 0.57              |
| 1:C:25:PHE:CD1   | 1:C:25:PHE:C     | 2.82                     | 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:F:25:PHE:CD1   | 1:F:25:PHE:C     | 2.82                     | 0.57              |
| 1:A:63:ALA:C     | 1:A:65:PRO:HD2   | 2.29                     | 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:A:25:PHE:CD1   | 1:A:25:PHE:C     | 2.81                     | 0.57              |
| 1:A:43:GLN:NE2   | 1:C:51:GLU:O     | 2.38                     | 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:D:136:ILE:O    | 1:D:140:GLY:HA3  | 2.04                     | 0.57              |
| 1:E:97:TYR:HD2   | 1:E:114:PHE:CE2  | 2.22                     | 0.57              |
| 1:F:75:GLY:C     | 1:F:76:LEU:HD13  | 2.30                     | 0.57              |
| 1:D:52:ARG:HH11  | 1:D:52:ARG:HG3   | 1.70                     | 0.56              |
| 1:D:101:TYR:HD1  | 1:D:109:THR:CG2  | 2.16                     | 0.56              |
| 1:F:133:TYR:C    | 1:F:133:TYR:HD1  | 2.12                     | 0.56              |
| 1:D:42:PHE:N     | 1:D:42:PHE:HD1   | 2.03                     | 0.56              |
| 1:A:42:PHE:CD1   | 1:C:112:TYR:CE1  | 2.93                     | 0.56              |
| 2:D:505:3CS:H341 | 1:E:21:VAL:HG22  | 1.86                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 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              |
| 2:F:504:3CS:C23  | 2:F:504:3CS:H371 | 2.35                     | 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:E:55:THR:HG1   | 1:F:42:PHE:HD2   | 1.54                     | 0.56              |
| 1:F:120:LEU:HD13 | 1:F:120:LEU:C    | 2.30                     | 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              |
| 1:A:42:PHE:HB2   | 1:C:112:TYR:OH   | 2.05                     | 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:13:ALA:O     | 1:A:17:LEU:HD23  | 2.05                     | 0.56              |
| 1:B:44:ARG:O     | 1:B:44:ARG:HG3   | 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:E:95:GLN:OE1   | 1:E:95:GLN:HA    | 2.04                     | 0.56              |
| 1:E:135:LEU:HD23 | 1:E:135:LEU:N    | 2.20                     | 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:F:120:LEU:HA   | 2:F:504:3CS:H313 | 1.87                     | 0.56              |
| 1:A:34:SER:HG    | 1:A:42:PHE:HE2   | 1.54                     | 0.56              |
| 1:B:18:ILE:CG2   | 1:B:91:LEU:HD23  | 2.36                     | 0.56              |
| 1:B:35:ARG:HE    | 1:B:35:ARG:HA    | 1.70                     | 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:E:72:TRP:O     | 1:E:76:LEU:HD22  | 2.05                     | 0.56              |
| 1:F:31:GLU:O     | 1:F:35:ARG:HG2   | 2.06                     | 0.56              |
| 1:B:142:ASP:O    | 1:B:143:PHE:HD1  | 1.89                     | 0.55              |
| 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: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:99:VAL:HG12  | 1:B:100:GLY:N    | 2.21                     | 0.55              |
| 1:B:137:PHE:CE2  | 1:B:138:PHE:HE1  | 2.24                     | 0.55              |
| 1:B:21:VAL:HG12  | 1:B:22:GLN:N     | 2.21                     | 0.55              |
| 1:B:97:TYR:HD1   | 1:B:109:THR:HG21 | 1.70                     | 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              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:37:GLN:OE1   | 1:F:37:GLN:HA    | 2.07                     | 0.55              |
| 1:A:20:VAL:HG22  | 1:C:66:THR:CG2   | 2.32                     | 0.55              |
| 1:A:120:LEU:HD13 | 1:A:124:LEU:HD22 | 1.89                     | 0.55              |
| 1:B:74:ALA:CB    | 1:B:125:MSE:HE2  | 2.29                     | 0.55              |
| 1:B:118:ILE:HG22 | 1:B:119:ILE:N    | 2.22                     | 0.55              |
| 1:E:47:THR:HG23  | 1:E:50:PHE:HB3   | 1.89                     | 0.55              |
| 1:A:58:GLN:HG3   | 1:A:58:GLN:O     | 2.07                     | 0.55              |
| 1:B:12:LEU:HG    | 1:B:80:GLN:HE21  | 1.72                     | 0.55              |
| 1:B:105:ARG:HH11 | 1:B:105:ARG:HB3  | 1.72                     | 0.55              |
| 1:B:113:ILE:HG12 | 1:B:114:PHE:N    | 2.20                     | 0.55              |
| 1:B:133:TYR:CE1  | 1:B:134:TYR:CD1  | 2.95                     | 0.55              |
| 1:E:81:VAL:HG22  | 1:E:82:PRO:HD3   | 1.88                     | 0.55              |
| 1:E:111:GLY:O    | 1:E:112:TYR:O    | 2.25                     | 0.55              |
| 2:A:503:3CS:C4   | 1:B:27:ALA:HB2   | 2.37                     | 0.55              |
| 1:B:120:LEU:HD13 | 1:B:120:LEU:C    | 2.31                     | 0.55              |
| 1:B:120:LEU:HB2  | 2:B:502:3CS:O35  | 2.07                     | 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:A:34:SER:O     | 1:A:37:GLN:O     | 2.24                     | 0.55              |
| 1:B:10:VAL:HG13  | 1:B:14:ILE:HD12  | 1.88                     | 0.55              |
| 1:C:18:ILE:HG22  | 1:C:91:LEU:HD23  | 1.88                     | 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:E:120:LEU:HD23 | 2:E:506:3CS:H322 | 1.89                     | 0.55              |
| 1:A:14:ILE:CD1   | 1:C:130:ILE:HD11 | 2.37                     | 0.54              |
| 1:B:104:GLU:O    | 1:B:105:ARG:HB2  | 2.07                     | 0.54              |
| 1:C:120:LEU:CD1  | 1:C:124:LEU:HD21 | 2.37                     | 0.54              |
| 1:D:30:VAL:HA    | 1:D:53:VAL:HG11  | 1.88                     | 0.54              |
| 2:D:505:3CS:O35  | 2:D:505:3CS:H382 | 2.07                     | 0.54              |
| 1:E:112:TYR:O    | 1:E:113:ILE:HB   | 2.07                     | 0.54              |
| 1:A:31:GLU:OE1   | 1:A:31:GLU:HA    | 2.07                     | 0.54              |
| 1:A:43:GLN:HA    | 1:C:44:ARG:HH21  | 1.72                     | 0.54              |
| 1:E:67:PHE:CD1   | 1:E:90:TYR:HD2   | 2.24                     | 0.54              |
| 1:E:66:THR:CG2   | 1:F:20:VAL:HG22  | 2.37                     | 0.54              |
| 1:F:30:VAL:HG22  | 1:F:53:VAL:HG12  | 1.89                     | 0.54              |
| 1:A:57:ASN:C     | 1:A:59:ASN:H     | 2.15                     | 0.54              |
| 1:B:114:PHE:N    | 1:B:114:PHE:CD1  | 2.76                     | 0.54              |
| 1:D:8:ASN:N      | 1:D:8:ASN:HD22   | 2.05                     | 0.54              |
| 1:D:18:ILE:HG21  | 1:D:91:LEU:HD23  | 1.90                     | 0.54              |
| 1:E:120:LEU:HD13 | 1:E:124:LEU:HD21 | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:132:ASN:ND2  | 1:E:136:ILE:HD11 | 2.22                     | 0.54              |
| 1:F:64:TYR:N     | 1:F:65:PRO:HD2   | 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:E:130:ILE:HD11 | 1:F:14:ILE:CD1   | 2.38                     | 0.54              |
| 1:F:94:ARG:HG2   | 1:F:114:PHE:CE2  | 2.42                     | 0.54              |
| 1:A:18:ILE:CG2   | 1:A:91:LEU:HD23  | 2.37                     | 0.54              |
| 2:B:502:3CS:H371 | 2:B:502:3CS:C19  | 2.38                     | 0.54              |
| 1:C:21:VAL:HG12  | 1:C:22:GLN:N     | 2.22                     | 0.54              |
| 1:C:119:ILE:CG1  | 2:C:501:3CS:H12  | 2.38                     | 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:F:131:PHE:CD1  | 1:F:132:ASN:N    | 2.75                     | 0.54              |
| 1:B:44:ARG:NE    | 1:C:44:ARG:HH12  | 2.05                     | 0.54              |
| 1:C:106:THR:HG22 | 1:C:107:GLN:H    | 1.72                     | 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:A:139:PHE:N    | 1:A:139:PHE:CD1  | 2.74                     | 0.54              |
| 1:E:120:LEU:CD1  | 1:E:124:LEU:HD21 | 2.38                     | 0.54              |
| 1:B:139:PHE:CD1  | 1:B:139:PHE:N    | 2.76                     | 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              |
| 2:D:505:3CS:H341 | 1:E:21:VAL:CG2   | 2.38                     | 0.54              |
| 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:79:SER:HB2   | 1:F:82:PRO:HD2   | 1.89                     | 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:E:97:TYR:CE2   | 1:E:114:PHE:CE1  | 2.95                     | 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:B:66:THR:CG2   | 1:C:20:VAL:HG22  | 2.38                     | 0.53              |
| 1:B:96:LYS:HD2   | 1:B:96:LYS:H     | 1.73                     | 0.53              |
| 1:D:143:PHE:N    | 1:D:143:PHE:CD1  | 2.75                     | 0.53              |
| 1:F:76:LEU:HD13  | 1:F:76:LEU:N     | 2.23                     | 0.53              |
| 1:D:45:THR:CG2   | 1:D:46:GLY:H     | 2.21                     | 0.53              |
| 1:D:110:PRO:CG   | 1:E:40:ARG:HD3   | 2.38                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:63:ALA:C     | 1:F:65:PRO:HD2   | 2.34                     | 0.53              |
| 1:F:143:PHE:O    | 1:F:144:GLU:O    | 2.27                     | 0.53              |
| 1:A:43:GLN:OE1   | 1:C:44:ARG:O     | 2.26                     | 0.53              |
| 2:C:501:3CS:C8   | 2:C:501:3CS:H13  | 2.39                     | 0.53              |
| 1:E:7:GLY:C      | 1:E:9:VAL:H      | 2.16                     | 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:B:114:PHE:N    | 1:B:114:PHE:HD1  | 2.05                     | 0.53              |
| 1:F:5:THR:O      | 1:F:9:VAL:HG13   | 2.08                     | 0.53              |
| 1:C:95:GLN:HA    | 1:C:95:GLN:OE1   | 2.07                     | 0.53              |
| 1:D:22:GLN:HG3   | 1:D:23:ASN:N     | 2.24                     | 0.53              |
| 1:D:42:PHE:HE1   | 1:F:110:PRO:HG2  | 1.73                     | 0.53              |
| 1:F:33:GLU:OE1   | 1:F:33:GLU:HA    | 2.09                     | 0.53              |
| 1:F:120:LEU:HD22 | 2:F:504:3CS:H313 | 1.91                     | 0.53              |
| 1:A:14:ILE:HD12  | 1:C:130:ILE:HD11 | 1.90                     | 0.53              |
| 1:B:88:LEU:HD13  | 1:B:88:LEU:C     | 2.34                     | 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              |
| 1:F:116:LYS:O    | 1:F:119:ILE:HD13 | 2.09                     | 0.53              |
| 1:D:40:ARG:O     | 1:D:41:SER:HB2   | 2.09                     | 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:B:81:VAL:CG1   | 1:B:82:PRO:HD3   | 2.34                     | 0.52              |
| 1:B:102:LEU:HD13 | 1:B:104:GLU:OE2  | 2.09                     | 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:F:142:ASP:C    | 1:F:144:GLU:N    | 2.67                     | 0.52              |
| 1:A:3:GLN:NE2    | 1:C:133:TYR:CE1  | 2.77                     | 0.52              |
| 1:D:139:PHE:CD1  | 1:D:139:PHE:N    | 2.76                     | 0.52              |
| 1:B:119:ILE:HD13 | 1:B:119:ILE:H    | 1.75                     | 0.52              |
| 1:B:137:PHE:CD2  | 1:B:138:PHE:CE1  | 2.98                     | 0.52              |
| 1:C:13:ALA:O     | 1:C:17:LEU:HD23  | 2.09                     | 0.52              |
| 1:E:58:GLN:O     | 1:E:58:GLN:HG3   | 2.10                     | 0.52              |
| 1:A:96:LYS:HD2   | 1:A:96:LYS:H     | 1.71                     | 0.52              |
| 1:B:31:GLU:HA    | 1:B:31:GLU:OE1   | 2.09                     | 0.52              |
| 1:D:94:ARG:HG2   | 1:D:114:PHE:CE1  | 2.45                     | 0.52              |
| 1:A:64:TYR:N     | 1:A:65:PRO:HD2   | 2.25                     | 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:D:124:LEU:HD13 | 1:D:124:LEU:N    | 2.25                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:64:TYR:CE1   | 1:E:68:LEU:HD22  | 2.45                     | 0.52              |
| 1:B:71:LEU:HD22  | 1:B:71:LEU:C     | 2.34                     | 0.52              |
| 1:B:131:PHE:CD1  | 1:B:132:ASN:N    | 2.78                     | 0.52              |
| 1:C:8:ASN:N      | 1:C:8:ASN:HD22   | 2.07                     | 0.52              |
| 1:D:63:ALA:C     | 1:D:65:PRO:HD2   | 2.34                     | 0.52              |
| 1:A:23:ASN:OD1   | 1:A:94:ARG:NH2   | 2.42                     | 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:F:97:TYR:HD1   | 1:F:97:TYR:O     | 1.92                     | 0.52              |
| 1:A:26:PHE:HB3   | 1:A:57:ASN:HD22  | 1.74                     | 0.52              |
| 1:B:19:SER:O     | 1:B:23:ASN:HB2   | 2.10                     | 0.52              |
| 1:D:42:PHE:O     | 1:D:43:GLN:HG3   | 2.10                     | 0.52              |
| 1:E:63:ALA:C     | 1:E:65:PRO:HD2   | 2.35                     | 0.52              |
| 1:F:135:LEU:N    | 1:F:135:LEU:HD23 | 2.25                     | 0.52              |
| 1:A:42:PHE:N     | 1:A:42:PHE:HD1   | 2.08                     | 0.52              |
| 1:F:57:ASN:C     | 1:F:59:ASN:H     | 2.17                     | 0.52              |
| 1:F:58:GLN:O     | 1:F:58:GLN:HG3   | 2.08                     | 0.52              |
| 1:B:102:LEU:C    | 1:B:102:LEU:HD22 | 2.35                     | 0.51              |
| 1:D:52:ARG:HH11  | 1:D:52:ARG:CG    | 2.23                     | 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:121:PHE:CD1  | 1:A:121:PHE:C    | 2.86                     | 0.51              |
| 1:D:133:TYR:CD1  | 1:D:134:TYR:CD1  | 2.98                     | 0.51              |
| 1:F:81:VAL:HG22  | 1:F:82:PRO:N     | 2.24                     | 0.51              |
| 1:A:97:TYR:HD2   | 1:A:114:PHE:CG   | 2.27                     | 0.51              |
| 1:C:63:ALA:CB    | 1:C:114:PHE:CE2  | 2.93                     | 0.51              |
| 1:C:116:LYS:HA   | 1:C:119:ILE:CD1  | 2.41                     | 0.51              |
| 1:D:71:LEU:HD22  | 1:D:71:LEU:O     | 2.10                     | 0.51              |
| 1:D:110:PRO:HG3  | 1:E:40:ARG:O     | 2.10                     | 0.51              |
| 2:D:505:3CS:H21  | 1:E:25:PHE:HB2   | 1.91                     | 0.51              |
| 1:E:131:PHE:CD1  | 1:E:132:ASN:N    | 2.78                     | 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:F:119:ILE:HG12 | 1:F:120:LEU:N    | 2.24                     | 0.51              |
| 1:D:31:GLU:HA    | 1:D:31:GLU:OE1   | 2.11                     | 0.51              |
| 1:A:104:GLU:O    | 1:A:105:ARG:HB2  | 2.10                     | 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:F:79:SER:CB    | 1:F:82:PRO:HD2   | 2.40                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:10:VAL:O     | 1:A:14:ILE:HD12  | 2.11                     | 0.51              |
| 1:C:139:PHE:N    | 1:C:139:PHE:HD1  | 2.09                     | 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:D:18:ILE:HG22  | 1:D:19:SER:N     | 2.26                     | 0.51              |
| 1:D:90:TYR:CE1   | 1:D:94:ARG:HG3   | 2.46                     | 0.51              |
| 1:D:90:TYR:HA    | 1:D:118:ILE:HD12 | 1.92                     | 0.51              |
| 1:E:120:LEU:CD2  | 2:E:506:3CS:H322 | 2.41                     | 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              |
| 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              |
| 2:F:504:3CS:H301 | 2:F:504:3CS:C37  | 2.27                     | 0.51              |
| 2:A:503:3CS:H20  | 1:B:24:GLY:C     | 2.35                     | 0.50              |
| 1:C:114:PHE:CD1  | 1:C:115:GLY:N    | 2.78                     | 0.50              |
| 1:D:25:PHE:HE2   | 1:D:95:GLN:HE22  | 1.59                     | 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              |
| 1:A:42:PHE:HD1   | 1:A:42:PHE:H     | 1.60                     | 0.50              |
| 2:A:503:3CS:C21  | 1:B:25:PHE:HB2   | 2.40                     | 0.50              |
| 1:B:33:GLU:HA    | 1:B:33:GLU:OE1   | 2.11                     | 0.50              |
| 1:E:64:TYR:N     | 1:E:65:PRO:HD2   | 2.25                     | 0.50              |
| 1:A:14:ILE:HD11  | 1:C:130:ILE:CD1  | 2.41                     | 0.50              |
| 1:A:22:GLN:HG3   | 1:A:23:ASN:N     | 2.26                     | 0.50              |
| 1:D:64:TYR:CZ    | 1:D:68:LEU:HD21  | 2.46                     | 0.50              |
| 1:B:133:TYR:CD1  | 1:B:134:TYR:HD1  | 2.29                     | 0.50              |
| 1:E:79:SER:OG    | 1:E:80:GLN:N     | 2.44                     | 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:B:72:TRP:O     | 1:B:76:LEU:HD22  | 2.12                     | 0.50              |
| 1:D:58:GLN:O     | 1:D:58:GLN:HG3   | 2.11                     | 0.50              |
| 1:D:79:SER:HB3   | 1:D:82:PRO:CD    | 2.42                     | 0.50              |
| 1:B:64:TYR:N     | 1:B:65:PRO:HD2   | 2.26                     | 0.50              |
| 1:B:142:ASP:C    | 1:B:143:PHE:HD1  | 2.20                     | 0.50              |
| 1:C:18:ILE:HG22  | 1:C:19:SER:N     | 2.26                     | 0.50              |
| 1:D:143:PHE:N    | 1:D:143:PHE:HD1  | 2.09                     | 0.50              |
| 1:F:90:TYR:CD1   | 1:F:90:TYR:C     | 2.89                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:96:LYS:HD2   | 1:C:96:LYS:H     | 1.72                     | 0.50              |
| 1:F:14:ILE:O     | 1:F:18:ILE:HD12  | 2.12                     | 0.50              |
| 1:A:95:GLN:HA    | 1:A:95:GLN:OE1   | 2.11                     | 0.50              |
| 1:B:64:TYR:CZ    | 1:B:68:LEU:CD2   | 2.95                     | 0.50              |
| 1:B:97:TYR:CD1   | 1:B:109:THR:HG21 | 2.46                     | 0.50              |
| 1:B:116:LYS:HE2  | 2:B:502:3CS:H383 | 1.93                     | 0.50              |
| 1:B:133:TYR:HE1  | 1:B:134:TYR:CE1  | 2.30                     | 0.50              |
| 1:C:74:ALA:CB    | 1:C:125:MSE:HE2  | 2.34                     | 0.50              |
| 1:D:105:ARG:O    | 1:D:107:GLN:HG3  | 2.12                     | 0.50              |
| 1:E:74:ALA:HB2   | 1:E:122:LEU:O    | 2.12                     | 0.50              |
| 1:F:79:SER:HB2   | 1:F:82:PRO:CD    | 2.42                     | 0.50              |
| 1:D:141:SER:O    | 1:D:142:ASP:OD1  | 2.29                     | 0.49              |
| 1:E:10:VAL:HG13  | 1:E:14:ILE:HD12  | 1.92                     | 0.49              |
| 1:E:45:THR:HB    | 1:F:43:GLN:NE2   | 2.27                     | 0.49              |
| 1:E:119:ILE:CD1  | 2:E:506:3CS:H12  | 2.42                     | 0.49              |
| 1:B:63:ALA:C     | 1:B:65:PRO:HD2   | 2.37                     | 0.49              |
| 1:B:119:ILE:CG1  | 2:B:502:3CS:H12  | 2.42                     | 0.49              |
| 1:D:21:VAL:HG12  | 1:D:22:GLN:N     | 2.26                     | 0.49              |
| 1:D:79:SER:C     | 1:D:82:PRO:HD2   | 2.37                     | 0.49              |
| 1:F:64:TYR:CZ    | 1:F:68:LEU:HD21  | 2.47                     | 0.49              |
| 1:F:67:PHE:CD1   | 1:F:67:PHE:C     | 2.89                     | 0.49              |
| 1:B:112:TYR:HD2  | 1:C:30:VAL:CG1   | 2.24                     | 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: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:A:30:VAL:HA    | 1:A:53:VAL:HG11  | 1.95                     | 0.49              |
| 1:E:105:ARG:O    | 1:E:106:THR:HB   | 2.12                     | 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: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:F:124:LEU:O    | 1:F:127:VAL:HG12 | 2.11                     | 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              |
| 1:C:133:TYR:CD1  | 1:C:133:TYR:C    | 2.90                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:22:GLN:HG3   | 1:C:23:ASN:N     | 2.24                     | 0.49              |
| 2:A:503:3CS:H371 | 2:A:503:3CS:C23  | 2.42                     | 0.49              |
| 1:C:77:LEU:CD1   | 1:C:77:LEU:N     | 2.75                     | 0.49              |
| 1:E:52:ARG:HD3   | 1:E:104:GLU:OE1  | 2.13                     | 0.49              |
| 1:F:97:TYR:CD2   | 1:F:114:PHE:CE1  | 3.01                     | 0.49              |
| 2:A:503:3CS:H13  | 2:A:503:3CS:N26  | 2.28                     | 0.48              |
| 1:B:120:LEU:HA   | 2:B:502:3CS:C31  | 2.39                     | 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:B:90:TYR:CD1   | 1:B:90:TYR:C     | 2.91                     | 0.48              |
| 1:D:41:SER:OG    | 1:F:110:PRO:HD2  | 2.13                     | 0.48              |
| 1:D:116:LYS:NZ   | 1:D:116:LYS:CB   | 2.77                     | 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:C:77:LEU:O     | 1:C:129:GLY:HA3  | 2.12                     | 0.48              |
| 1:D:119:ILE:HG12 | 1:D:120:LEU:N    | 2.27                     | 0.48              |
| 1:A:94:ARG:HG2   | 1:A:114:PHE:CZ   | 2.48                     | 0.48              |
