



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:17 PM UTC

PDB ID : 3MV3 / pdb\_00003mv3  
Title : Crystal Structure of  $\alpha$ -COP in Complex with e-COP  
Authors : Hoelz, A.; Hsia, K.C.  
Deposited on : 2010-05-03  
Resolution : 3.25 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:

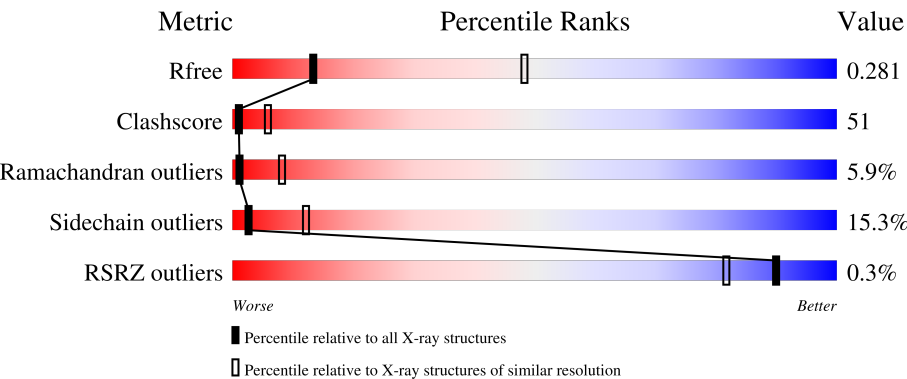
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| 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 i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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                      | 1605 (3.30-3.22)                                      |
| Clashscore            | 190562                      | 1660 (3.30-3.22)                                      |
| Ramachandran outliers | 187476                      | 1630 (3.30-3.22)                                      |
| Sidechain outliers    | 187428                      | 1629 (3.30-3.22)                                      |
| RSRZ outliers         | 180081                      | 1605 (3.30-3.22)                                      |

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     | 325    | <div><div></div><div>28%52%12%• 7%</div></div>   |
| 1   | C     | 325    | <div><div></div><div>30%50%11%• 7%</div></div>   |
| 1   | E     | 325    | <div><div>2%</div><div>29%51%11%• 7%</div></div> |
| 2   | B     | 310    | <div><div></div><div>30%46%17%• 5%</div></div>   |
| 2   | D     | 310    | <div><div></div><div>30%46%16%• 5%</div></div>   |

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| Mol | Chain | Length | Quality of chain                                                                |
|-----|-------|--------|---------------------------------------------------------------------------------|
| 2   | F     | 310    | <div><div></div><div>31%</div><div>46%</div><div>15%</div><div>• 5%</div></div> |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14256 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 Coatomer subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
| 1   | A     | 303      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 2388  | 1531 | 399 | 447 | 4 | 7  |         |         |       |
| 1   | C     | 303      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 2388  | 1531 | 399 | 447 | 4 | 7  |         |         |       |
| 1   | E     | 303      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 2388  | 1531 | 399 | 447 | 4 | 7  |         |         |       |