| 1:B:26:PHE:CD2   | 1:B:98:PHE:CD2   | 3.02                     | 0.48              |
| 1:B:130:ILE:HD11 | 1:C:14:ILE:CD1   | 2.43                     | 0.48              |
| 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:A:26:PHE:N     | 1:A:26:PHE:HD1   | 2.12                     | 0.48              |
| 1:B:18:ILE:HG22  | 1:B:19:SER:N     | 2.28                     | 0.48              |
| 1:B:47:THR:HA    | 1:B:51:GLU:CG    | 2.44                     | 0.48              |
| 1:D:136:ILE:HA   | 1:D:140:GLY:CA   | 2.44                     | 0.48              |
| 1:F:12:LEU:HB3   | 1:F:72:TRP:CH2   | 2.48                     | 0.48              |
| 1:F:140:GLY:C    | 1:F:142:ASP:N    | 2.71                     | 0.48              |
| 1:A:30:VAL:HG23  | 1:A:53:VAL:HG12  | 1.94                     | 0.48              |
| 1:A:111:GLY:HA2  | 1:B:31:GLU:CD    | 2.38                     | 0.48              |
| 1:C:7:GLY:C      | 1:C:9:VAL:H      | 2.22                     | 0.48              |
| 1:C:90:TYR:HD1   | 1:C:118:ILE:HG21 | 1.79                     | 0.48              |
| 1:D:57:ASN:C     | 1:D:59:ASN:H     | 2.21                     | 0.48              |
| 1:D:108:SER:C    | 1:E:40:ARG:HD2   | 2.38                     | 0.48              |
| 2:F:504:3CS:H371 | 2:F:504:3CS:C19  | 2.44                     | 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:B:57:ASN:C     | 1:B:59:ASN:H     | 2.21                     | 0.48              |
| 1:B:133:TYR:CE1  | 1:B:134:TYR:HD1  | 2.31                     | 0.48              |
| 1:E:96:LYS:HD2   | 1:E:96:LYS:H     | 1.74                     | 0.48              |
| 1:C:114:PHE:CZ   | 2:C:501:3CS:C8   | 2.97                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:133:TYR:CE1  | 1:C:137:PHE:HB2  | 2.49                     | 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:F:133:TYR:HA   | 1:F:136:ILE:HD12 | 1.96                     | 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:D:26:PHE:CE2   | 1:D:98:PHE:HB2   | 2.49                     | 0.48              |
| 1:E:90:TYR:N     | 1:E:118:ILE:CD1  | 2.77                     | 0.48              |
| 1:F:42:PHE:HD1   | 1:F:43:GLN:H     | 1.60                     | 0.48              |
| 1:A:26:PHE:CD2   | 1:A:98:PHE:CD2   | 3.02                     | 0.47              |
| 1:A:85:PHE:O     | 1:A:88:LEU:HB3   | 2.14                     | 0.47              |
| 1:B:97:TYR:CD2   | 1:B:114:PHE:CD2  | 3.00                     | 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              |
| 1:A:81:VAL:HB    | 1:A:82:PRO:HD3   | 1.96                     | 0.47              |
| 2:A:503:3CS:N17  | 2:A:503:3CS:H393 | 2.28                     | 0.47              |
| 1:B:141:SER:O    | 1:B:143:PHE:N    | 2.47                     | 0.47              |
| 1:C:26:PHE:N     | 1:C:26:PHE:CD1   | 2.82                     | 0.47              |
| 1:F:56:ALA:CB    | 1:F:101:TYR:CD2  | 2.97                     | 0.47              |
| 1:A:67:PHE:CD1   | 1:A:67:PHE:C     | 2.92                     | 0.47              |
| 2:A:503:3CS:C20  | 1:B:25:PHE:N     | 2.76                     | 0.47              |
| 1:F:120:LEU:HD13 | 1:F:124:LEU:CD2  | 2.43                     | 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              |
| 1:C:25:PHE:O     | 1:C:25:PHE:HD1   | 1.97                     | 0.47              |
| 1:D:42:PHE:CE2   | 1:F:111:GLY:C    | 2.93                     | 0.47              |
| 1:D:124:LEU:O    | 1:D:127:VAL:HG12 | 2.14                     | 0.47              |
| 1:F:121:PHE:HE1  | 1:F:125:MSE:HG3  | 1.79                     | 0.47              |
| 1:A:19:SER:O     | 1:A:23:ASN:HB2   | 2.15                     | 0.47              |
| 1:A:29:LYS:HD2   | 1:A:29:LYS:HA    | 1.62                     | 0.47              |
| 1:A:118:ILE:HG22 | 1:A:119:ILE:N    | 2.30                     | 0.47              |
| 1:B:25:PHE:HE1   | 1:B:29:LYS:HG2   | 1.77                     | 0.47              |
| 1:B:132:ASN:O    | 1:B:136:ILE:HD12 | 2.14                     | 0.47              |
| 1:C:29:LYS:HD2   | 1:C:29:LYS:HA    | 1.61                     | 0.47              |
| 1:C:58:GLN:HG3   | 1:C:58:GLN:O     | 2.15                     | 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:D:101:TYR:HD1  | 1:D:109:THR:HG22 | 1.75                     | 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              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:90:TYR:HD1   | 1:A:90:TYR:O     | 1.98                     | 0.47              |
| 1:B:64:TYR:CE1   | 1:B:68:LEU:HD22  | 2.49                     | 0.47              |
| 1:B:74:ALA:HB2   | 1:B:122:LEU:O    | 2.13                     | 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:91:LEU:HD12  | 1:B:91:LEU:HA    | 1.72                     | 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:C:115:GLY:O    | 1:C:119:ILE:HD12 | 2.14                     | 0.47              |
| 1:D:37:GLN:O     | 1:D:38:ASN:HB2   | 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:31:GLU:OE1   | 1:F:31:GLU:HA    | 2.14                     | 0.47              |
| 1:B:39:GLY:O     | 1:B:42:PHE:N     | 2.48                     | 0.47              |
| 1:B:135:LEU:C    | 1:B:137:PHE:H    | 2.22                     | 0.47              |
| 1:D:116:LYS:HE3  | 2:D:505:3CS:C16  | 2.44                     | 0.47              |
| 1:D:116:LYS:O    | 1:D:119:ILE:HD13 | 2.14                     | 0.47              |
| 1:E:75:GLY:O     | 1:E:79:SER:O     | 2.33                     | 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              |
| 1:E:45:THR:HA    | 1:F:43:GLN:NE2   | 2.29                     | 0.47              |
| 2:E:506:3CS:H372 | 2:E:506:3CS:C32  | 2.33                     | 0.47              |
| 1:F:7:GLY:C      | 1:F:9:VAL:H      | 2.23                     | 0.47              |
| 1:C:76:LEU:HD12  | 1:C:76:LEU:HA    | 1.78                     | 0.47              |
| 1:D:119:ILE:HD11 | 2:D:505:3CS:H12  | 1.96                     | 0.47              |
| 1:E:11:LEU:CD2   | 1:E:80:GLN:NE2   | 2.78                     | 0.47              |
| 1:E:11:LEU:HB2   | 1:E:80:GLN:NE2   | 2.29                     | 0.47              |
| 1:F:139:PHE:C    | 1:F:141:SER:H    | 2.20                     | 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:D:90:TYR:CD1   | 1:D:90:TYR:C     | 2.94                     | 0.46              |
| 1:F:124:LEU:C    | 1:F:127:VAL:HG12 | 2.40                     | 0.46              |
| 1:A:120:LEU:CD2  | 2:A:503:3CS:H313 | 2.45                     | 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:B:90:TYR:C     | 1:B:90:TYR:HD1   | 2.24                     | 0.46              |
| 1:C:18:ILE:HG22  | 1:C:91:LEU:CD2   | 2.45                     | 0.46              |
| 1:D:48:LEU:HD22  | 1:D:48:LEU:H     | 1.81                     | 0.46              |
| 1:D:106:THR:O    | 1:D:107:GLN:HB2  | 2.16                     | 0.46              |
| 1:E:64:TYR:CZ    | 1:E:68:LEU:CD2   | 2.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:114:PHE:O    | 1:E:115:GLY:C    | 2.58                     | 0.46              |
| 1:F:12:LEU:HD13  | 1:F:72:TRP:CE3   | 2.50                     | 0.46              |
| 1:A:18:ILE:HG22  | 1:A:19:SER:N     | 2.30                     | 0.46              |
| 1:B:105:ARG:O    | 1:B:106:THR:O    | 2.33                     | 0.46              |
| 1:B:120:LEU:CD2  | 2:B:502:3CS:H313 | 2.46                     | 0.46              |
| 1:C:124:LEU:O    | 1:C:127:VAL:HG12 | 2.15                     | 0.46              |
| 1:C:124:LEU:C    | 1:C:127:VAL:HG12 | 2.40                     | 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:124:LEU:O    | 1:A:128:ALA:N    | 2.49                     | 0.46              |
| 1:B:21:VAL:CG1   | 1:B:22:GLN:N     | 2.79                     | 0.46              |
| 1:B:52:ARG:HH11  | 1:B:52:ARG:CG    | 2.26                     | 0.46              |
| 1:B:73:SER:O     | 1:B:77:LEU:HB2   | 2.15                     | 0.46              |
| 1:D:29:LYS:HD2   | 1:D:29:LYS:HA    | 1.48                     | 0.46              |
| 1:A:52:ARG:HG3   | 1:A:52:ARG:NH1   | 2.25                     | 0.46              |
| 1:A:116:LYS:O    | 1:A:120:LEU:HB2  | 2.14                     | 0.46              |
| 1:B:146:TYR:O    | 1:B:148:ALA:N    | 2.48                     | 0.46              |
| 1:C:37:GLN:HG3   | 1:C:47:THR:OG1   | 2.15                     | 0.46              |
| 1:D:31:GLU:CG    | 1:F:113:ILE:HD11 | 2.37                     | 0.46              |
| 1:D:67:PHE:CD1   | 1:D:67:PHE:C     | 2.91                     | 0.46              |
| 1:D:88:LEU:C     | 1:D:88:LEU:HD13  | 2.40                     | 0.46              |
| 1:E:8:ASN:O      | 1:E:9:VAL:HG12   | 2.16                     | 0.46              |
| 1:F:56:ALA:CA    | 1:F:101:TYR:CD2  | 2.97                     | 0.46              |
| 2:F:504:3CS:H382 | 2:F:504:3CS:C29  | 2.45                     | 0.46              |
| 1:A:9:VAL:N      | 1:A:80:GLN:NE2   | 2.63                     | 0.46              |
| 1:A:90:TYR:N     | 1:A:118:ILE:CD1  | 2.78                     | 0.46              |
| 1:B:22:GLN:HG3   | 1:B:23:ASN:N     | 2.29                     | 0.46              |
| 1:E:48:LEU:HD13  | 1:E:48:LEU:C     | 2.40                     | 0.46              |
| 1:E:95:GLN:O     | 1:E:99:VAL:HB    | 2.16                     | 0.46              |
| 1:F:1:MSE:HB3    | 1:F:6:VAL:CG2    | 2.46                     | 0.46              |
| 1:A:56:ALA:O     | 1:A:59:ASN:HB2   | 2.15                     | 0.46              |
| 1:B:109:THR:N    | 1:B:110:PRO:CD   | 2.78                     | 0.46              |
| 1:C:5:THR:O      | 1:C:9:VAL:HG13   | 2.15                     | 0.46              |
| 1:E:77:LEU:CD1   | 1:E:77:LEU:N     | 2.78                     | 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:D:135:LEU:N    | 1:D:135:LEU:HD23 | 2.30                     | 0.46              |
| 1:F:10:VAL:HG13  | 1:F:14:ILE:HD12  | 1.96                     | 0.46              |
| 1:F:25:PHE:O     | 1:F:28:HIS:HB3   | 2.16                     | 0.46              |
| 1:A:91:LEU:HD12  | 1:A:91:LEU:HA    | 1.78                     | 0.46              |
| 1:C:35:ARG:HA    | 1:C:35:ARG:NE    | 2.28                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:18:ILE:CG2   | 1:E:91:LEU:HD23  | 2.46                     | 0.46              |
| 1:E:67:PHE:CB    | 1:E:90:TYR:HE2   | 2.25                     | 0.46              |
| 1:E:113:ILE:C    | 1:E:114:PHE:HD1  | 2.23                     | 0.46              |
| 1:F:77:LEU:O     | 1:F:78:CYS:HB3   | 2.16                     | 0.46              |
| 1:D:27:ALA:HB2   | 2:F:504:3CS:C3   | 2.46                     | 0.46              |
| 1:D:124:LEU:C    | 1:D:127:VAL:HG12 | 2.41                     | 0.46              |
| 1:D:136:ILE:HA   | 1:D:140:GLY:HA3  | 1.98                     | 0.46              |
| 1:E:60:CYS:HG    | 1:E:114:PHE:HZ   | 1.59                     | 0.46              |
| 1:E:91:LEU:HD12  | 1:E:91:LEU:HA    | 1.74                     | 0.46              |
| 1:A:8:ASN:C      | 1:A:9:VAL:HG12   | 2.41                     | 0.45              |
| 1:B:25:PHE:CE1   | 1:B:29:LYS:HG2   | 2.51                     | 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:D:44:ARG:HB3   | 1:E:44:ARG:HH21  | 1.79                     | 0.45              |
| 1:E:11:LEU:H     | 1:E:11:LEU:CD2   | 2.18                     | 0.45              |
| 1:E:22:GLN:HG3   | 1:E:23:ASN:N     | 2.28                     | 0.45              |
| 1:F:77:LEU:CD1   | 1:F:77:LEU:N     | 2.79                     | 0.45              |
| 1:A:133:TYR:CD1  | 1:A:133:TYR:C    | 2.94                     | 0.45              |
| 1:B:10:VAL:HG13  | 1:B:14:ILE:CD1   | 2.45                     | 0.45              |
| 1:B:38:ASN:C     | 1:B:40:ARG:N     | 2.74                     | 0.45              |
| 1:B:135:LEU:C    | 1:B:137:PHE:N    | 2.72                     | 0.45              |
| 1:D:10:VAL:CG2   | 1:F:133:TYR:CD2  | 2.98                     | 0.45              |
| 1:D:91:LEU:HD12  | 1:D:91:LEU:HA    | 1.75                     | 0.45              |
| 1:E:26:PHE:CD2   | 1:E:98:PHE:CD2   | 3.04                     | 0.45              |
| 1:E:90:TYR:HA    | 1:E:118:ILE:HD12 | 1.97                     | 0.45              |
| 1:B:35:ARG:C     | 1:B:37:GLN:H     | 2.24                     | 0.45              |
| 1:C:120:LEU:HD23 | 2:C:501:3CS:H323 | 1.99                     | 0.45              |
| 1:D:133:TYR:CE1  | 1:D:134:TYR:CD1  | 3.05                     | 0.45              |
| 1:E:18:ILE:HG22  | 1:E:19:SER:N     | 2.31                     | 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:A:74:ALA:O     | 1:A:78:CYS:O     | 2.33                     | 0.45              |
| 1:B:25:PHE:CD1   | 1:B:25:PHE:C     | 2.94                     | 0.45              |
| 1:C:26:PHE:N     | 1:C:26:PHE:HD1   | 2.14                     | 0.45              |
| 1:C:52:ARG:CG    | 1:C:52:ARG:HH11  | 2.30                     | 0.45              |
| 1:D:121:PHE:CD1  | 1:D:121:PHE:C    | 2.94                     | 0.45              |
| 1:E:83:ALA:CB    | 1:E:125:MSE:HE1  | 2.37                     | 0.45              |
| 1:B:18:ILE:HG22  | 1:B:91:LEU:CD2   | 2.47                     | 0.45              |
| 1:B:112:TYR:HD2  | 1:C:30:VAL:HG11  | 1.81                     | 0.45              |
| 1:C:26:PHE:CD2   | 1:C:98:PHE:CD2   | 3.05                     | 0.45              |
| 1:D:12:LEU:HG    | 1:D:80:GLN:HE21  | 1.81                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:90:TYR:HE1   | 1:D:94:ARG:CG    | 2.30                     | 0.45              |
| 1:D:132:ASN:O    | 1:D:135:LEU:HB2  | 2.17                     | 0.45              |
| 1:E:90:TYR:CD1   | 1:E:90:TYR:C     | 2.91                     | 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: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:D:79:SER:HB3   | 1:D:82:PRO:HD2   | 1.97                     | 0.45              |
| 1:A:81:VAL:O     | 1:A:84:ALA:HB3   | 2.17                     | 0.45              |
| 1:B:90:TYR:N     | 1:B:118:ILE:HD13 | 2.32                     | 0.45              |
| 1:B:113:ILE:O    | 1:B:114:PHE:HB3  | 2.16                     | 0.45              |
| 1:B:116:LYS:N    | 1:B:119:ILE:CD1  | 2.80                     | 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              |
| 2:C:501:3CS:H182 | 2:C:501:3CS:C41  | 2.47                     | 0.45              |
| 1:E:8:ASN:C      | 1:E:9:VAL:CG1    | 2.89                     | 0.45              |
| 1:F:102:LEU:HD22 | 1:F:102:LEU:HA   | 1.69                     | 0.45              |
| 1:B:85:PHE:CD1   | 1:B:85:PHE:C     | 2.94                     | 0.45              |
| 1:C:50:PHE:CD1   | 1:C:50:PHE:C     | 2.94                     | 0.45              |
| 1:C:85:PHE:CD1   | 1:C:85:PHE:C     | 2.95                     | 0.45              |
| 1:D:81:VAL:N     | 1:D:82:PRO:CD    | 2.80                     | 0.45              |
| 1:E:25:PHE:O     | 1:E:28:HIS:HB3   | 2.17                     | 0.45              |
| 1:E:121:PHE:CE1  | 1:E:125:MSE:HG3  | 2.51                     | 0.45              |
| 1:F:70:VAL:HG23  | 1:F:71:LEU:N     | 2.31                     | 0.45              |
| 1:A:3:GLN:NE2    | 1:C:133:TYR:CD1  | 2.85                     | 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:90:TYR:HE1   | 1:A:114:PHE:CE2  | 2.35                     | 0.45              |
| 1:A:95:GLN:O     | 1:A:99:VAL:HB    | 2.17                     | 0.45              |
| 1:A:124:LEU:HD13 | 1:A:124:LEU:N    | 2.31                     | 0.45              |
| 1:B:106:THR:O    | 1:B:108:SER:N    | 2.50                     | 0.45              |
| 1:A:56:ALA:HA    | 1:A:101:TYR:HD2  | 1.81                     | 0.45              |
| 2:A:503:3CS:H382 | 2:A:503:3CS:C23  | 2.44                     | 0.45              |
| 2:A:503:3CS:H13  | 2:A:503:3CS:C9   | 2.47                     | 0.45              |
| 2:A:503:3CS:I25  | 1:B:25:PHE:HB2   | 2.87                     | 0.45              |
| 1:B:139:PHE:CD2  | 1:F:121:PHE:HB2  | 2.52                     | 0.45              |
| 1:D:64:TYR:N     | 1:D:65:PRO:HD2   | 2.32                     | 0.45              |
| 1:E:22:GLN:CG    | 1:E:23:ASN:N     | 2.80                     | 0.45              |
| 1:E:109:THR:N    | 1:E:110:PRO:HD3  | 2.32                     | 0.45              |
| 1:E:123:PHE:CD1  | 1:E:123:PHE:C    | 2.95                     | 0.45              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:130:ILE:CD1 | 1:F:14:ILE:HD11  | 2.47                     | 0.45              |
| 2:E:506:3CS:H23 | 2:E:506:3CS:O42  | 2.16                     | 0.45              |
| 1:F:123:PHE:CD1 | 1:F:123:PHE:C    | 2.95                     | 0.45              |
| 1:A:76:LEU:HD12 | 1:A:76:LEU:HA    | 1.81                     | 0.44              |
| 1:B:2:ASP:OD1   | 1:B:5:THR:HG23   | 2.17                     | 0.44              |
| 1:C:11:LEU:CD2  | 1:C:80:GLN:NE2   | 2.69                     | 0.44              |
| 1:C:116:LYS:HA  | 1:C:119:ILE:HD11 | 1.99                     | 0.44              |
| 1:D:123:PHE:HB2 | 2:D:505:3CS:H313 | 1.98                     | 0.44              |
| 1:E:56:ALA:HA   | 1:E:101:TYR:CD2  | 2.52                     | 0.44              |
| 1:E:59:ASN:ND2  | 1:E:112:TYR:H    | 2.15                     | 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:D:79:SER:O    | 1:D:82:PRO:HD2   | 2.18                     | 0.44              |
| 1:E:67:PHE:CD1  | 1:E:67:PHE:C     | 2.93                     | 0.44              |
| 1:F:11:LEU:HD22 | 1:F:80:GLN:HE22  | 1.82                     | 0.44              |
| 1:F:90:TYR:C    | 1:F:90:TYR:HD1   | 2.26                     | 0.44              |
| 1:F:121:PHE:C   | 1:F:121:PHE:HD1  | 2.25                     | 0.44              |
| 1:A:22:GLN:OE1  | 1:A:94:ARG:NE    | 2.49                     | 0.44              |
| 1:A:43:GLN:CD   | 1:C:54:TYR:HD2   | 2.26                     | 0.44              |
| 1:A:137:PHE:CE2 | 1:A:138:PHE:HE1  | 2.36                     | 0.44              |
| 1:B:77:LEU:N    | 1:B:77:LEU:CD1   | 2.80                     | 0.44              |
| 1:D:2:ASP:OD2   | 1:D:5:THR:HG23   | 2.17                     | 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:E:44:ARG:HH11 | 1:E:44:ARG:HB2   | 1.82                     | 0.44              |
| 1:B:74:ALA:CB   | 1:B:122:LEU:HD12 | 2.48                     | 0.44              |
| 1:E:8:ASN:C     | 1:E:9:VAL:HG12   | 2.42                     | 0.44              |
| 1:A:102:LEU:CG  | 1:A:103:GLY:H    | 2.15                     | 0.44              |
| 2:B:502:3CS:H21 | 1:C:25:PHE:N     | 2.32                     | 0.44              |
| 1:C:64:TYR:N    | 1:C:65:PRO:HD2   | 2.33                     | 0.44              |
| 1:D:6:VAL:HG12  | 1:F:133:TYR:CD2  | 2.52                     | 0.44              |
| 1:D:15:VAL:O    | 1:D:18:ILE:HB    | 2.18                     | 0.44              |
| 1:D:143:PHE:CE2 | 1:D:144:GLU:HG2  | 2.53                     | 0.44              |
| 1:E:12:LEU:HD13 | 1:E:72:TRP:CE3   | 2.52                     | 0.44              |
| 1:F:55:THR:HG21 | 1:F:101:TYR:OH   | 2.18                     | 0.44              |
| 1:F:78:CYS:O    | 1:F:79:SER:CB    | 2.65                     | 0.44              |
| 1:F:104:GLU:C   | 1:F:106:THR:H    | 2.26                     | 0.44              |
| 1:B:123:PHE:CD1 | 1:B:123:PHE:C    | 2.95                     | 0.44              |
| 1:C:26:PHE:HD1  | 1:C:26:PHE:H     | 1.65                     | 0.44              |
| 1:D:89:MSE:O    | 1:D:93:VAL:HG23  | 2.16                     | 0.44              |
| 1:D:97:TYR:CD1  | 1:D:97:TYR:C     | 2.94                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:14:ILE:HD11  | 1:C:130:ILE:HD12 | 1.99                     | 0.44              |
| 1:B:7:GLY:C      | 1:B:9:VAL:H      | 2.25                     | 0.44              |
| 1:B:90:TYR:N     | 1:B:118:ILE:CD1  | 2.81                     | 0.44              |
| 1:C:90:TYR:CD1   | 1:C:118:ILE:HG21 | 2.53                     | 0.44              |
| 1:C:120:LEU:CD2  | 2:C:501:3CS:H323 | 2.47                     | 0.44              |
| 1:D:66:THR:CG2   | 1:E:20:VAL:HG22  | 2.44                     | 0.44              |
| 1:E:25:PHE:CD1   | 1:E:25:PHE:C     | 2.95                     | 0.44              |
| 1:E:97:TYR:C     | 1:E:97:TYR:CD1   | 2.94                     | 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:D:47:THR:HG22  | 1:D:49:ALA:H     | 1.83                     | 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              |