There are 69 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -22     | MSE      | -      | expression tag | UNP P53622 |
| A     | -21     | GLY      | -      | expression tag | UNP P53622 |
| A     | -20     | SER      | -      | expression tag | UNP P53622 |
| A     | -19     | SER      | -      | expression tag | UNP P53622 |
| A     | -18     | HIS      | -      | expression tag | UNP P53622 |
| A     | -17     | HIS      | -      | expression tag | UNP P53622 |
| A     | -16     | HIS      | -      | expression tag | UNP P53622 |
| A     | -15     | HIS      | -      | expression tag | UNP P53622 |
| A     | -14     | HIS      | -      | expression tag | UNP P53622 |
| A     | -13     | HIS      | -      | expression tag | UNP P53622 |
| A     | -12     | SER      | -      | expression tag | UNP P53622 |
| A     | -11     | SER      | -      | expression tag | UNP P53622 |
| A     | -10     | GLY      | -      | expression tag | UNP P53622 |
| A     | -9      | LEU      | -      | expression tag | UNP P53622 |
| A     | -8      | GLU      | -      | expression tag | UNP P53622 |
| A     | -7      | VAL      | -      | expression tag | UNP P53622 |
| A     | -6      | LEU      | -      | expression tag | UNP P53622 |
| A     | -5      | PHE      | -      | expression tag | UNP P53622 |
| A     | -4      | GLN      | -      | expression tag | UNP P53622 |
| A     | -3      | GLY      | -      | expression tag | UNP P53622 |
| A     | -2      | PRO      | -      | expression tag | UNP P53622 |
| A     | -1      | HIS      | -      | expression tag | UNP P53622 |
| A     | 0       | MSE      | -      | expression tag | UNP P53622 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | -22     | MSE      | -      | expression tag | UNP P53622 |
| C     | -21     | GLY      | -      | expression tag | UNP P53622 |
| C     | -20     | SER      | -      | expression tag | UNP P53622 |
| C     | -19     | SER      | -      | expression tag | UNP P53622 |
| C     | -18     | HIS      | -      | expression tag | UNP P53622 |
| C     | -17     | HIS      | -      | expression tag | UNP P53622 |
| C     | -16     | HIS      | -      | expression tag | UNP P53622 |
| C     | -15     | HIS      | -      | expression tag | UNP P53622 |
| C     | -14     | HIS      | -      | expression tag | UNP P53622 |
| C     | -13     | HIS      | -      | expression tag | UNP P53622 |
| C     | -12     | SER      | -      | expression tag | UNP P53622 |
| C     | -11     | SER      | -      | expression tag | UNP P53622 |
| C     | -10     | GLY      | -      | expression tag | UNP P53622 |
| C     | -9      | LEU      | -      | expression tag | UNP P53622 |
| C     | -8      | GLU      | -      | expression tag | UNP P53622 |
| C     | -7      | VAL      | -      | expression tag | UNP P53622 |
| C     | -6      | LEU      | -      | expression tag | UNP P53622 |
| C     | -5      | PHE      | -      | expression tag | UNP P53622 |
| C     | -4      | GLN      | -      | expression tag | UNP P53622 |
| C     | -3      | GLY      | -      | expression tag | UNP P53622 |
| C     | -2      | PRO      | -      | expression tag | UNP P53622 |
| C     | -1      | HIS      | -      | expression tag | UNP P53622 |
| C     | 0       | MSE      | -      | expression tag | UNP P53622 |
| E     | -22     | MSE      | -      | expression tag | UNP P53622 |
| E     | -21     | GLY      | -      | expression tag | UNP P53622 |
| E     | -20     | SER      | -      | expression tag | UNP P53622 |
| E     | -19     | SER      | -      | expression tag | UNP P53622 |
| E     | -18     | HIS      | -      | expression tag | UNP P53622 |
| E     | -17     | HIS      | -      | expression tag | UNP P53622 |
| E     | -16     | HIS      | -      | expression tag | UNP P53622 |
| E     | -15     | HIS      | -      | expression tag | UNP P53622 |
| E     | -14     | HIS      | -      | expression tag | UNP P53622 |
| E     | -13     | HIS      | -      | expression tag | UNP P53622 |
| E     | -12     | SER      | -      | expression tag | UNP P53622 |
| E     | -11     | SER      | -      | expression tag | UNP P53622 |
| E     | -10     | GLY      | -      | expression tag | UNP P53622 |
| E     | -9      | LEU      | -      | expression tag | UNP P53622 |
| E     | -8      | GLU      | -      | expression tag | UNP P53622 |
| E     | -7      | VAL      | -      | expression tag | UNP P53622 |
| E     | -6      | LEU      | -      | expression tag | UNP P53622 |
| E     | -5      | PHE      | -      | expression tag | UNP P53622 |
| E     | -4      | GLN      | -      | expression tag | UNP P53622 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| E     | -3      | GLY      | -      | expression tag | UNP P53622 |
| E     | -2      | PRO      | -      | expression tag | UNP P53622 |
| E     | -1      | HIS      | -      | expression tag | UNP P53622 |
| E     | 0       | MSE      | -      | expression tag | UNP P53622 |

- Molecule 2 is a protein called Coatomer subunit epsilon.

| Mol | Chain | Residues | Atoms |      |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
| 2   | B     | 293      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 2364  | 1508 | 371 | 480 | 2 | 3  |         |         |       |
| 2   | D     | 293      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 2364  | 1508 | 371 | 480 | 2 | 3  |         |         |       |
| 2   | F     | 293      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 2364  | 1508 | 371 | 480 | 2 | 3  |         |         |       |

There are 42 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | -13     | MSE      | -      | expression tag | UNP P40509 |
| B     | -12     | GLY      | -      | expression tag | UNP P40509 |
| B     | -11     | SER      | -      | expression tag | UNP P40509 |
| B     | -10     | SER      | -      | expression tag | UNP P40509 |
| B     | -9      | HIS      | -      | expression tag | UNP P40509 |
| B     | -8      | HIS      | -      | expression tag | UNP P40509 |
| B     | -7      | HIS      | -      | expression tag | UNP P40509 |
| B     | -6      | HIS      | -      | expression tag | UNP P40509 |
| B     | -5      | HIS      | -      | expression tag | UNP P40509 |
| B     | -4      | HIS      | -      | expression tag | UNP P40509 |
| B     | -3      | SER      | -      | expression tag | UNP P40509 |
| B     | -2      | GLN      | -      | expression tag | UNP P40509 |
| B     | -1      | ASP      | -      | expression tag | UNP P40509 |
| B     | 0       | PRO      | -      | expression tag | UNP P40509 |
| D     | -13     | MSE      | -      | expression tag | UNP P40509 |
| D     | -12     | GLY      | -      | expression tag | UNP P40509 |
| D     | -11     | SER      | -      | expression tag | UNP P40509 |
| D     | -10     | SER      | -      | expression tag | UNP P40509 |
| D     | -9      | HIS      | -      | expression tag | UNP P40509 |
| D     | -8      | HIS      | -      | expression tag | UNP P40509 |
| D     | -7      | HIS      | -      | expression tag | UNP P40509 |
| D     | -6      | HIS      | -      | expression tag | UNP P40509 |
| D     | -5      | HIS      | -      | expression tag | UNP P40509 |
| D     | -4      | HIS      | -      | expression tag | UNP P40509 |