| 1:F:121:PHE:HE1  | 1:F:125:MSE:CG   | 2.30                     | 0.44              |
| 1:A:35:ARG:NH2   | 1:C:113:ILE:CD1  | 2.81                     | 0.44              |
| 1:A:90:TYR:HB2   | 1:A:118:ILE:HG21 | 1.99                     | 0.44              |
| 1:A:110:PRO:CB   | 1:B:42:PHE:HB2   | 2.48                     | 0.44              |
| 1:B:110:PRO:HB3  | 1:C:35:ARG:HH22  | 1.83                     | 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:F:106:THR:O    | 1:F:107:GLN:HB2  | 2.16                     | 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:HE    | 1:D:44:ARG:CA    | 2.31                     | 0.43              |
| 1:D:99:VAL:HG12  | 1:D:100:GLY:N    | 2.32                     | 0.43              |
| 1:A:25:PHE:HD1   | 1:A:25:PHE:O     | 2.01                     | 0.43              |
| 1:B:145:ASN:HD22 | 1:B:145:ASN:N    | 2.01                     | 0.43              |
| 1:C:119:ILE:HD13 | 1:C:119:ILE:H    | 1.82                     | 0.43              |
| 1:D:44:ARG:HH11  | 1:F:51:GLU:HG2   | 1.81                     | 0.43              |
| 1:E:80:GLN:H     | 1:E:82:PRO:HD2   | 1.83                     | 0.43              |
| 1:E:133:TYR:CD1  | 1:E:134:TYR:HD1  | 2.34                     | 0.43              |
| 1:F:97:TYR:HB3   | 1:F:114:PHE:CZ   | 2.53                     | 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:C:87:GLY:O     | 1:C:90:TYR:HB3   | 2.19                     | 0.43              |
| 1:D:52:ARG:CG    | 1:D:52:ARG:NH1   | 2.81                     | 0.43              |
| 1:D:85:PHE:O     | 1:D:88:LEU:HB3   | 2.18                     | 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:F:64:TYR:CE1   | 1:F:68:LEU:HD22  | 2.53                     | 0.43              |
| 1:A:90:TYR:CD1   | 1:A:90:TYR:C     | 2.93                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:502:3CS:C21  | 1:C:25:PHE:N     | 2.81                     | 0.43              |
| 1:C:33:GLU:CG    | 1:C:50:PHE:HA    | 2.48                     | 0.43              |
| 1:F:104:GLU:OE1  | 1:F:104:GLU:HA   | 2.17                     | 0.43              |
| 1:A:74:ALA:CB    | 1:A:122:LEU:HD12 | 2.49                     | 0.43              |
| 1:B:97:TYR:CD1   | 1:B:97:TYR:C     | 2.96                     | 0.43              |
| 1:C:22:GLN:HE21  | 1:C:22:GLN:HB2   | 1.67                     | 0.43              |
| 1:C:81:VAL:N     | 1:C:82:PRO:CD    | 2.81                     | 0.43              |
| 1:C:144:GLU:OE1  | 1:C:147:ILE:HD11 | 2.19                     | 0.43              |
| 1:D:21:VAL:HG23  | 1:F:123:PHE:CE2  | 2.53                     | 0.43              |
| 1:D:133:TYR:HD1  | 1:D:134:TYR:CD1  | 2.37                     | 0.43              |
| 1:E:10:VAL:O     | 1:E:14:ILE:HD12  | 2.19                     | 0.43              |
| 1:E:29:LYS:HD2   | 1:E:29:LYS:HA    | 1.55                     | 0.43              |
| 1:F:137:PHE:CD1  | 1:F:137:PHE:C    | 2.95                     | 0.43              |
| 1:A:30:VAL:HG23  | 1:A:53:VAL:CG1   | 2.48                     | 0.43              |
| 1:F:1:MSE:HB3    | 1:F:6:VAL:HG22   | 1.99                     | 0.43              |
| 1:F:29:LYS:HD2   | 1:F:29:LYS:HA    | 1.51                     | 0.43              |
| 1:F:79:SER:HB2   | 1:F:82:PRO:HG2   | 2.01                     | 0.43              |
| 1:B:35:ARG:C     | 1:B:37:GLN:N     | 2.76                     | 0.43              |
| 1:B:67:PHE:CD1   | 1:B:67:PHE:C     | 2.97                     | 0.43              |
| 1:C:71:LEU:HD22  | 1:C:71:LEU:C     | 2.43                     | 0.43              |
| 1:D:10:VAL:CG2   | 1:F:133:TYR:CE2  | 3.00                     | 0.43              |
| 1:D:116:LYS:NZ   | 2:D:505:3CS:C12  | 2.76                     | 0.43              |
| 1:E:74:ALA:HB1   | 1:E:125:MSE:HE2  | 2.00                     | 0.43              |
| 1:B:26:PHE:CG    | 1:B:98:PHE:CD2   | 3.06                     | 0.43              |
| 1:B:90:TYR:HA    | 1:B:118:ILE:HD13 | 1.99                     | 0.43              |
| 1:B:124:LEU:HD13 | 1:B:124:LEU:N    | 2.34                     | 0.43              |
| 1:D:26:PHE:N     | 1:D:26:PHE:CD1   | 2.87                     | 0.43              |
| 1:D:28:HIS:C     | 1:D:30:VAL:N     | 2.77                     | 0.43              |
| 2:E:506:3CS:C19  | 2:E:506:3CS:H371 | 2.49                     | 0.43              |
| 1:F:12:LEU:HD11  | 1:F:75:GLY:HA3   | 1.99                     | 0.43              |
| 1:F:90:TYR:N     | 1:F:118:ILE:CD1  | 2.81                     | 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:B:67:PHE:HB2   | 1:B:90:TYR:CE2   | 2.53                     | 0.43              |
| 1:C:90:TYR:CB    | 1:C:118:ILE:HG21 | 2.46                     | 0.43              |
| 1:D:16:THR:O     | 1:D:19:SER:OG    | 2.35                     | 0.43              |
| 1:E:47:THR:CG2   | 1:E:50:PHE:HB3   | 2.48                     | 0.43              |
| 1:F:26:PHE:HB3   | 1:F:57:ASN:HD22  | 1.84                     | 0.43              |
| 1:F:90:TYR:HD1   | 1:F:90:TYR:O     | 2.01                     | 0.43              |
| 1:A:9:VAL:O      | 1:A:9:VAL:HG23   | 2.18                     | 0.43              |
| 1:B:120:LEU:CD1  | 1:B:124:LEU:HD21 | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:502:3CS:I25  | 1:C:25:PHE:HB2   | 2.88                     | 0.43              |
| 1:D:120:LEU:HD23 | 2:D:505:3CS:C29  | 2.48                     | 0.43              |
| 1:D:133:TYR:CD1  | 1:D:134:TYR:HD1  | 2.36                     | 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:A:81:VAL:N     | 1:A:82:PRO:HD2   | 2.33                     | 0.42              |
| 1:B:121:PHE:CD1  | 1:B:121:PHE:C    | 2.93                     | 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:C:131:PHE:CD1  | 1:C:132:ASN:N    | 2.87                     | 0.42              |
| 1:D:2:ASP:OD1    | 1:D:2:ASP:N      | 2.51                     | 0.42              |
| 1:D:124:LEU:HA   | 1:D:124:LEU:HD12 | 1.82                     | 0.42              |
| 1:B:30:VAL:CG2   | 1:B:53:VAL:CG1   | 2.97                     | 0.42              |
| 1:B:113:ILE:HD13 | 1:B:113:ILE:C    | 2.44                     | 0.42              |
| 1:B:144:GLU:O    | 1:F:89:MSE:HE3   | 2.19                     | 0.42              |
| 1:C:1:MSE:HE3    | 1:C:5:THR:OG1    | 2.19                     | 0.42              |
| 1:C:55:THR:HG22  | 1:C:101:TYR:CE2  | 2.54                     | 0.42              |
| 1:D:120:LEU:HD13 | 1:D:120:LEU:C    | 2.44                     | 0.42              |
| 1:E:121:PHE:CD1  | 1:E:121:PHE:C    | 2.95                     | 0.42              |
| 1:E:133:TYR:HD1  | 1:E:134:TYR:CD1  | 2.36                     | 0.42              |
| 1:C:83:ALA:HB2   | 1:C:125:MSE:CE   | 2.25                     | 0.42              |
| 2:D:505:3CS:C21  | 1:E:25:PHE:HB2   | 2.49                     | 0.42              |
| 1:F:132:ASN:ND2  | 1:F:136:ILE:HD11 | 2.34                     | 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:116:LYS:CA   | 1:B:119:ILE:HD11 | 2.50                     | 0.42              |
| 1:A:11:LEU:HD13  | 1:A:11:LEU:N     | 2.34                     | 0.42              |
| 2:A:503:3CS:C38  | 2:A:503:3CS:C23  | 2.96                     | 0.42              |
| 1:B:18:ILE:HG22  | 1:B:91:LEU:HD23  | 2.00                     | 0.42              |
| 1:C:135:LEU:HD23 | 1:C:135:LEU:HA   | 1.78                     | 0.42              |
| 1:D:141:SER:C    | 1:D:143:PHE:N    | 2.77                     | 0.42              |
| 1:E:7:GLY:O      | 1:E:9:VAL:N      | 2.52                     | 0.42              |
| 1:E:33:GLU:OE1   | 1:E:33:GLU:HA    | 2.20                     | 0.42              |
| 1:B:133:TYR:CE1  | 1:B:134:TYR:CE1  | 3.08                     | 0.42              |
| 1:B:144:GLU:CG   | 1:B:146:TYR:CE1  | 3.02                     | 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:D:47:THR:HB    | 1:D:50:PHE:HB3   | 2.02                     | 0.42              |
| 1:D:116:LYS:CA   | 1:D:116:LYS:NZ   | 2.79                     | 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              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:48:LEU:HD23  | 1:A:48:LEU:HA    | 1.80                     | 0.42              |
| 2:A:503:3CS:H182 | 2:A:503:3CS:H393 | 2.02                     | 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:HA   | 1:F:124:LEU:HD12 | 1.78                     | 0.42              |
| 2:A:503:3CS:H181 | 1:B:28:HIS:HB2   | 2.02                     | 0.42              |
| 1:B:143:PHE:C    | 1:B:143:PHE:CD1  | 2.97                     | 0.42              |
| 2:B:502:3CS:C21  | 1:C:25:PHE:CA    | 2.98                     | 0.42              |
| 1:C:53:VAL:HG12  | 1:C:54:TYR:N     | 2.35                     | 0.42              |
| 1:D:85:PHE:CD1   | 1:D:85:PHE:C     | 2.96                     | 0.42              |
| 1:E:81:VAL:CB    | 1:E:82:PRO:HD3   | 2.50                     | 0.42              |
| 1:F:104:GLU:C    | 1:F:106:THR:N    | 2.78                     | 0.42              |
| 1:A:126:SER:O    | 1:A:130:ILE:HB   | 2.19                     | 0.42              |
| 1:B:8:ASN:C      | 1:B:9:VAL:HG12   | 2.45                     | 0.42              |
| 1:B:133:TYR:HD1  | 1:B:134:TYR:CD1  | 2.38                     | 0.42              |
| 1:B:138:PHE:N    | 1:B:138:PHE:CD1  | 2.87                     | 0.42              |
| 1:C:57:ASN:C     | 1:C:59:ASN:H     | 2.28                     | 0.42              |
| 1:D:90:TYR:C     | 1:D:90:TYR:HD1   | 2.28                     | 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:F:35:ARG:HA    | 1:F:38:ASN:OD1   | 2.19                     | 0.42              |
| 1:A:11:LEU:CD2   | 1:A:80:GLN:NE2   | 2.80                     | 0.42              |
| 1:A:15:VAL:CG1   | 1:A:16:THR:N     | 2.83                     | 0.42              |
| 1:A:124:LEU:HA   | 1:A:124:LEU:HD12 | 1.87                     | 0.42              |
| 1:B:29:LYS:HA    | 1:B:29:LYS:HD2   | 1.57                     | 0.42              |
| 1:C:72:TRP:O     | 1:C:76:LEU:HD22  | 2.20                     | 0.42              |
| 1:C:74:ALA:HB2   | 1:C:122:LEU:O    | 2.20                     | 0.42              |
| 1:F:39:GLY:C     | 1:F:41:SER:N     | 2.73                     | 0.42              |
| 1:F:111:GLY:C    | 1:F:113:ILE:H    | 2.28                     | 0.42              |
| 1:B:38:ASN:C     | 1:B:40:ARG:H     | 2.28                     | 0.41              |
| 1:B:137:PHE:CD1  | 1:B:137:PHE:C    | 2.97                     | 0.41              |
| 1:B:142:ASP:C    | 1:B:144:GLU:N    | 2.78                     | 0.41              |
| 1:D:22:GLN:CG    | 1:D:23:ASN:N     | 2.81                     | 0.41              |
| 1:D:26:PHE:HD1   | 1:D:26:PHE:H     | 1.67                     | 0.41              |
| 1:D:56:ALA:HB2   | 1:D:101:TYR:HB3  | 2.02                     | 0.41              |
| 1:D:123:PHE:HD1  | 1:D:124:LEU:HD13 | 1.85                     | 0.41              |
| 1:F:85:PHE:CD1   | 1:F:85:PHE:C     | 2.97                     | 0.41              |
| 1:A:25:PHE:CA    | 2:C:501:3CS:C21  | 2.98                     | 0.41              |
| 1:A:97:TYR:CD1   | 1:A:97:TYR:C     | 2.95                     | 0.41              |
| 1:B:108:SER:C    | 1:B:110:PRO:HD3  | 2.44                     | 0.41              |
| 1:B:116:LYS:HA   | 1:B:119:ILE:HD11 | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:62:ASP:OD1   | 1:C:62:ASP:N     | 2.53                     | 0.41              |
| 1:C:113:ILE:O    | 1:C:114:PHE:CG   | 2.73                     | 0.41              |
| 1:A:42:PHE:CD2   | 1:A:50:PHE:CZ    | 2.96                     | 0.41              |
| 1:B:50:PHE:HD1   | 1:B:50:PHE:O     | 2.03                     | 0.41              |
| 1:B:85:PHE:HZ    | 1:B:89:MSE:HE2   | 1.85                     | 0.41              |
| 1:C:85:PHE:O     | 1:C:88:LEU:HB3   | 2.20                     | 0.41              |
| 1:C:135:LEU:O    | 1:C:139:PHE:N    | 2.53                     | 0.41              |
| 1:D:112:TYR:CE2  | 1:E:30:VAL:CG1   | 2.99                     | 0.41              |
| 1:D:120:LEU:O    | 1:D:124:LEU:HD22 | 2.20                     | 0.41              |
| 1:E:15:VAL:O     | 1:E:18:ILE:HB    | 2.20                     | 0.41              |
| 1:B:107:GLN:CG   | 1:C:40:ARG:HD2   | 2.50                     | 0.41              |
| 1:C:113:ILE:HG22 | 1:C:114:PHE:O    | 2.20                     | 0.41              |
| 1:D:33:GLU:HA    | 1:D:33:GLU:OE1   | 2.21                     | 0.41              |
| 1:F:64:TYR:O     | 1:F:67:PHE:HB3   | 2.20                     | 0.41              |
| 1:A:12:LEU:O     | 1:A:15:VAL:HG12  | 2.21                     | 0.41              |
| 1:B:124:LEU:C    | 1:B:127:VAL:HG12 | 2.45                     | 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: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:2:ASP:OD1    | 1:E:5:THR:HG23   | 2.21                     | 0.41              |
| 1:E:44:ARG:H     | 1:E:44:ARG:HG2   | 1.44                     | 0.41              |
| 1:E:50:PHE:CD1   | 1:E:50:PHE:C     | 2.97                     | 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:F:79:SER:OG    | 1:F:82:PRO:HD2   | 2.20                     | 0.41              |
| 1:A:64:TYR:CE1   | 1:A:68:LEU:HD22  | 2.55                     | 0.41              |
| 1:A:71:LEU:O     | 1:A:71:LEU:HD22  | 2.20                     | 0.41              |
| 1:B:26:PHE:CD1   | 1:B:26:PHE:N     | 2.89                     | 0.41              |
| 1:B:120:LEU:CD1  | 1:B:124:LEU:CD2  | 2.97                     | 0.41              |
| 1:C:26:PHE:CE2   | 1:C:98:PHE:CD2   | 3.09                     | 0.41              |
| 1:D:8:ASN:C      | 1:D:9:VAL:HG12   | 2.46                     | 0.41              |
| 1:D:138:PHE:CD1  | 1:D:138:PHE:N    | 2.88                     | 0.41              |
| 2:D:505:3CS:C21  | 1:E:25:PHE:CA    | 2.99                     | 0.41              |
| 1:A:22:GLN:CG    | 1:A:23:ASN:N     | 2.83                     | 0.41              |
| 1:B:65:PRO:HG2   | 1:B:66:THR:H     | 1.84                     | 0.41              |
| 1:C:121:PHE:CD1  | 1:C:121:PHE:C    | 2.99                     | 0.41              |
| 1:F:10:VAL:CG1   | 1:F:14:ILE:CD1   | 2.98                     | 0.41              |
| 1:F:91:LEU:HD12  | 1:F:91:LEU:HA    | 1.78                     | 0.41              |
| 1:F:121:PHE:HD1  | 1:F:121:PHE:O    | 2.04                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:25:PHE:N     | 2:C:501:3CS:C21  | 2.83                     | 0.41              |
| 1:A:33:GLU:OE2   | 1:A:49:ALA:HB1   | 2.20                     | 0.41              |
| 1:A:56:ALA:HA    | 1:A:101:TYR:CD2  | 2.56                     | 0.41              |
| 1:B:26:PHE:CG    | 1:B:98:PHE:CE2   | 3.09                     | 0.41              |
| 1:B:81:VAL:N     | 1:B:82:PRO:CD    | 2.84                     | 0.41              |
| 1:B:112:TYR:CD2  | 1:C:30:VAL:CG1   | 2.97                     | 0.41              |
| 1:C:10:VAL:HG13  | 1:C:14:ILE:HD13  | 2.00                     | 0.41              |
| 1:C:37:GLN:CD    | 1:C:47:THR:OG1   | 2.63                     | 0.41              |
| 1:C:95:GLN:O     | 1:C:99:VAL:HB    | 2.20                     | 0.41              |
| 1:D:19:SER:HB2   | 1:D:64:TYR:CE1   | 2.56                     | 0.41              |
| 1:D:78:CYS:HB2   | 1:D:125:MSE:O    | 2.21                     | 0.41              |
| 1:E:22:GLN:HE21  | 1:E:22:GLN:HB2   | 1.72                     | 0.41              |
| 1:E:52:ARG:CG    | 1:E:52:ARG:NH1   | 2.83                     | 0.41              |
| 1:E:55:THR:OG1   | 1:F:42:PHE:HD2   | 2.02                     | 0.41              |
| 1:E:57:ASN:C     | 1:E:59:ASN:H     | 2.29                     | 0.41              |
| 1:F:8:ASN:C      | 1:F:9:VAL:CG1    | 2.94                     | 0.41              |
| 1:F:11:LEU:HD23  | 1:F:80:GLN:CD    | 2.45                     | 0.41              |
| 1:F:30:VAL:CG2   | 1:F:53:VAL:HG12  | 2.51                     | 0.41              |
| 1:F:79:SER:O     | 1:F:80:GLN:CB    | 2.69                     | 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:B:10:VAL:HG12  | 1:B:11:LEU:N     | 2.34                     | 0.41              |
| 1:B:56:ALA:HB2   | 1:B:101:TYR:HB3  | 2.03                     | 0.41              |
| 1:D:5:THR:O      | 1:D:9:VAL:HG13   | 2.21                     | 0.41              |
| 1:D:25:PHE:CA    | 2:F:504:3CS:C21  | 2.99                     | 0.41              |
| 1:D:50:PHE:CD1   | 1:D:50:PHE:C     | 2.98                     | 0.41              |
| 1:D:74:ALA:CB    | 1:D:122:LEU:HD12 | 2.51                     | 0.41              |
| 1:E:135:LEU:N    | 1:E:135:LEU:CD2  | 2.84                     | 0.41              |
| 1:F:67:PHE:CG    | 1:F:90:TYR:HE2   | 2.37                     | 0.41              |
| 1:F:146:TYR:O    | 1:F:147:ILE:HD13 | 2.21                     | 0.41              |
| 1:A:97:TYR:CD2   | 1:A:114:PHE:HB3  | 2.56                     | 0.40              |
| 1:A:124:LEU:C    | 1:A:127:VAL:HG12 | 2.46                     | 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:F:78:CYS:O     | 1:F:78:CYS:SG    | 2.79                     | 0.40              |
| 1:A:10:VAL:HG21  | 1:C:133:TYR:HD2  | 1.80                     | 0.40              |
| 1:C:147:ILE:HG22 | 1:C:147:ILE:O    | 2.20                     | 0.40              |
| 1:D:133:TYR:CD1  | 1:D:133:TYR:C    | 2.97                     | 0.40              |
| 1:E:28:HIS:C     | 1:E:30:VAL:N     | 2.78                     | 0.40              |
| 2:E:506:3CS:C21  | 1:F:25:PHE:N     | 2.84                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:33:GLU:OE1   | 1:A:33:GLU:HA    | 2.21                     | 0.40              |
| 1:A:40:ARG:HD3   | 1:C:52:ARG:HH22  | 1.86                     | 0.40              |
| 1:A:42:PHE:CG    | 1:C:112:TYR:HE1  | 2.40                     | 0.40              |
| 1:A:50:PHE:C     | 1:A:50:PHE:CD1   | 2.98                     | 0.40              |
| 1:A:111:GLY:C    | 1:A:113:ILE:N    | 2.77                     | 0.40              |
| 1:A:137:PHE:O    | 1:A:137:PHE:CD1  | 2.74                     | 0.40              |
| 1:B:11:LEU:HD22  | 1:B:11:LEU:N     | 2.09                     | 0.40              |
| 1:C:52:ARG:NE    | 1:C:102:LEU:HA   | 2.36                     | 0.40              |
| 1:D:25:PHE:CE1   | 1:D:29:LYS:HG2   | 2.57                     | 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:D:132:ASN:ND2  | 1:D:136:ILE:HD11 | 2.37                     | 0.40              |
| 1:E:133:TYR:CD1  | 1:E:133:TYR:C    | 2.98                     | 0.40              |
| 1:F:81:VAL:N     | 1:F:82:PRO:CD    | 2.84                     | 0.40              |
| 1:A:22:GLN:NE2   | 1:A:26:PHE:CZ    | 2.89                     | 0.40              |
| 1:B:8:ASN:C      | 1:B:9:VAL:CG1    | 2.94                     | 0.40              |
| 1:D:11:LEU:HB2   | 1:D:80:GLN:NE2   | 2.36                     | 0.40              |
| 1:D:133:TYR:CE1  | 1:D:134:TYR:HD1  | 2.40                     | 0.40              |
| 1:E:45:THR:CB    | 1:F:43:GLN:NE2   | 2.85                     | 0.40              |
| 1:A:11:LEU:HB3   | 1:A:84:ALA:CB    | 2.51                     | 0.40              |
| 1:A:136:ILE:H    | 1:A:136:ILE:HG13 | 1.63                     | 0.40              |
| 1:B:26:PHE:N     | 1:B:26:PHE:HD1   | 2.19                     | 0.40              |
| 1:B:50:PHE:C     | 1:B:50:PHE:CD1   | 2.98                     | 0.40              |
| 1:B:57:ASN:C     | 1:B:59:ASN:N     | 2.79                     | 0.40              |
| 1:D:26:PHE:N     | 1:D:26:PHE:HD1   | 2.20                     | 0.40              |
| 1:D:57:ASN:C     | 1:D:59:ASN:N     | 2.80                     | 0.40              |
| 1:E:130:ILE:CD1  | 1:F:14:ILE:CD1   | 2.99                     | 0.40              |
| 1:F:90:TYR:CE1   | 1:F:94:ARG:HG3   | 2.56                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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%)   | 1           | 15 |
| 1   | B     | 146/161 (91%) | 98 (67%)  | 26 (18%)  | 22 (15%) | 0           | 3  |
| 1   | C     | 147/161 (91%) | 115 (78%) | 25 (17%)  | 7 (5%)   | 2           | 19 |
| 1   | D     | 146/161 (91%) | 109 (75%) | 31 (21%)  | 6 (4%)   | 2           | 21 |
| 1   | E     | 138/161 (86%) | 110 (80%) | 17 (12%)  | 11 (8%)  | 1           | 12 |
| 1   | F     | 147/161 (91%) | 107 (73%) | 26 (18%)  | 14 (10%) | 0           | 9  |
| All | All   | 862/966 (89%) | 647 (75%) | 146 (17%) | 69 (8%)  | 1           | 12 |