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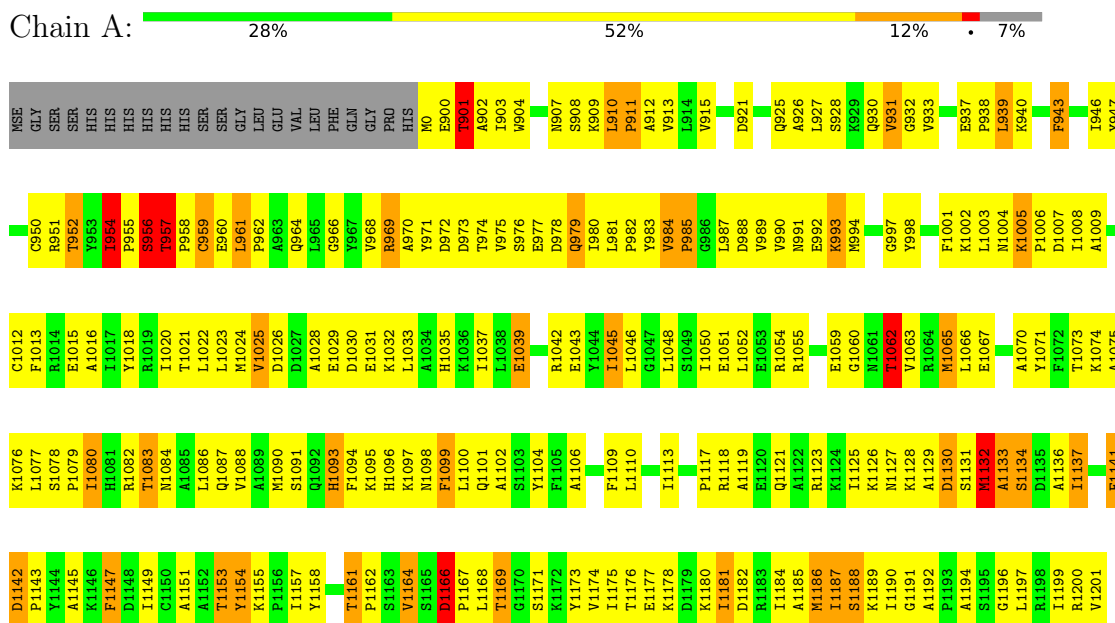
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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | -3      | SER      | -      | expression tag | UNP P40509 |
| D     | -2      | GLN      | -      | expression tag | UNP P40509 |
| D     | -1      | ASP      | -      | expression tag | UNP P40509 |
| D     | 0       | PRO      | -      | expression tag | UNP P40509 |
| F     | -13     | MSE      | -      | expression tag | UNP P40509 |
| F     | -12     | GLY      | -      | expression tag | UNP P40509 |
| F     | -11     | SER      | -      | expression tag | UNP P40509 |
| F     | -10     | SER      | -      | expression tag | UNP P40509 |
| F     | -9      | HIS      | -      | expression tag | UNP P40509 |
| F     | -8      | HIS      | -      | expression tag | UNP P40509 |
| F     | -7      | HIS      | -      | expression tag | UNP P40509 |
| F     | -6      | HIS      | -      | expression tag | UNP P40509 |
| F     | -5      | HIS      | -      | expression tag | UNP P40509 |
| F     | -4      | HIS      | -      | expression tag | UNP P40509 |
| F     | -3      | SER      | -      | expression tag | UNP P40509 |
| F     | -2      | GLN      | -      | expression tag | UNP P40509 |
| F     | -1      | ASP      | -      | expression tag | UNP P40509 |
| F     | 0       | PRO      | -      | expression tag | UNP P40509 |