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  |
| 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  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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  |
| 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%) | 70 (60%)  | 47 (40%)  | 0           | 0 |
| 1   | B     | 124/134 (92%) | 70 (56%)  | 54 (44%)  | 0           | 0 |
| 1   | C     | 125/134 (93%) | 79 (63%)  | 46 (37%)  | 0           | 1 |
| 1   | D     | 124/134 (92%) | 72 (58%)  | 52 (42%)  | 0           | 0 |
| 1   | E     | 117/134 (87%) | 66 (56%)  | 51 (44%)  | 0           | 0 |
| 1   | F     | 125/134 (93%) | 73 (58%)  | 52 (42%)  | 0           | 0 |
| All | All   | 732/804 (91%) | 430 (59%) | 302 (41%) | 0           | 0 |

All (302) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | MSE  |
| 1   | A     | 8   | ASN  |
| 1   | A     | 9   | VAL  |
| 1   | A     | 10  | VAL  |
| 1   | A     | 11  | LEU  |
| 1   | A     | 14  | ILE  |
| 1   | A     | 18  | ILE  |
| 1   | A     | 20  | VAL  |
| 1   | A     | 21  | 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  |
| 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     | 66  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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     | 91  | LEU  |
| 1   | A     | 93  | VAL  |
| 1   | A     | 94  | ARG  |
| 1   | A     | 95  | GLN  |
| 1   | A     | 96  | LYS  |
| 1   | A     | 99  | VAL  |
| 1   | A     | 101 | TYR  |
| 1   | A     | 109 | THR  |
| 1   | A     | 112 | TYR  |
| 1   | A     | 117 | ARG  |
| 1   | A     | 118 | ILE  |
| 1   | A     | 119 | ILE  |
| 1   | A     | 122 | LEU  |
| 1   | A     | 124 | LEU  |
| 1   | A     | 130 | ILE  |
| 1   | A     | 131 | PHE  |
| 1   | A     | 132 | ASN  |
| 1   | A     | 135 | LEU  |
| 1   | A     | 136 | ILE  |
| 1   | B     | 1   | MSE  |
| 1   | B     | 8   | ASN  |
| 1   | B     | 9   | VAL  |
| 1   | B     | 10  | VAL  |
| 1   | B     | 11  | LEU  |
| 1   | B     | 14  | ILE  |
| 1   | B     | 18  | ILE  |
| 1   | B     | 20  | VAL  |
| 1   | B     | 21  | VAL  |
| 1   | B     | 22  | GLN  |
| 1   | B     | 29  | LYS  |
| 1   | B     | 30  | VAL  |
| 1   | B     | 32  | HIS  |
| 1   | B     | 35  | ARG  |
| 1   | B     | 37  | GLN  |
| 1   | B     | 48  | LEU  |
| 1   | B     | 52  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 62  | ASP  |
| 1   | B     | 66  | THR  |
| 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     | 107 | GLN  |
| 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     | 122 | LEU  |
| 1   | B     | 124 | LEU  |
| 1   | B     | 130 | ILE  |
| 1   | B     | 131 | PHE  |
| 1   | B     | 132 | ASN  |
| 1   | B     | 135 | LEU  |
| 1   | B     | 136 | ILE  |
| 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     | 9   | VAL  |
| 1   | C     | 10  | VAL  |
| 1   | C     | 11  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 14  | ILE  |
| 1   | C     | 17  | LEU  |
| 1   | C     | 18  | ILE  |
| 1   | C     | 20  | VAL  |
| 1   | C     | 21  | VAL  |
| 1   | C     | 22  | GLN  |
| 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     | 53  | VAL  |
| 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     | 77  | 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     | 99  | VAL  |
| 1   | C     | 101 | TYR  |
| 1   | C     | 102 | LEU  |
| 1   | C     | 108 | SER  |
| 1   | C     | 118 | ILE  |
| 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  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 8   | ASN  |
| 1   | D     | 9   | VAL  |
| 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     | 40  | ARG  |
| 1   | D     | 41  | SER  |
| 1   | D     | 42  | PHE  |
| 1   | D     | 44  | ARG  |
| 1   | D     | 52  | ARG  |
| 1   | D     | 61  | VAL  |
| 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     | 80  | GLN  |
| 1   | D     | 89  | MSE  |
| 1   | D     | 91  | LEU  |
| 1   | D     | 93  | VAL  |
| 1   | D     | 94  | ARG  |
| 1   | D     | 95  | GLN  |
| 1   | D     | 96  | LYS  |
| 1   | D     | 99  | VAL  |
| 1   | D     | 102 | LEU  |
| 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  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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     | 136 | ILE  |
| 1   | D     | 142 | ASP  |
| 1   | D     | 143 | PHE  |
| 1   | E     | 1   | MSE  |
| 1   | E     | 8   | ASN  |
| 1   | E     | 9   | VAL  |
| 1   | E     | 10  | VAL  |
| 1   | E     | 11  | LEU  |
| 1   | E     | 14  | ILE  |
| 1   | E     | 18  | ILE  |
| 1   | E     | 20  | VAL  |
| 1   | E     | 21  | VAL  |
| 1   | E     | 22  | GLN  |
| 1   | E     | 29  | LYS  |
| 1   | E     | 30  | VAL  |
| 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     | 52  | ARG  |
| 1   | E     | 61  | VAL  |
| 1   | E     | 62  | ASP  |
| 1   | E     | 66  | THR  |
| 1   | E     | 68  | LEU  |
| 1   | E     | 71  | LEU  |
| 1   | E     | 76  | LEU  |
| 1   | E     | 80  | GLN  |
| 1   | E     | 81  | VAL  |
| 1   | E     | 89  | MSE  |
| 1   | E     | 91  | LEU  |
| 1   | E     | 93  | VAL  |
| 1   | E     | 94  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 96  | LYS  |
| 1   | E     | 99  | VAL  |
| 1   | E     | 101 | TYR  |
| 1   | E     | 102 | LEU  |
| 1   | E     | 104 | GLU  |
| 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     | 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     | 9   | VAL  |
| 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     | 30  | VAL  |
| 1   | F     | 32  | HIS  |
| 1   | F     | 33  | GLU  |
| 1   | F     | 43  | GLN  |
| 1   | F     | 52  | ARG  |
| 1   | F     | 53  | VAL  |
| 1   | F     | 62  | ASP  |
| 1   | F     | 66  | THR  |
| 1   | F     | 68  | LEU  |
| 1   | F     | 71  | LEU  |
| 1   | F     | 76  | LEU  |
| 1   | F     | 78  | CYS  |
| 1   | F     | 81  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 89  | MSE  |
| 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     | 99  | VAL  |
| 1   | F     | 102 | LEU  |
| 1   | F     | 104 | GLU  |
| 1   | F     | 107 | GLN  |
| 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  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 8   | ASN  |
| 1   | A     | 57  | ASN  |
| 1   | A     | 132 | ASN  |
| 1   | B     | 8   | ASN  |
| 1   | B     | 38  | ASN  |
| 1   | B     | 80  | GLN  |
| 1   | B     | 132 | ASN  |
| 1   | B     | 145 | ASN  |
| 1   | C     | 8   | ASN  |
| 1   | C     | 32  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 38  | ASN  |
| 1   | C     | 57  | ASN  |
| 1   | C     | 58  | GLN  |
| 1   | C     | 80  | GLN  |
| 1   | D     | 3   | GLN  |
| 1   | D     | 8   | ASN  |
| 1   | D     | 57  | ASN  |
| 1   | D     | 59  | ASN  |
| 1   | D     | 80  | GLN  |
| 1   | E     | 8   | ASN  |
| 1   | E     | 32  | HIS  |
| 1   | E     | 57  | ASN  |
| 1   | E     | 80  | GLN  |
| 1   | E     | 132 | ASN  |
| 1   | F     | 8   | ASN  |
| 1   | F     | 43  | GLN  |
| 1   | F     | 57  | ASN  |
| 1   | F     | 80  | GLN  |
| 1   | F     | 132 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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  | B     | 502 | -    | 47,47,47     | 2.07 | 22 (46%)    | 65,70,70    | 1.98 | 18 (27%)    |
| 2   | 3CS  | E     | 506 | -    | 47,47,47     | 1.95 | 18 (38%)    | 65,70,70    | 1.96 | 19 (29%)    |
| 2   | 3CS  | A     | 503 | -    | 47,47,47     | 2.07 | 21 (44%)    | 65,70,70    | 2.02 | 22 (33%)    |
| 2   | 3CS  | D     | 505 | -    | 47,47,47     | 2.09 | 20 (42%)    | 65,70,70    | 2.01 | 18 (27%)    |
| 2   | 3CS  | C     | 501 | -    | 47,47,47     | 2.03 | 16 (34%)    | 65,70,70    | 1.99 | 19 (29%)    |
| 2   | 3CS  | F     | 504 | -    | 47,47,47     | 2.00 | 17 (36%)    | 65,70,70    | 1.84 | 17 (26%)    |

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  | B     | 502 | -    | -       | 15/29/29/29 | 0/5/5/5 |
| 2   | 3CS  | E     | 506 | -    | -       | 17/29/29/29 | 0/5/5/5 |
| 2   | 3CS  | A     | 503 | -    | -       | 16/29/29/29 | 0/5/5/5 |
| 2   | 3CS  | D     | 505 | -    | -       | 16/29/29/29 | 0/5/5/5 |
| 2   | 3CS  | C     | 501 | -    | -       | 12/29/29/29 | 0/5/5/5 |
| 2   | 3CS  | F     | 504 | -    | -       | 13/29/29/29 | 0/5/5/5 |

All (114) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | C     | 501 | 3CS  | O27-C11 | -6.17 | 1.23        | 1.37     |
| 2   | C     | 501 | 3CS  | C30-C29 | -5.34 | 1.45        | 1.51     |
| 2   | F     | 504 | 3CS  | O27-C11 | -5.18 | 1.25        | 1.37     |
| 2   | E     | 506 | 3CS  | O27-C11 | -5.15 | 1.25        | 1.37     |
| 2   | D     | 505 | 3CS  | C30-C29 | -5.12 | 1.45        | 1.51     |
| 2   | A     | 503 | 3CS  | O27-C11 | -4.84 | 1.26        | 1.37     |
| 2   | D     | 505 | 3CS  | O27-C11 | -4.78 | 1.26        | 1.37     |
| 2   | B     | 502 | 3CS  | O27-C11 | -4.69 | 1.27        | 1.37     |
| 2   | F     | 504 | 3CS  | C30-C29 | -4.35 | 1.46        | 1.51     |
| 2   | E     | 506 | 3CS  | C30-C29 | -4.22 | 1.46        | 1.51     |
| 2   | B     | 502 | 3CS  | C30-C29 | -4.09 | 1.46        | 1.51     |
| 2   | C     | 501 | 3CS  | C18-C19 | -4.08 | 1.44        | 1.51     |
| 2   | A     | 503 | 3CS  | C37-C36 | -3.87 | 1.46        | 1.50     |
| 2   | D     | 505 | 3CS  | C18-C19 | -3.77 | 1.44        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | A     | 503 | 3CS  | C30-C29 | -3.75 | 1.47        | 1.51     |
| 2   | C     | 501 | 3CS  | O27-C10 | -3.71 | 1.31        | 1.43     |
| 2   | F     | 504 | 3CS  | C23-C22 | 3.71  | 1.44        | 1.38     |
| 2   | B     | 502 | 3CS  | C18-C19 | -3.45 | 1.45        | 1.51     |
| 2   | A     | 503 | 3CS  | C9-N26  | 3.41  | 1.38        | 1.32     |
| 2   | B     | 502 | 3CS  | C37-C36 | -3.22 | 1.47        | 1.50     |
| 2   | A     | 503 | 3CS  | C18-C19 | -3.21 | 1.45        | 1.51     |
| 2   | E     | 506 | 3CS  | O27-C10 | -3.11 | 1.33        | 1.43     |
| 2   | F     | 504 | 3CS  | C18-C19 | -3.05 | 1.45        | 1.51     |
| 2   | A     | 503 | 3CS  | C24-I25 | -3.04 | 2.02        | 2.10     |
| 2   | D     | 505 | 3CS  | O27-C10 | -2.98 | 1.34        | 1.43     |
| 2   | F     | 504 | 3CS  | C22-C24 | 2.96  | 1.45        | 1.38     |
| 2   | B     | 502 | 3CS  | C4-C5   | 2.96  | 1.43        | 1.36     |
| 2   | D     | 505 | 3CS  | C18-N17 | -2.95 | 1.42        | 1.46     |
| 2   | D     | 505 | 3CS  | C9-N26  | 2.86  | 1.37        | 1.32     |
| 2   | C     | 501 | 3CS  | C10-C9  | -2.85 | 1.43        | 1.50     |
| 2   | B     | 502 | 3CS  | O27-C10 | -2.85 | 1.34        | 1.43     |
| 2   | B     | 502 | 3CS  | C9-N26  | 2.84  | 1.37        | 1.32     |
| 2   | A     | 503 | 3CS  | C1-C6   | 2.84  | 1.46        | 1.42     |
| 2   | A     | 503 | 3CS  | O27-C10 | -2.83 | 1.34        | 1.43     |
| 2   | F     | 504 | 3CS  | O27-C10 | -2.82 | 1.34        | 1.43     |
| 2   | B     | 502 | 3CS  | C12-C11 | 2.81  | 1.43        | 1.39     |
| 2   | A     | 503 | 3CS  | C3-C2   | 2.81  | 1.42        | 1.36     |
| 2   | B     | 502 | 3CS  | C3-C2   | 2.75  | 1.42        | 1.36     |
| 2   | E     | 506 | 3CS  | C4-C5   | 2.74  | 1.42        | 1.36     |
| 2   | B     | 502 | 3CS  | C1-C6   | 2.74  | 1.46        | 1.42     |
| 2   | A     | 503 | 3CS  | C4-C5   | 2.73  | 1.42        | 1.36     |
| 2   | F     | 504 | 3CS  | C9-N26  | 2.72  | 1.37        | 1.32     |
| 2   | D     | 505 | 3CS  | C12-C16 | 2.71  | 1.44        | 1.39     |
| 2   | C     | 501 | 3CS  | C14-C15 | 2.70  | 1.43        | 1.39     |
| 2   | E     | 506 | 3CS  | C18-C19 | -2.68 | 1.46        | 1.51     |
| 2   | A     | 503 | 3CS  | C15-N17 | -2.65 | 1.34        | 1.39     |
| 2   | D     | 505 | 3CS  | C37-C36 | -2.63 | 1.47        | 1.50     |
| 2   | D     | 505 | 3CS  | C15-N17 | -2.63 | 1.34        | 1.39     |
| 2   | F     | 504 | 3CS  | C4-C5   | 2.61  | 1.42        | 1.36     |
| 2   | E     | 506 | 3CS  | C3-C2   | 2.60  | 1.42        | 1.36     |
| 2   | A     | 503 | 3CS  | C36-N17 | -2.58 | 1.34        | 1.38     |
| 2   | D     | 505 | 3CS  | C10-C9  | -2.54 | 1.44        | 1.50     |
| 2   | A     | 503 | 3CS  | O43-C41 | -2.53 | 1.21        | 1.30     |
| 2   | B     | 502 | 3CS  | C14-C15 | 2.52  | 1.43        | 1.39     |
| 2   | C     | 501 | 3CS  | C4-C5   | 2.51  | 1.42        | 1.36     |
| 2   | E     | 506 | 3CS  | C14-C15 | 2.50  | 1.43        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | E     | 506 | 3CS  | C1-C6   | 2.49  | 1.45        | 1.42     |
| 2   | D     | 505 | 3CS  | C4-C5   | 2.49  | 1.42        | 1.36     |
| 2   | B     | 502 | 3CS  | C15-N17 | -2.47 | 1.35        | 1.39     |
| 2   | F     | 504 | 3CS  | C21-C20 | 2.47  | 1.42        | 1.38     |
| 2   | D     | 505 | 3CS  | C3-C2   | 2.45  | 1.41        | 1.36     |
| 2   | F     | 504 | 3CS  | C3-C2   | 2.44  | 1.41        | 1.36     |
| 2   | D     | 505 | 3CS  | O43-C41 | -2.43 | 1.21        | 1.30     |
| 2   | E     | 506 | 3CS  | C10-C9  | -2.42 | 1.44        | 1.50     |
| 2   | E     | 506 | 3CS  | C4-C3   | 2.42  | 1.43        | 1.38     |
| 2   | C     | 501 | 3CS  | C3-C2   | 2.42  | 1.41        | 1.36     |
| 2   | E     | 506 | 3CS  | C13-C11 | 2.40  | 1.43        | 1.38     |
| 2   | F     | 504 | 3CS  | C21-C24 | 2.38  | 1.43        | 1.38     |
| 2   | A     | 503 | 3CS  | C12-C11 | 2.34  | 1.42        | 1.39     |
| 2   | B     | 502 | 3CS  | C13-C11 | 2.34  | 1.43        | 1.38     |
| 2   | D     | 505 | 3CS  | C14-C13 | 2.34  | 1.42        | 1.38     |
| 2   | C     | 501 | 3CS  | C37-C36 | -2.34 | 1.48        | 1.50     |
| 2   | C     | 501 | 3CS  | C24-I25 | -2.31 | 2.04        | 2.10     |
| 2   | F     | 504 | 3CS  | C37-C36 | -2.30 | 1.48        | 1.50     |
| 2   | E     | 506 | 3CS  | C16-C28 | -2.30 | 1.41        | 1.46     |
| 2   | B     | 502 | 3CS  | C36-N17 | -2.30 | 1.34        | 1.38     |
| 2   | B     | 502 | 3CS  | C4-C3   | 2.29  | 1.43        | 1.38     |
| 2   | B     | 502 | 3CS  | C23-C22 | 2.29  | 1.42        | 1.38     |
| 2   | F     | 504 | 3CS  | O43-C41 | -2.29 | 1.22        | 1.30     |
| 2   | F     | 504 | 3CS  | C15-N17 | -2.29 | 1.35        | 1.39     |
| 2   | B     | 502 | 3CS  | C12-C16 | 2.27  | 1.43        | 1.39     |
| 2   | E     | 506 | 3CS  | C12-C11 | 2.27  | 1.42        | 1.39     |
| 2   | A     | 503 | 3CS  | C10-C9  | -2.26 | 1.45        | 1.50     |
| 2   | B     | 502 | 3CS  | O43-C41 | -2.25 | 1.22        | 1.30     |
| 2   | D     | 505 | 3CS  | C23-C22 | 2.25  | 1.42        | 1.38     |
| 2   | C     | 501 | 3CS  | C15-N17 | -2.22 | 1.35        | 1.39     |
| 2   | D     | 505 | 3CS  | C14-C15 | 2.21  | 1.43        | 1.39     |
| 2   | A     | 503 | 3CS  | C7-C8   | 2.19  | 1.41        | 1.36     |
| 2   | D     | 505 | 3CS  | C13-C11 | 2.18  | 1.42        | 1.38     |
| 2   | A     | 503 | 3CS  | C40-C41 | -2.18 | 1.41        | 1.51     |
| 2   | C     | 501 | 3CS  | C36-N17 | -2.17 | 1.34        | 1.38     |
| 2   | C     | 501 | 3CS  | C6-N26  | -2.16 | 1.34        | 1.37     |
| 2   | B     | 502 | 3CS  | C10-C9  | -2.16 | 1.45        | 1.50     |
| 2   | A     | 503 | 3CS  | C4-C3   | 2.15  | 1.43        | 1.38     |
| 2   | B     | 502 | 3CS  | C24-I25 | -2.15 | 2.04        | 2.10     |
| 2   | F     | 504 | 3CS  | C23-C19 | 2.15  | 1.43        | 1.38     |
| 2   | A     | 503 | 3CS  | C16-C28 | -2.14 | 1.41        | 1.46     |
| 2   | A     | 503 | 3CS  | C14-C15 | 2.14  | 1.42        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | E     | 506 | 3CS  | C18-N17 | -2.13 | 1.43        | 1.46     |
| 2   | B     | 502 | 3CS  | C7-C8   | 2.11  | 1.41        | 1.36     |
| 2   | B     | 502 | 3CS  | C16-C28 | -2.10 | 1.41        | 1.46     |
| 2   | E     | 506 | 3CS  | C15-N17 | -2.09 | 1.35        | 1.39     |
| 2   | C     | 501 | 3CS  | C16-C28 | -2.07 | 1.41        | 1.46     |
| 2   | D     | 505 | 3CS  | C20-C19 | 2.05  | 1.43        | 1.38     |
| 2   | F     | 504 | 3CS  | C10-C9  | -2.05 | 1.45        | 1.50     |
| 2   | D     | 505 | 3CS  | C7-C8   | 2.04  | 1.41        | 1.36     |
| 2   | F     | 504 | 3CS  | C14-C15 | 2.03  | 1.42        | 1.39     |
| 2   | E     | 506 | 3CS  | C21-C20 | 2.03  | 1.42        | 1.38     |
| 2   | A     | 503 | 3CS  | C18-N17 | -2.03 | 1.43        | 1.46     |
| 2   | C     | 501 | 3CS  | O43-C41 | -2.02 | 1.23        | 1.30     |
| 2   | C     | 501 | 3CS  | C4-C3   | 2.02  | 1.42        | 1.38     |
| 2   | E     | 506 | 3CS  | C21-C24 | 2.02  | 1.43        | 1.38     |
| 2   | E     | 506 | 3CS  | C9-N26  | 2.02  | 1.35        | 1.32     |
| 2   | D     | 505 | 3CS  | C4-C3   | 2.01  | 1.42        | 1.38     |