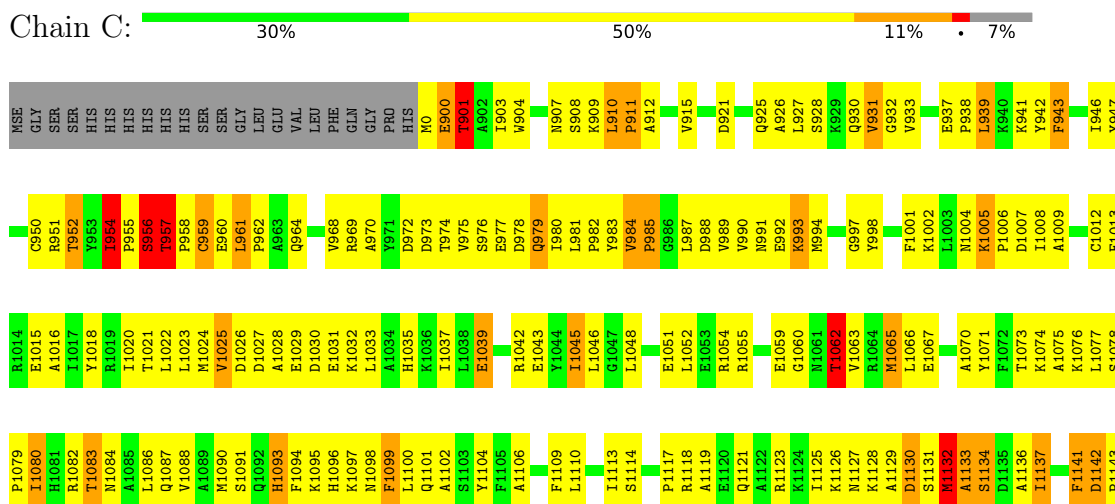
### 3 Residue-property plots

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: Coatomer subunit alpha



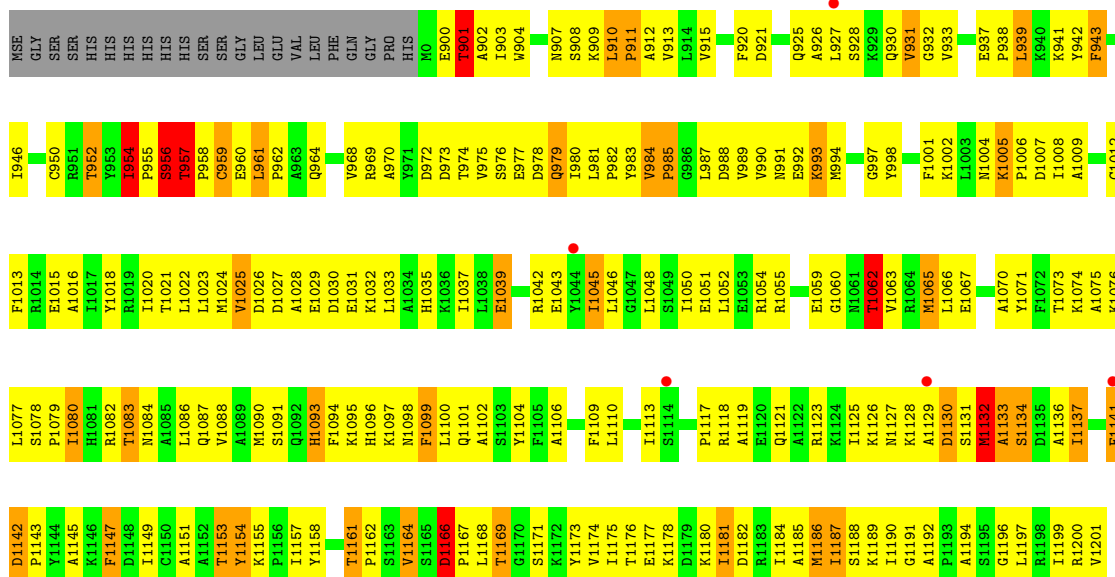
#### • Molecule 1: Coatomer subunit alpha