All (113) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 503 | 3CS  | C16-C28-C36 | -6.02 | 102.59      | 107.79   |
| 2   | C     | 501 | 3CS  | C16-C28-C36 | -5.91 | 102.69      | 107.79   |
| 2   | D     | 505 | 3CS  | C16-C28-C36 | -5.76 | 102.82      | 107.79   |
| 2   | B     | 502 | 3CS  | C16-C28-C36 | -5.45 | 103.08      | 107.79   |
| 2   | D     | 505 | 3CS  | O35-C29-C30 | -5.31 | 110.88      | 121.76   |
| 2   | C     | 501 | 3CS  | O35-C29-C30 | -5.27 | 110.95      | 121.76   |
| 2   | F     | 504 | 3CS  | C16-C28-C36 | -5.06 | 103.42      | 107.79   |
| 2   | B     | 502 | 3CS  | O35-C29-C30 | -4.84 | 111.83      | 121.76   |
| 2   | E     | 506 | 3CS  | O43-C41-O42 | -4.83 | 108.40      | 123.86   |
| 2   | F     | 504 | 3CS  | O35-C29-C30 | -4.77 | 111.99      | 121.76   |
| 2   | B     | 502 | 3CS  | O43-C41-O42 | -4.59 | 109.16      | 123.86   |
| 2   | B     | 502 | 3CS  | C10-O27-C11 | 4.53  | 128.40      | 117.62   |
| 2   | E     | 506 | 3CS  | O35-C29-C30 | -4.50 | 112.53      | 121.76   |
| 2   | A     | 503 | 3CS  | O35-C29-C30 | -4.46 | 112.62      | 121.76   |
| 2   | A     | 503 | 3CS  | C28-C36-N17 | 4.44  | 113.06      | 109.16   |
| 2   | E     | 506 | 3CS  | C16-C28-C36 | -4.39 | 104.00      | 107.79   |
| 2   | E     | 506 | 3CS  | O43-C41-C40 | 4.16  | 126.32      | 114.41   |
| 2   | D     | 505 | 3CS  | O43-C41-O42 | -4.07 | 110.83      | 123.86   |
| 2   | B     | 502 | 3CS  | C28-C36-N17 | 4.01  | 112.68      | 109.16   |
| 2   | A     | 503 | 3CS  | C10-O27-C11 | 3.98  | 127.09      | 117.62   |
| 2   | B     | 502 | 3CS  | O43-C41-C40 | 3.91  | 125.64      | 114.41   |
| 2   | C     | 501 | 3CS  | C28-C36-N17 | 3.79  | 112.49      | 109.16   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | C     | 501 | 3CS  | O43-C41-O42 | -3.79 | 111.73      | 123.86   |
| 2   | D     | 505 | 3CS  | O43-C41-C40 | 3.77  | 125.21      | 114.41   |
| 2   | D     | 505 | 3CS  | C30-C29-C28 | 3.64  | 126.12      | 118.87   |
| 2   | D     | 505 | 3CS  | C1-C6-N26   | -3.56 | 117.35      | 122.25   |
| 2   | F     | 504 | 3CS  | C28-C36-N17 | 3.54  | 112.27      | 109.16   |
| 2   | F     | 504 | 3CS  | O43-C41-O42 | -3.51 | 112.63      | 123.86   |
| 2   | E     | 506 | 3CS  | C22-C24-I25 | -3.50 | 114.47      | 119.69   |
| 2   | C     | 501 | 3CS  | O43-C41-C40 | 3.50  | 124.43      | 114.41   |
| 2   | E     | 506 | 3CS  | C39-C40-C38 | -3.49 | 100.24      | 109.19   |
| 2   | C     | 501 | 3CS  | C1-C6-N26   | -3.47 | 117.47      | 122.25   |
| 2   | D     | 505 | 3CS  | C10-O27-C11 | 3.47  | 125.88      | 117.62   |
| 2   | A     | 503 | 3CS  | C1-C6-N26   | -3.43 | 117.53      | 122.25   |
| 2   | F     | 504 | 3CS  | O43-C41-C40 | 3.40  | 124.15      | 114.41   |
| 2   | E     | 506 | 3CS  | C4-C5-C6    | -3.39 | 115.46      | 120.09   |
| 2   | E     | 506 | 3CS  | C5-C6-C1    | 3.32  | 122.36      | 119.04   |
| 2   | A     | 503 | 3CS  | C5-C6-C1    | 3.32  | 122.36      | 119.04   |
| 2   | F     | 504 | 3CS  | C10-O27-C11 | 3.30  | 125.48      | 117.62   |
| 2   | C     | 501 | 3CS  | C5-C6-C1    | 3.26  | 122.30      | 119.04   |
| 2   | D     | 505 | 3CS  | C28-C36-N17 | 3.22  | 111.99      | 109.16   |
| 2   | A     | 503 | 3CS  | O43-C41-O42 | -3.17 | 113.71      | 123.86   |
| 2   | A     | 503 | 3CS  | C22-C24-C21 | 3.05  | 124.67      | 120.64   |
| 2   | E     | 506 | 3CS  | C10-O27-C11 | 3.04  | 124.87      | 117.62   |
| 2   | E     | 506 | 3CS  | C3-C2-C1    | -3.03 | 116.27      | 120.48   |
| 2   | D     | 505 | 3CS  | C5-C6-C1    | 3.02  | 122.06      | 119.04   |
| 2   | A     | 503 | 3CS  | C18-N17-C15 | 3.01  | 129.42      | 124.79   |
| 2   | B     | 502 | 3CS  | C1-C6-N26   | -2.94 | 118.20      | 122.25   |
| 2   | D     | 505 | 3CS  | C34-C33-C30 | 2.94  | 119.28      | 109.70   |
| 2   | B     | 502 | 3CS  | C4-C5-C6    | -2.93 | 116.08      | 120.09   |
| 2   | F     | 504 | 3CS  | C1-C6-N26   | -2.92 | 118.23      | 122.25   |
| 2   | B     | 502 | 3CS  | C3-C2-C1    | -2.90 | 116.45      | 120.48   |
| 2   | A     | 503 | 3CS  | C4-C5-C6    | -2.88 | 116.15      | 120.09   |
| 2   | A     | 503 | 3CS  | C21-C24-I25 | -2.88 | 115.39      | 119.69   |
| 2   | C     | 501 | 3CS  | C30-C29-C28 | 2.86  | 124.56      | 118.87   |
| 2   | D     | 505 | 3CS  | C4-C5-C6    | -2.85 | 116.19      | 120.09   |
| 2   | E     | 506 | 3CS  | C30-C29-C28 | 2.82  | 124.50      | 118.87   |
| 2   | D     | 505 | 3CS  | C38-C40-C41 | -2.81 | 103.04      | 108.98   |
| 2   | C     | 501 | 3CS  | C4-C5-C6    | -2.80 | 116.26      | 120.09   |
| 2   | C     | 501 | 3CS  | C13-C11-C12 | 2.78  | 124.25      | 120.50   |
| 2   | F     | 504 | 3CS  | O27-C10-C9  | 2.78  | 117.25      | 109.56   |
| 2   | D     | 505 | 3CS  | C7-C8-C9    | -2.74 | 116.15      | 119.20   |
| 2   | E     | 506 | 3CS  | C1-C6-N26   | -2.73 | 118.49      | 122.25   |
| 2   | C     | 501 | 3CS  | C18-N17-C15 | 2.72  | 128.97      | 124.79   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | F     | 504 | 3CS  | C34-C33-C30 | 2.71  | 118.53      | 109.70   |
| 2   | F     | 504 | 3CS  | O35-C29-C28 | 2.68  | 124.76      | 120.78   |
| 2   | D     | 505 | 3CS  | C15-C16-C28 | 2.67  | 109.53      | 106.92   |
| 2   | A     | 503 | 3CS  | O43-C41-C40 | 2.67  | 122.06      | 114.41   |
| 2   | C     | 501 | 3CS  | C15-C16-C28 | 2.65  | 109.51      | 106.92   |
| 2   | E     | 506 | 3CS  | C34-C33-C30 | 2.62  | 118.23      | 109.70   |
| 2   | B     | 502 | 3CS  | C34-C33-C30 | 2.61  | 118.21      | 109.70   |
| 2   | B     | 502 | 3CS  | C30-C29-C28 | 2.59  | 124.03      | 118.87   |
| 2   | A     | 503 | 3CS  | C30-C29-C28 | 2.57  | 123.99      | 118.87   |
| 2   | D     | 505 | 3CS  | C18-N17-C15 | 2.50  | 128.63      | 124.79   |
| 2   | A     | 503 | 3CS  | C3-C2-C1    | -2.50 | 117.01      | 120.48   |
| 2   | D     | 505 | 3CS  | C3-C2-C1    | -2.49 | 117.02      | 120.48   |
| 2   | D     | 505 | 3CS  | C9-N26-C6   | 2.49  | 121.86      | 118.06   |
| 2   | F     | 504 | 3CS  | C4-C5-C6    | -2.48 | 116.70      | 120.09   |
| 2   | C     | 501 | 3CS  | C22-C24-C21 | 2.48  | 123.92      | 120.64   |
| 2   | E     | 506 | 3CS  | C7-C1-C2    | -2.46 | 117.39      | 123.01   |
| 2   | C     | 501 | 3CS  | O35-C29-C28 | 2.46  | 124.42      | 120.78   |
| 2   | B     | 502 | 3CS  | C5-C6-C1    | 2.43  | 121.47      | 119.04   |
| 2   | F     | 504 | 3CS  | C39-C40-C38 | -2.41 | 103.01      | 109.19   |
| 2   | C     | 501 | 3CS  | C7-C1-C2    | -2.38 | 117.59      | 123.01   |
| 2   | B     | 502 | 3CS  | C39-C40-C38 | -2.38 | 103.10      | 109.19   |
| 2   | A     | 503 | 3CS  | C38-C40-C37 | 2.37  | 115.28      | 109.41   |
| 2   | B     | 502 | 3CS  | C2-C1-C6    | 2.34  | 121.58      | 118.43   |
| 2   | C     | 501 | 3CS  | C7-C1-C6    | 2.33  | 121.57      | 118.43   |
| 2   | E     | 506 | 3CS  | O27-C10-C9  | 2.31  | 115.93      | 109.56   |
| 2   | F     | 504 | 3CS  | C5-C6-C1    | 2.31  | 121.34      | 119.04   |
| 2   | F     | 504 | 3CS  | C22-C24-I25 | 2.30  | 123.12      | 119.69   |
| 2   | E     | 506 | 3CS  | C21-C24-I25 | 2.26  | 123.07      | 119.69   |
| 2   | A     | 503 | 3CS  | C15-C16-C28 | 2.26  | 109.13      | 106.92   |
| 2   | B     | 502 | 3CS  | O35-C29-C28 | 2.26  | 124.12      | 120.78   |
| 2   | A     | 503 | 3CS  | C34-C33-C30 | 2.23  | 116.99      | 109.70   |
| 2   | B     | 502 | 3CS  | O27-C10-C9  | 2.23  | 115.73      | 109.56   |
| 2   | A     | 503 | 3CS  | C7-C1-C6    | 2.23  | 121.44      | 118.43   |
| 2   | F     | 504 | 3CS  | C3-C2-C1    | -2.22 | 117.40      | 120.48   |
| 2   | F     | 504 | 3CS  | C7-C1-C2    | -2.22 | 117.95      | 123.01   |
| 2   | B     | 502 | 3CS  | C7-C1-C2    | -2.21 | 117.98      | 123.01   |
| 2   | F     | 504 | 3CS  | C30-C29-C28 | 2.20  | 123.24      | 118.87   |
| 2   | A     | 503 | 3CS  | C7-C8-C9    | -2.18 | 116.77      | 119.20   |
| 2   | C     | 501 | 3CS  | C3-C2-C1    | -2.18 | 117.45      | 120.48   |
| 2   | E     | 506 | 3CS  | C2-C1-C6    | 2.18  | 121.36      | 118.43   |
| 2   | E     | 506 | 3CS  | C15-C16-C28 | 2.18  | 109.05      | 106.92   |
| 2   | C     | 501 | 3CS  | C7-C8-C9    | -2.18 | 116.78      | 119.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 502 | 3CS  | C18-N17-C15 | 2.17  | 128.12      | 124.79   |
| 2   | A     | 503 | 3CS  | C20-C21-C24 | -2.16 | 116.78      | 119.55   |
| 2   | A     | 503 | 3CS  | C23-C22-C24 | -2.14 | 116.81      | 119.55   |
| 2   | C     | 501 | 3CS  | C20-C21-C24 | -2.14 | 116.81      | 119.55   |
| 2   | D     | 505 | 3CS  | C39-C40-C38 | -2.10 | 103.80      | 109.19   |
| 2   | E     | 506 | 3CS  | C7-C1-C6    | 2.09  | 121.24      | 118.43   |
| 2   | A     | 503 | 3CS  | C7-C1-C2    | -2.08 | 118.28      | 123.01   |

There are no chirality outliers.

All (89) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 503 | 3CS  | C36-C37-C40-C38 |
| 2   | A     | 503 | 3CS  | C36-C37-C40-C39 |
| 2   | A     | 503 | 3CS  | C36-C37-C40-C41 |
| 2   | B     | 502 | 3CS  | C16-C28-C29-C30 |
| 2   | B     | 502 | 3CS  | C36-C28-C29-C30 |
| 2   | B     | 502 | 3CS  | C36-C37-C40-C38 |
| 2   | B     | 502 | 3CS  | C36-C37-C40-C39 |
| 2   | B     | 502 | 3CS  | C36-C37-C40-C41 |
| 2   | C     | 501 | 3CS  | C16-C28-C29-C30 |
| 2   | C     | 501 | 3CS  | C36-C28-C29-C30 |
| 2   | C     | 501 | 3CS  | C36-C28-C29-O35 |
| 2   | D     | 505 | 3CS  | C28-C29-C30-C33 |
| 2   | D     | 505 | 3CS  | C16-C28-C29-C30 |
| 2   | D     | 505 | 3CS  | C36-C28-C29-O35 |
| 2   | E     | 506 | 3CS  | C29-C30-C33-C31 |
| 2   | E     | 506 | 3CS  | C29-C30-C33-C32 |
| 2   | E     | 506 | 3CS  | C29-C30-C33-C34 |
| 2   | E     | 506 | 3CS  | C28-C29-C30-C33 |
| 2   | E     | 506 | 3CS  | C16-C28-C29-C30 |
| 2   | E     | 506 | 3CS  | C36-C28-C29-C30 |
| 2   | E     | 506 | 3CS  | C36-C28-C29-O35 |
| 2   | F     | 504 | 3CS  | C28-C29-C30-C33 |
| 2   | F     | 504 | 3CS  | C36-C37-C40-C39 |
| 2   | C     | 501 | 3CS  | C12-C11-O27-C10 |
| 2   | C     | 501 | 3CS  | C13-C11-O27-C10 |
| 2   | F     | 504 | 3CS  | C12-C11-O27-C10 |
| 2   | F     | 504 | 3CS  | C13-C11-O27-C10 |
| 2   | E     | 506 | 3CS  | C12-C11-O27-C10 |
| 2   | E     | 506 | 3CS  | C13-C11-O27-C10 |
| 2   | E     | 506 | 3CS  | C16-C28-C29-O35 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | C     | 501 | 3CS  | C29-C30-C33-C31 |
| 2   | C     | 501 | 3CS  | C29-C30-C33-C32 |
| 2   | F     | 504 | 3CS  | C19-C18-N17-C15 |
| 2   | E     | 506 | 3CS  | C19-C18-N17-C15 |
| 2   | B     | 502 | 3CS  | C16-C28-C29-O35 |
| 2   | D     | 505 | 3CS  | C12-C11-O27-C10 |
| 2   | D     | 505 | 3CS  | C13-C11-O27-C10 |
| 2   | F     | 504 | 3CS  | C36-C37-C40-C38 |
| 2   | A     | 503 | 3CS  | C12-C11-O27-C10 |
| 2   | B     | 502 | 3CS  | C38-C40-C41-O43 |
| 2   | C     | 501 | 3CS  | C39-C40-C41-O42 |
| 2   | E     | 506 | 3CS  | C39-C40-C41-O43 |
| 2   | A     | 503 | 3CS  | C13-C11-O27-C10 |
| 2   | A     | 503 | 3CS  | C16-C28-C29-O35 |
| 2   | F     | 504 | 3CS  | C16-C28-C29-O35 |
| 2   | A     | 503 | 3CS  | C36-C28-C29-C30 |
| 2   | D     | 505 | 3CS  | C36-C28-C29-C30 |
| 2   | F     | 504 | 3CS  | C36-C28-C29-C30 |
| 2   | F     | 504 | 3CS  | C36-C37-C40-C41 |
| 2   | C     | 501 | 3CS  | C19-C18-N17-C15 |
| 2   | B     | 502 | 3CS  | C19-C18-N17-C15 |
| 2   | A     | 503 | 3CS  | C36-C28-C29-O35 |
| 2   | B     | 502 | 3CS  | C36-C28-C29-O35 |
| 2   | B     | 502 | 3CS  | C37-C40-C41-O43 |
| 2   | D     | 505 | 3CS  | C37-C40-C41-O42 |
| 2   | B     | 502 | 3CS  | C38-C40-C41-O42 |
| 2   | C     | 501 | 3CS  | C39-C40-C41-O43 |
| 2   | D     | 505 | 3CS  | C38-C40-C41-O43 |
| 2   | D     | 505 | 3CS  | C39-C40-C41-O42 |
| 2   | E     | 506 | 3CS  | C39-C40-C41-O42 |
| 2   | A     | 503 | 3CS  | C19-C18-N17-C15 |
| 2   | D     | 505 | 3CS  | O35-C29-C30-C33 |
| 2   | E     | 506 | 3CS  | O35-C29-C30-C33 |
| 2   | F     | 504 | 3CS  | O35-C29-C30-C33 |
| 2   | C     | 501 | 3CS  | C29-C30-C33-C34 |
| 2   | C     | 501 | 3CS  | C19-C18-N17-C36 |
| 2   | F     | 504 | 3CS  | C19-C18-N17-C36 |
| 2   | B     | 502 | 3CS  | C39-C40-C41-O43 |
| 2   | D     | 505 | 3CS  | C19-C18-N17-C15 |
| 2   | A     | 503 | 3CS  | C19-C18-N17-C36 |
| 2   | B     | 502 | 3CS  | C19-C18-N17-C36 |
| 2   | D     | 505 | 3CS  | C19-C18-N17-C36 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | E     | 506 | 3CS  | C19-C18-N17-C36 |
| 2   | A     | 503 | 3CS  | C39-C40-C41-O42 |
| 2   | D     | 505 | 3CS  | C38-C40-C41-O42 |
| 2   | E     | 506 | 3CS  | C38-C40-C41-O43 |
| 2   | D     | 505 | 3CS  | O27-C10-C9-N26  |
| 2   | E     | 506 | 3CS  | C37-C40-C41-O43 |
| 2   | F     | 504 | 3CS  | C36-C28-C29-O35 |
| 2   | A     | 503 | 3CS  | O27-C10-C9-N26  |
| 2   | B     | 502 | 3CS  | O27-C10-C9-N26  |
| 2   | A     | 503 | 3CS  | C16-C28-C29-C30 |
| 2   | F     | 504 | 3CS  | C16-C28-C29-C30 |
| 2   | D     | 505 | 3CS  | O27-C10-C9-C8   |
| 2   | B     | 502 | 3CS  | O27-C10-C9-C8   |
| 2   | A     | 503 | 3CS  | C38-C40-C41-O43 |
| 2   | A     | 503 | 3CS  | C39-C40-C41-O43 |
| 2   | D     | 505 | 3CS  | C39-C40-C41-O43 |
| 2   | A     | 503 | 3CS  | O27-C10-C9-C8   |

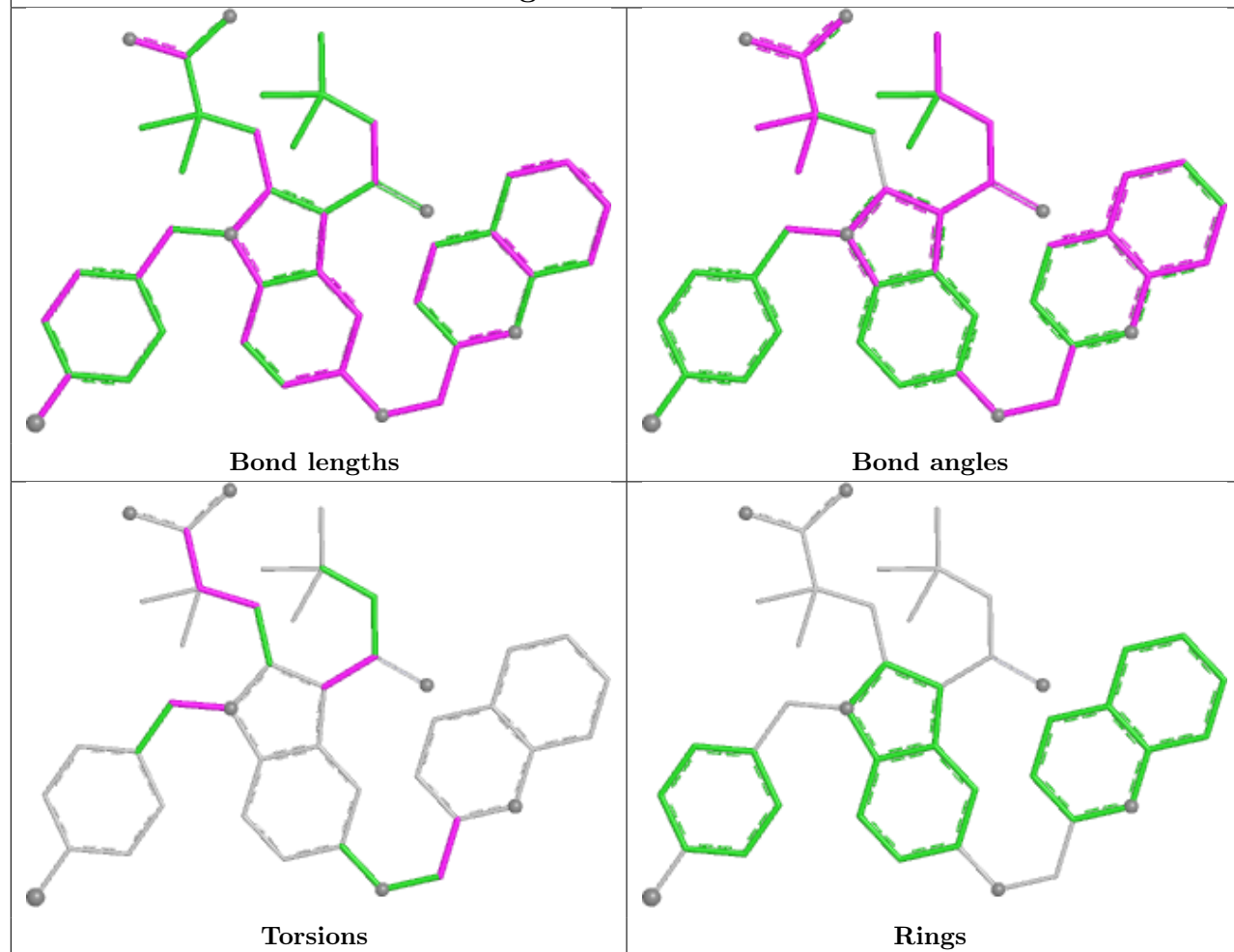
There are no ring outliers.