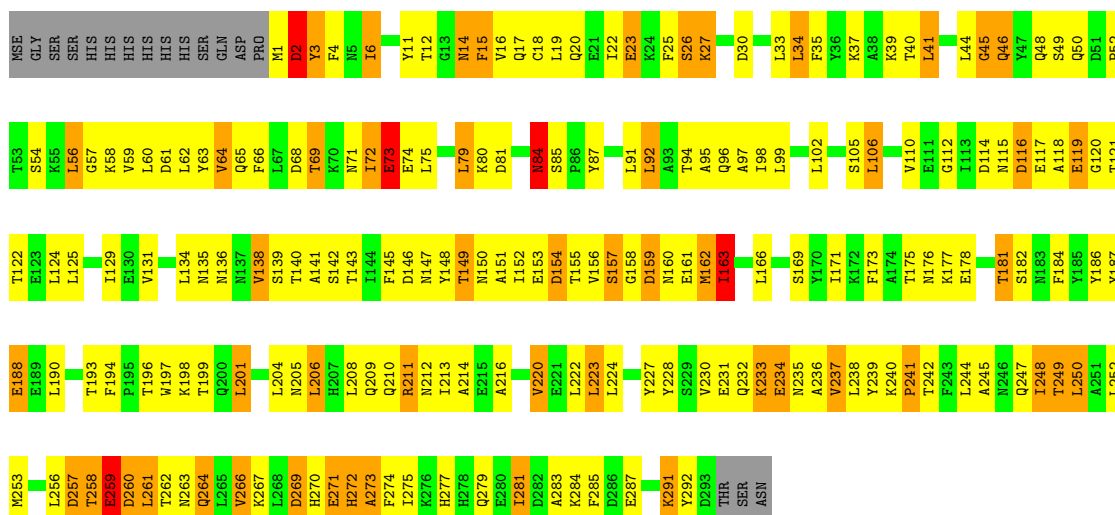




• Molecule 1: Coatomer subunit alpha



• Molecule 2: Coatomer subunit epsilon



• Molecule 2: Coatomer subunit epsilon





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 328.13Å 74.31Å 96.40Å<br>90.00° 101.98° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 50.00 – 3.25<br>50.00 – 3.25                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 89.7 (50.00-3.25)<br>91.0 (50.00-3.25)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.10                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.88 (at 3.25Å)                                             | Xtriage          |
| Refinement program                                                      | CNS                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.241 , 0.287<br>0.244 , 0.281                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3391 reflections (4.95%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 85.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.537                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 131.9                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 14256                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 129.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.65         | 0/2429         | 1.24        | 29/3273 (0.9%)   |
| 1   | C     | 0.64         | 0/2429         | 1.24        | 29/3273 (0.9%)   |
| 1   | E     | 0.61         | 0/2429         | 1.24        | 29/3273 (0.9%)   |
| 2   | B     | 0.66         | 0/2401         | 1.11        | 18/3255 (0.6%)   |
| 2   | D     | 0.66         | 2/2401 (0.1%)  | 1.10        | 15/3255 (0.5%)   |
| 2   | F     | 0.63         | 1/2401 (0.0%)  | 1.09        | 12/3255 (0.4%)   |
| All | All   | 0.64         | 3/14490 (0.0%) | 1.17        | 132/19584 (0.7%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | D     | 157 | SER  | C-N   | -6.21 | 1.24        | 1.33     |
| 2   | F     | 266 | VAL  | CA-CB | 5.09  | 1.60        | 1.54     |
| 2   | D     | 266 | VAL  | CA-CB | 5.07  | 1.60        | 1.54     |