6 monomers are involved in 141 short contacts:

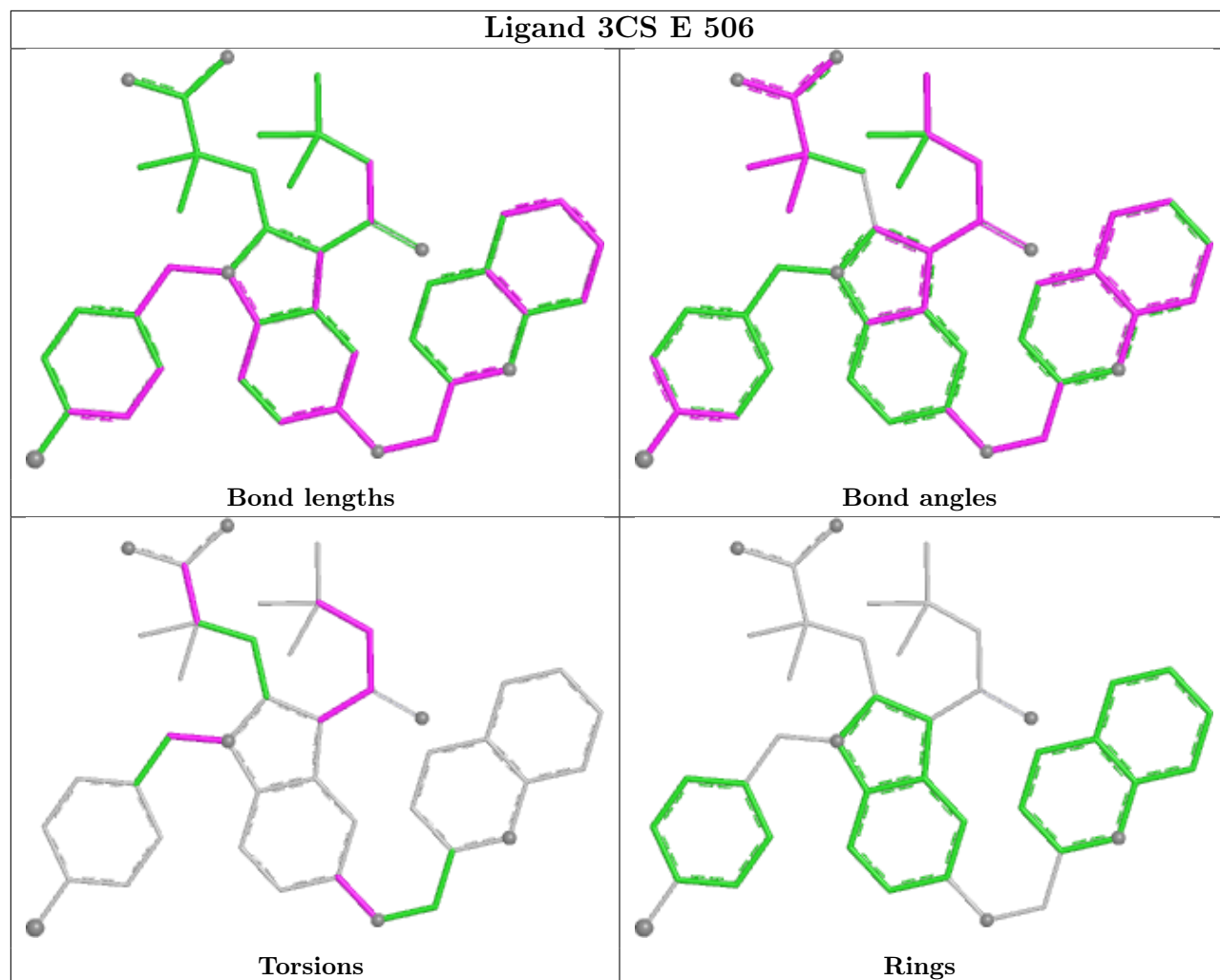
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | B     | 502 | 3CS  | 19      | 0            |
| 2   | E     | 506 | 3CS  | 23      | 0            |
| 2   | A     | 503 | 3CS  | 29      | 0            |
| 2   | D     | 505 | 3CS  | 28      | 0            |
| 2   | C     | 501 | 3CS  | 21      | 0            |
| 2   | F     | 504 | 3CS  | 21      | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

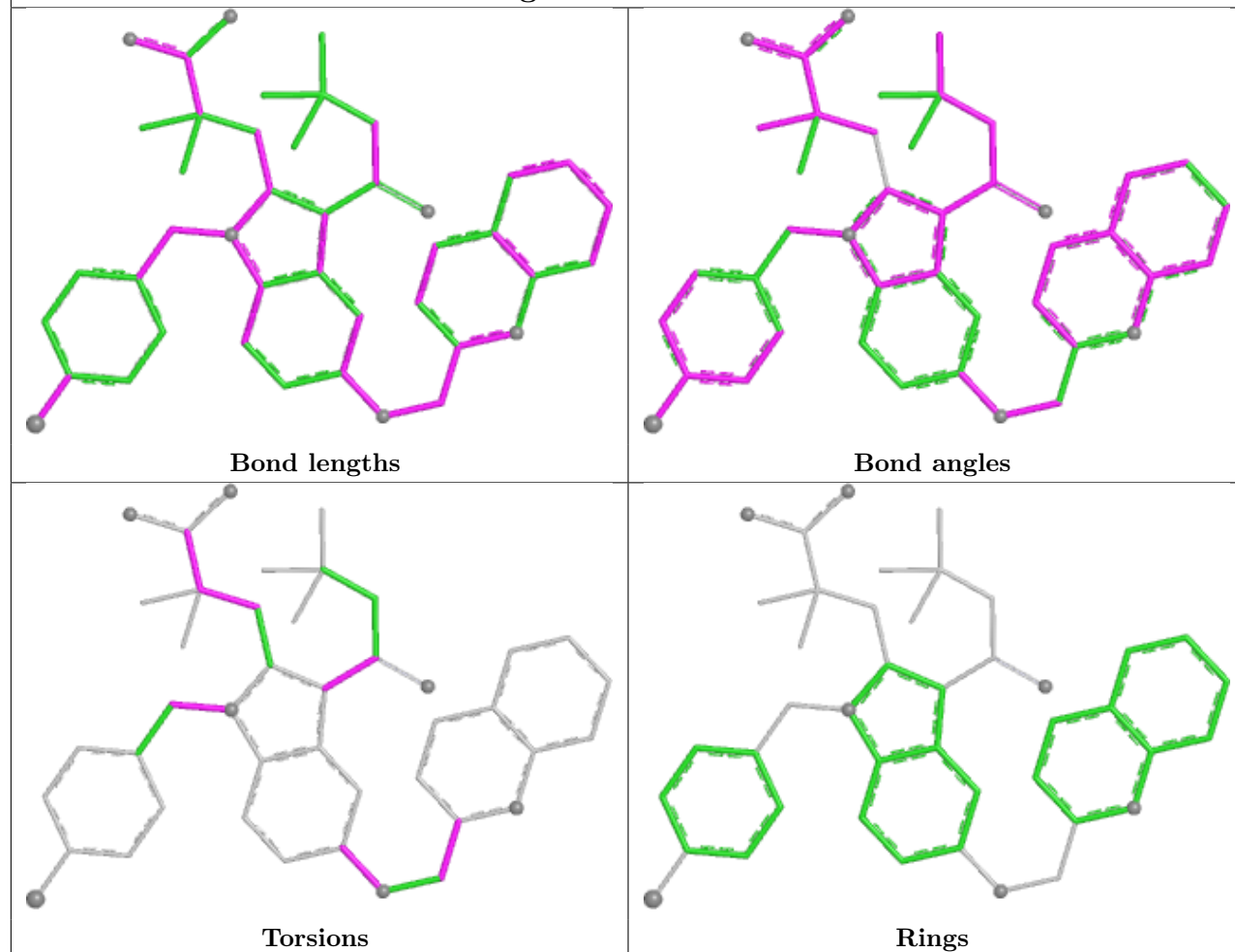
## Ligand 3CS B 502



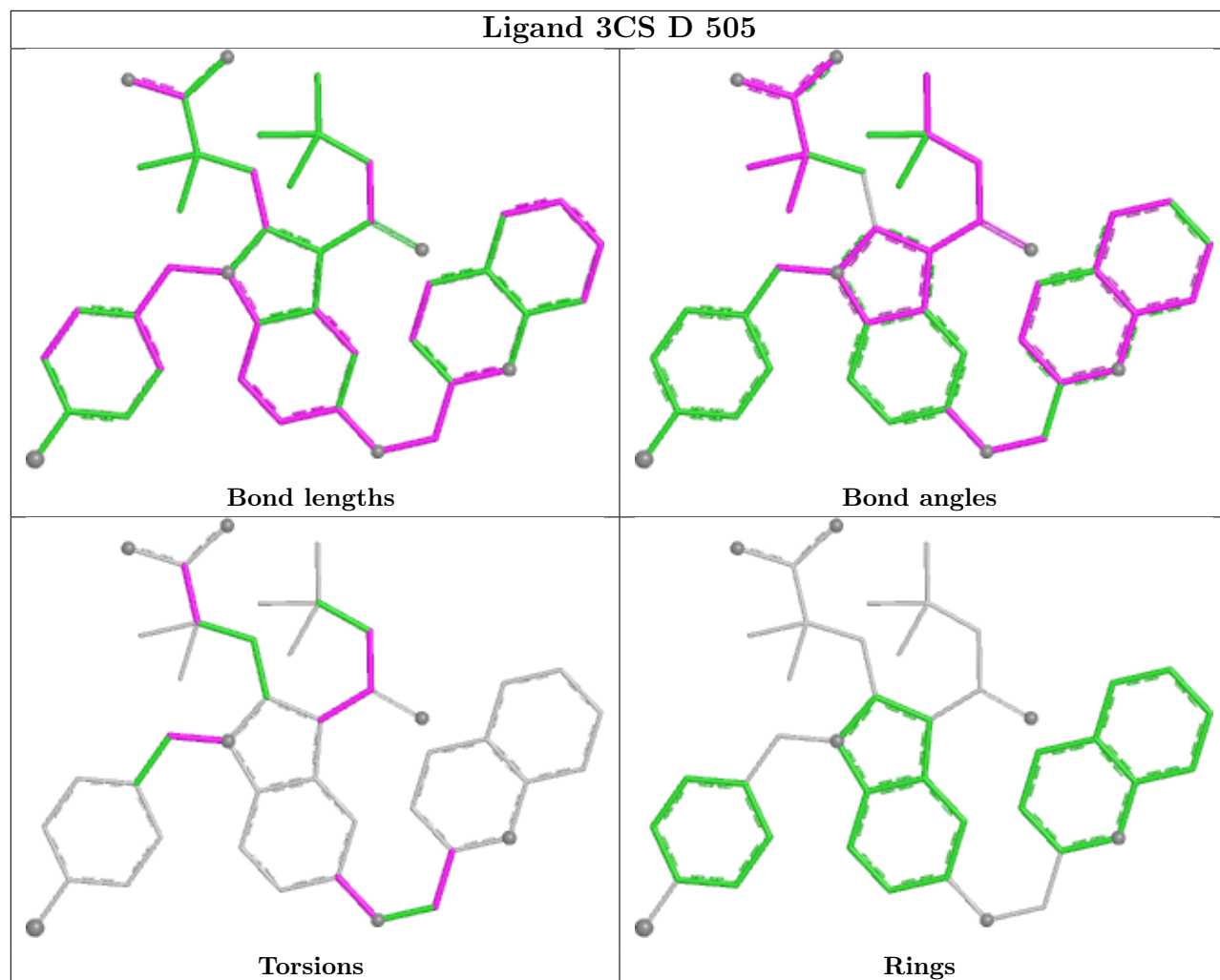
## Ligand 3CS E 506



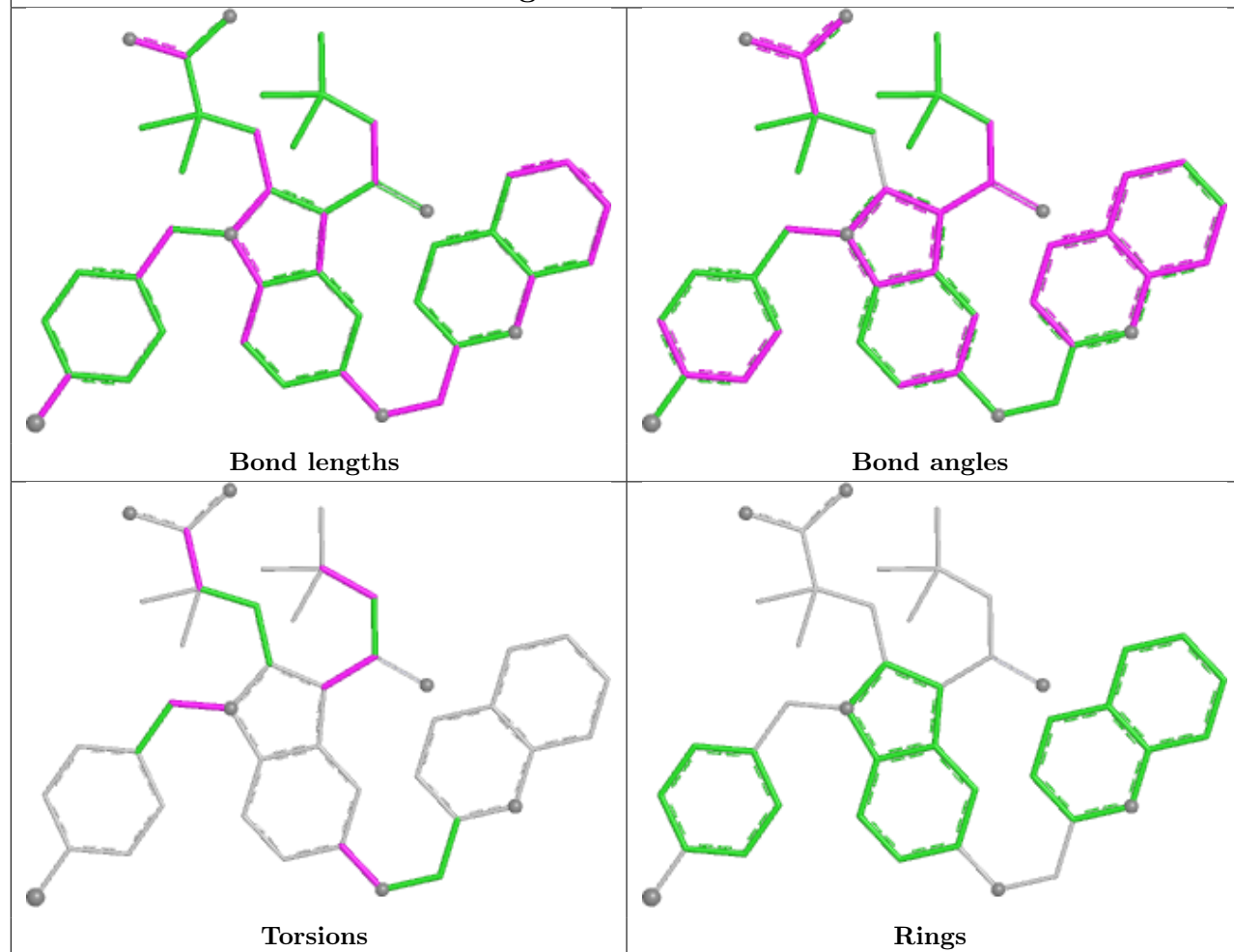
## Ligand 3CS A 503

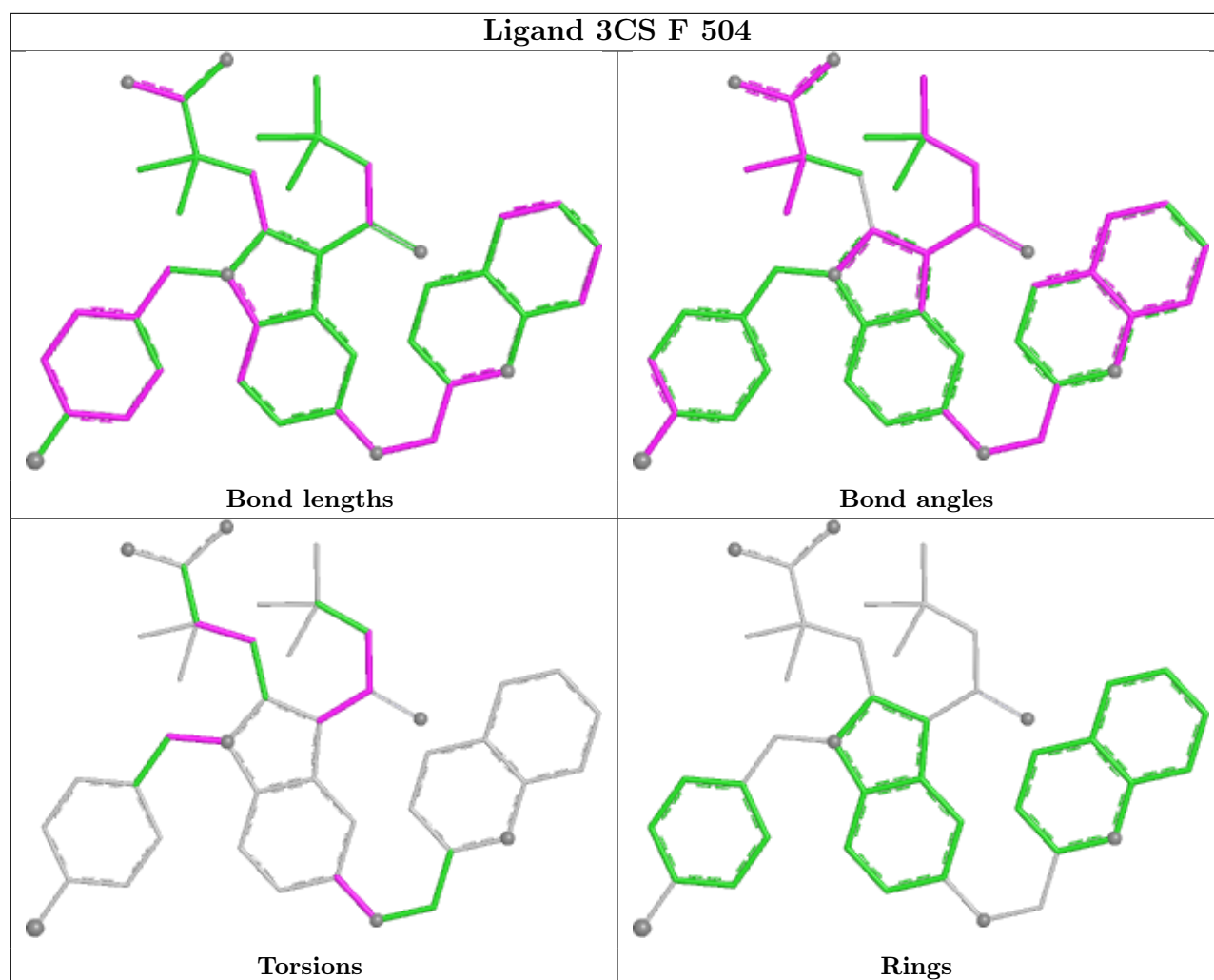


## Ligand 3CS D 505



## Ligand 3CS C 501





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|----------------|-----------------------|-------|
| 1   | A     | 137/161 (85%) | 0.41   | 6 (4%) 39 31   | 78, 114, 163, 182     | 0     |
| 1   | B     | 145/161 (90%) | 0.32   | 6 (4%) 41 32   | 75, 112, 162, 171     | 0     |
| 1   | C     | 146/161 (90%) | 0.38   | 11 (7%) 20 20  | 67, 105, 158, 173     | 0     |
| 1   | D     | 145/161 (90%) | 0.23   | 4 (2%) 55 40   | 74, 114, 163, 170     | 0     |
| 1   | E     | 137/161 (85%) | 0.40   | 8 (5%) 29 25   | 83, 117, 170, 188     | 0     |
| 1   | F     | 146/161 (90%) | 0.60   | 16 (10%) 10 13 | 80, 117, 172, 205     | 0     |
| All | All   | 856/966 (88%) | 0.39   | 51 (5%) 27 24  | 67, 114, 165, 205     | 0     |

All (51) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 112 | TYR  | 7.0  |
| 1   | F     | 44  | ARG  | 6.1  |
| 1   | E     | 107 | GLN  | 4.8  |
| 1   | F     | 43  | GLN  | 4.8  |
| 1   | D     | 45  | THR  | 4.1  |
| 1   | E     | 108 | SER  | 4.1  |
| 1   | F     | 37  | GLN  | 3.9  |
| 1   | A     | 39  | GLY  | 3.7  |
| 1   | E     | 42  | PHE  | 3.6  |
| 1   | F     | 29  | LYS  | 3.4  |
| 1   | B     | 140 | GLY  | 3.2  |
| 1   | D     | 112 | TYR  | 3.2  |
| 1   | A     | 42  | PHE  | 3.1  |
| 1   | F     | 48  | LEU  | 2.9  |
| 1   | A     | 36  | THR  | 2.9  |
| 1   | C     | 48  | LEU  | 2.9  |
| 1   | E     | 110 | PRO  | 2.9  |
| 1   | B     | 27  | ALA  | 2.8  |
| 1   | F     | 110 | PRO  | 2.8  |

*Continued on next page...*

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 43  | GLN  | 2.7  |
| 1   | F     | 109 | THR  | 2.7  |
| 1   | E     | 106 | THR  | 2.7  |
| 1   | B     | 43  | GLN  | 2.7  |
| 1   | C     | 44  | ARG  | 2.6  |
| 1   | E     | 34  | SER  | 2.6  |
| 1   | F     | 57  | ASN  | 2.6  |
| 1   | C     | 143 | PHE  | 2.6  |
| 1   | F     | 80  | GLN  | 2.6  |
| 1   | A     | 38  | ASN  | 2.6  |
| 1   | A     | 112 | TYR  | 2.6  |
| 1   | F     | 115 | GLY  | 2.5  |
| 1   | F     | 45  | THR  | 2.4  |
| 1   | C     | 35  | ARG  | 2.4  |
| 1   | F     | 47  | THR  | 2.4  |
| 1   | B     | 143 | PHE  | 2.3  |
| 1   | D     | 46  | GLY  | 2.3  |
| 1   | E     | 44  | ARG  | 2.3  |
| 1   | A     | 5   | THR  | 2.3  |
| 1   | C     | 52  | ARG  | 2.2  |
| 1   | C     | 80  | GLN  | 2.2  |
| 1   | C     | 45  | THR  | 2.2  |
| 1   | D     | 148 | ALA  | 2.1  |
| 1   | F     | 36  | THR  | 2.1  |
| 1   | C     | 47  | THR  | 2.1  |
| 1   | F     | 54  | TYR  | 2.1  |
| 1   | F     | 146 | TYR  | 2.1  |
| 1   | B     | 147 | ILE  | 2.1  |
| 1   | E     | 43  | GLN  | 2.1  |
| 1   | C     | 114 | PHE  | 2.1  |
| 1   | B     | 44  | ARG  | 2.0  |
| 1   | F     | 40  | ARG  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands

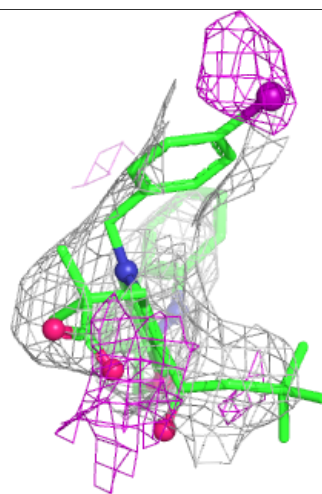
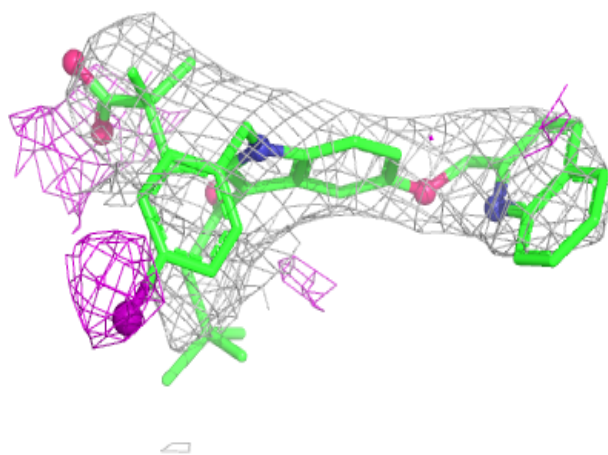
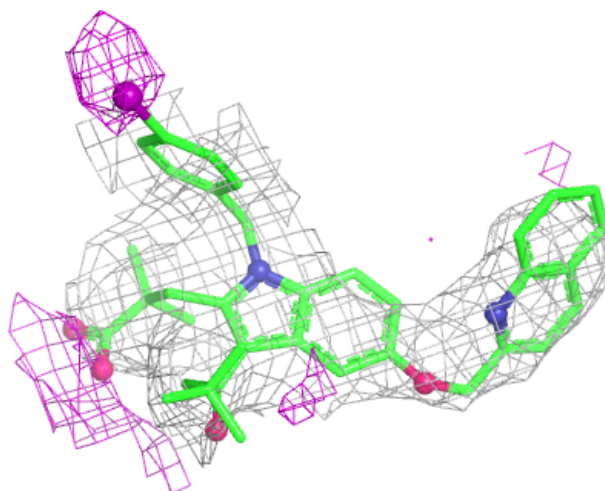
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | 3CS  | A     | 503 | 43/43 | 0.91 | 0.21 | 159,159,159,159            | 0     |
| 2   | 3CS  | D     | 505 | 43/43 | 0.92 | 0.20 | 159,159,159,159            | 0     |
| 2   | 3CS  | C     | 501 | 43/43 | 0.93 | 0.17 | 155,155,155,155            | 0     |
| 2   | 3CS  | B     | 502 | 43/43 | 0.93 | 0.20 | 152,152,152,152            | 0     |
| 2   | 3CS  | F     | 504 | 43/43 | 0.93 | 0.18 | 155,155,155,155            | 0     |
| 2   | 3CS  | E     | 506 | 43/43 | 0.94 | 0.18 | 160,160,160,160            | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

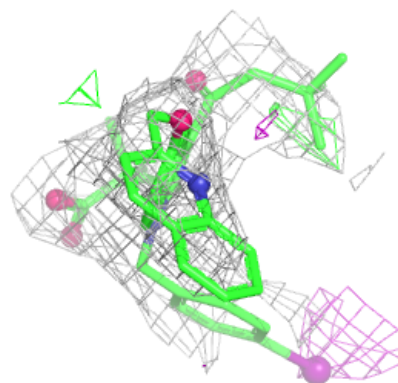
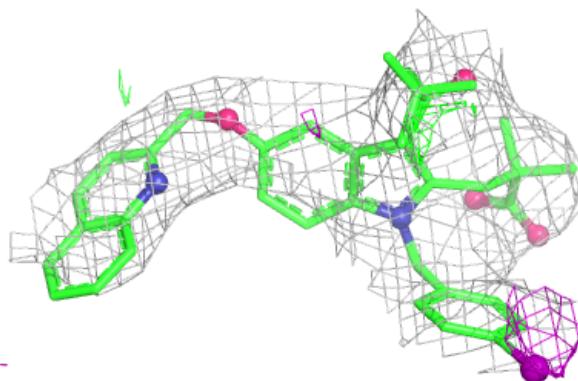
**Electron density around 3CS A 503:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



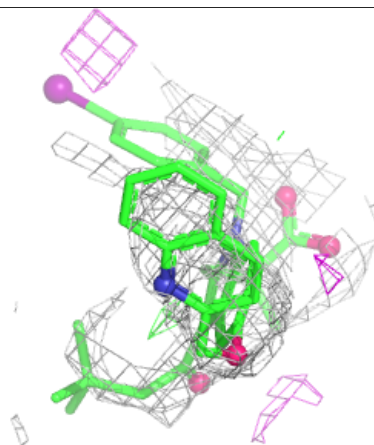
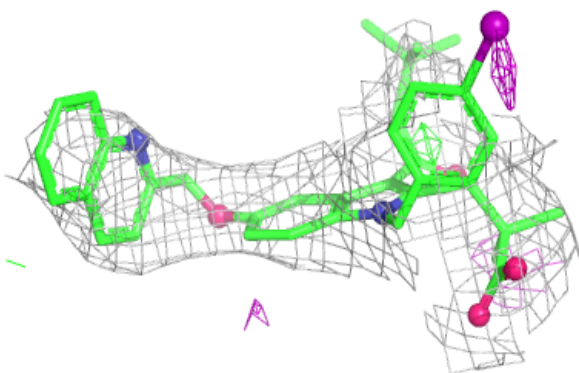
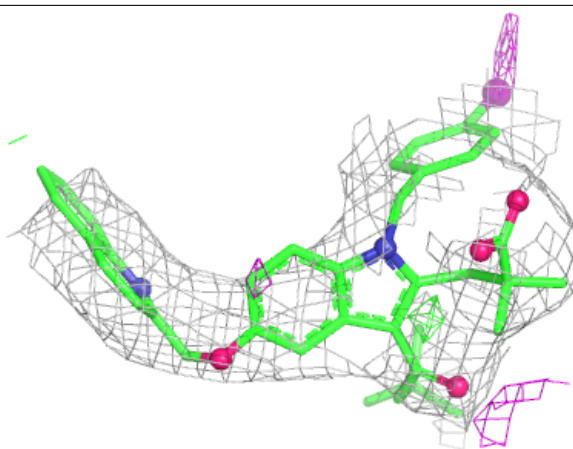
**Electron density around 3CS D 505:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



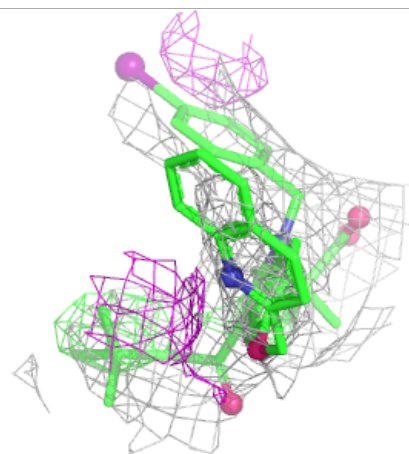
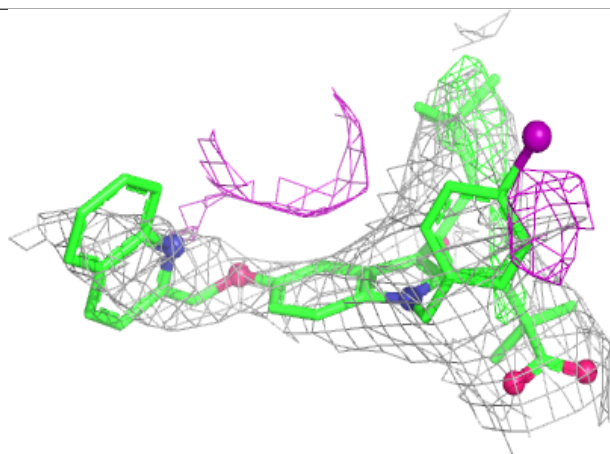
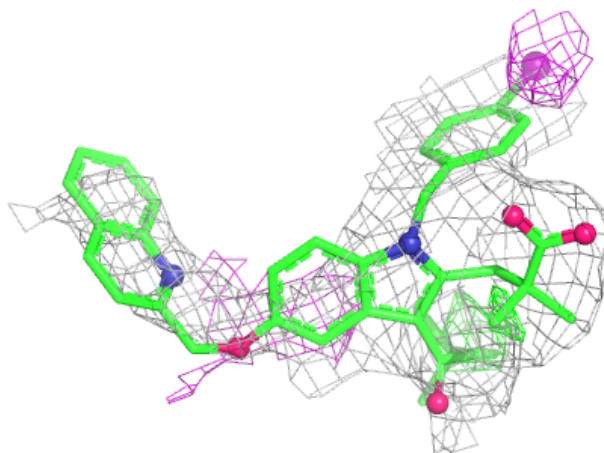
**Electron density around 3CS C 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



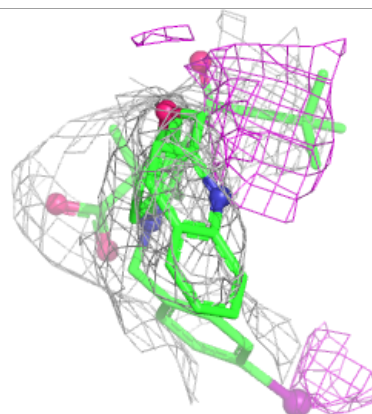
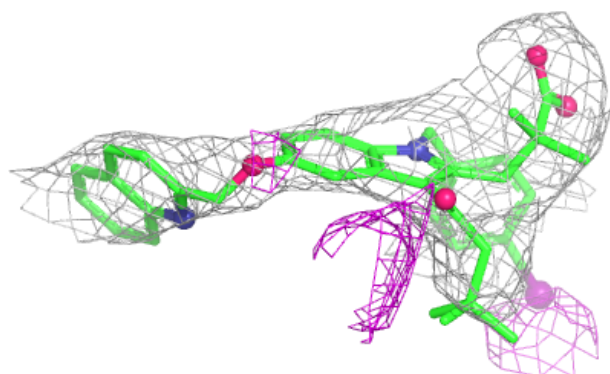
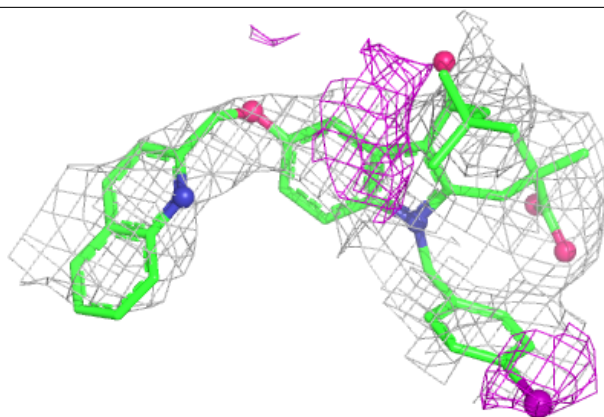
**Electron density around 3CS B 502:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

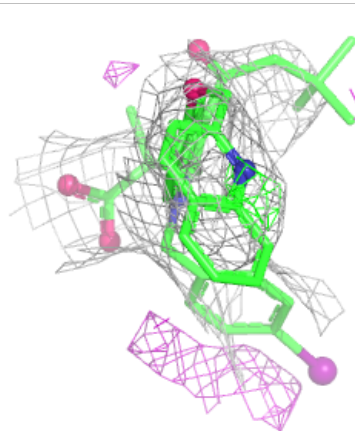
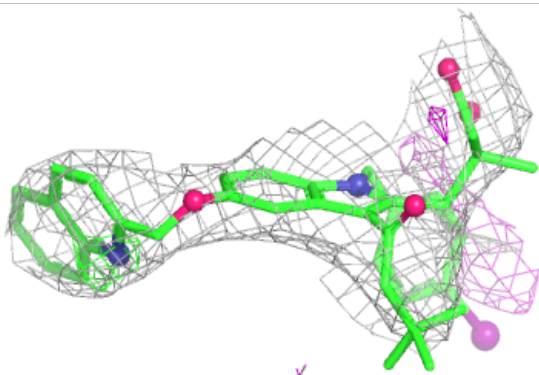
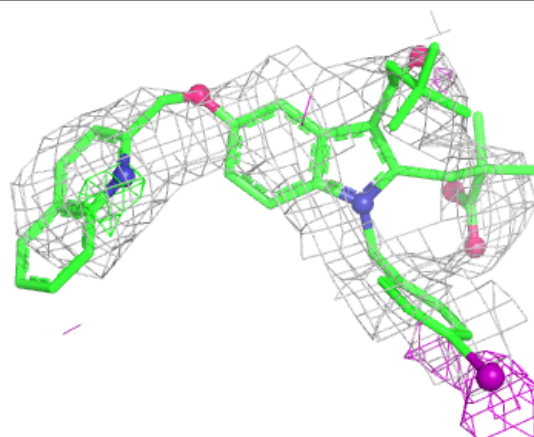


**Electron density around 3CS F 504:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 3CS E 506:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.