All (132) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | A     | 1095 | LYS  | N-CA-C | -9.52 | 101.83      | 113.15   |
| 1   | C     | 1095 | LYS  | N-CA-C | -9.47 | 101.88      | 113.15   |
| 1   | C     | 1155 | LYS  | N-CA-C | -9.46 | 95.63       | 110.10   |
| 1   | E     | 1095 | LYS  | N-CA-C | -9.46 | 101.89      | 113.15   |
| 1   | A     | 1155 | LYS  | N-CA-C | -9.45 | 95.65       | 110.10   |
| 1   | E     | 1155 | LYS  | N-CA-C | -9.43 | 95.67       | 110.10   |
| 2   | D     | 264  | GLN  | N-CA-C | -7.82 | 102.84      | 111.36   |
| 2   | B     | 264  | GLN  | N-CA-C | -7.78 | 102.88      | 111.36   |
| 2   | F     | 264  | GLN  | N-CA-C | -7.77 | 102.89      | 111.36   |
| 1   | E     | 1025 | VAL  | N-CA-C | 7.33  | 120.14      | 108.85   |
| 1   | C     | 1025 | VAL  | N-CA-C | 7.31  | 120.11      | 108.85   |
| 1   | E     | 1187 | ILE  | N-CA-C | 7.30  | 117.84      | 111.56   |
| 1   | A     | 1187 | ILE  | N-CA-C | 7.26  | 117.81      | 111.56   |
| 1   | C     | 1187 | ILE  | N-CA-C | 7.25  | 117.80      | 111.56   |
| 1   | A     | 1025 | VAL  | N-CA-C | 7.25  | 120.01      | 108.85   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | C     | 1078 | SER  | N-CA-C | -7.25 | 100.44      | 109.64   |
| 1   | E     | 1078 | SER  | N-CA-C | -7.22 | 100.46      | 109.64   |
| 1   | A     | 1045 | ILE  | N-CA-C | -7.21 | 103.26      | 110.62   |
| 1   | C     | 1045 | ILE  | N-CA-C | -7.20 | 103.28      | 110.62   |
| 1   | E     | 1045 | ILE  | N-CA-C | -7.18 | 103.30      | 110.62   |
| 1   | A     | 1078 | SER  | N-CA-C | -7.17 | 100.53      | 109.64   |
| 1   | E     | 1169 | THR  | N-CA-C | 6.70  | 118.37      | 111.14   |
| 1   | A     | 1169 | THR  | N-CA-C | 6.64  | 118.31      | 111.14   |
| 1   | A     | 1005 | LYS  | CA-C-N | 6.62  | 128.12      | 119.84   |
| 1   | A     | 1005 | LYS  | C-N-CA | 6.62  | 128.12      | 119.84   |
| 1   | C     | 1005 | LYS  | CA-C-N | 6.60  | 128.09      | 119.84   |
| 1   | C     | 1005 | LYS  | C-N-CA | 6.60  | 128.09      | 119.84   |
| 1   | C     | 1169 | THR  | N-CA-C | 6.60  | 118.27      | 111.14   |
| 1   | E     | 1005 | LYS  | CA-C-N | 6.52  | 127.99      | 119.84   |
| 1   | E     | 1005 | LYS  | C-N-CA | 6.52  | 127.99      | 119.84   |
| 2   | B     | 291  | LYS  | CA-C-N | -6.48 | 111.78      | 122.08   |
| 2   | B     | 291  | LYS  | C-N-CA | -6.48 | 111.78      | 122.08   |
| 2   | B     | 46   | GLN  | N-CA-C | 6.34  | 118.03      | 108.46   |
| 1   | C     | 1161 | THR  | N-CA-C | 6.33  | 117.68      | 109.64   |
| 1   | C     | 1166 | ASP  | CA-C-N | 6.29  | 127.70      | 119.84   |
| 1   | C     | 1166 | ASP  | C-N-CA | 6.29  | 127.70      | 119.84   |
| 1   | E     | 1161 | THR  | N-CA-C | 6.29  | 117.63      | 109.64   |
| 1   | A     | 1161 | THR  | N-CA-C | 6.29  | 117.62      | 109.64   |
| 1   | E     | 1166 | ASP  | CA-C-N | 6.28  | 127.68      | 119.84   |
| 1   | E     | 1166 | ASP  | C-N-CA | 6.28  | 127.68      | 119.84   |
| 1   | A     | 1166 | ASP  | CA-C-N | 6.27  | 127.68      | 119.84   |
| 1   | A     | 1166 | ASP  | C-N-CA | 6.27  | 127.68      | 119.84   |
| 2   | F     | 46   | GLN  | N-CA-C | 6.23  | 117.87      | 108.46   |
| 1   | C     | 1054 | ARG  | N-CA-C | -6.23 | 104.59      | 111.82   |
| 1   | E     | 1054 | ARG  | N-CA-C | -6.22 | 104.61      | 111.82   |
| 1   | E     | 1177 | GLU  | N-CA-C | 6.22  | 118.47      | 109.71   |
| 1   | A     | 1054 | ARG  | N-CA-C | -6.18 | 104.65      | 111.82   |
| 1   | A     | 1177 | GLU  | N-CA-C | 6.18  | 118.42      | 109.71   |
| 1   | C     | 1177 | GLU  | N-CA-C | 6.11  | 118.33      | 109.71   |
| 1   | A     | 956  | SER  | N-CA-C | 6.03  | 118.96      | 107.75   |
| 1   | C     | 956  | SER  | N-CA-C | 6.01  | 118.93      | 107.75   |
| 1   | E     | 956  | SER  | N-CA-C | 5.97  | 118.86      | 107.75   |
| 1   | A     | 957  | THR  | CA-C-N | -5.94 | 112.41      | 119.84   |
| 1   | A     | 957  | THR  | C-N-CA | -5.94 | 112.41      | 119.84   |
| 2   | D     | 46   | GLN  | N-CA-C | 5.93  | 118.16      | 108.55   |
| 1   | C     | 1141 | PHE  | N-CA-C | 5.93  | 118.79      | 109.96   |
| 1   | C     | 1188 | SER  | N-CA-C | 5.90  | 119.57      | 110.42   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | E     | 1141 | PHE  | N-CA-C | 5.90  | 118.75      | 109.96   |
| 1   | A     | 1141 | PHE  | N-CA-C | 5.89  | 118.74      | 109.96   |
| 1   | C     | 957  | THR  | CA-C-N | -5.89 | 112.48      | 119.84   |
| 1   | C     | 957  | THR  | C-N-CA | -5.89 | 112.48      | 119.84   |
| 1   | E     | 957  | THR  | CA-C-N | -5.87 | 112.50      | 119.84   |
| 1   | E     | 957  | THR  | C-N-CA | -5.87 | 112.50      | 119.84   |
| 1   | E     | 1188 | SER  | N-CA-C | 5.85  | 119.49      | 110.42   |
| 2   | B     | 224  | LEU  | N-CA-C | -5.84 | 105.99      | 113.23   |
| 1   | A     | 1188 | SER  | N-CA-C | 5.83  | 119.46      | 110.42   |
| 2   | D     | 224  | LEU  | N-CA-C | -5.83 | 106.00      | 113.23   |
| 2   | B     | 52   | PRO  | N-CA-C | -5.83 | 107.98      | 114.92   |
| 2   | F     | 52   | PRO  | N-CA-C | -5.82 | 108.00      | 114.92   |
| 2   | F     | 224  | LEU  | N-CA-C | -5.80 | 106.04      | 113.23   |
| 2   | D     | 52   | PRO  | N-CA-C | -5.75 | 108.08      | 114.92   |
| 1   | A     | 954  | ILE  | CA-C-N | -5.74 | 114.05      | 120.14   |
| 1   | A     | 954  | ILE  | C-N-CA | -5.74 | 114.05      | 120.14   |
| 1   | E     | 1137 | ILE  | CA-C-N | 5.74  | 125.92      | 119.90   |
| 1   | E     | 1137 | ILE  | C-N-CA | 5.74  | 125.92      | 119.90   |
| 1   | C     | 943  | PHE  | N-CA-C | -5.72 | 104.96      | 111.14   |
| 1   | A     | 1137 | ILE  | CA-C-N | 5.72  | 125.90      | 119.90   |
| 1   | A     | 1137 | ILE  | C-N-CA | 5.72  | 125.90      | 119.90   |
| 2   | F     | 84   | ASN  | N-CA-C | 5.71  | 117.65      | 109.14   |
| 1   | C     | 1137 | ILE  | CA-C-N | 5.71  | 125.90      | 119.90   |
| 1   | C     | 1137 | ILE  | C-N-CA | 5.71  | 125.90      | 119.90   |
| 2   | D     | 84   | ASN  | N-CA-C | 5.70  | 117.64      | 109.14   |
| 2   | F     | 65   | GLN  | N-CA-C | -5.70 | 105.07      | 111.28   |
| 1   | A     | 943  | PHE  | N-CA-C | -5.70 | 104.99      | 111.14   |
| 2   | B     | 65   | GLN  | N-CA-C | -5.70 | 105.07      | 111.28   |
| 2   | B     | 84   | ASN  | N-CA-C | 5.69  | 117.62      | 109.14   |
| 2   | D     | 65   | GLN  | N-CA-C | -5.68 | 105.08      | 111.28   |
| 1   | E     | 943  | PHE  | N-CA-C | -5.66 | 105.03      | 111.14   |
| 2   | F     | 163  | ILE  | N-CA-C | -5.64 | 105.03      | 110.72   |
| 1   | E     | 954  | ILE  | CA-C-N | -5.60 | 114.20      | 120.14   |
| 1   | E     | 954  | ILE  | C-N-CA | -5.60 | 114.20      | 120.14   |
| 2   | D     | 163  | ILE  | N-CA-C | -5.60 | 105.06      | 110.72   |
| 1   | C     | 954  | ILE  | CA-C-N | -5.54 | 114.27      | 120.14   |
| 1   | C     | 954  | ILE  | C-N-CA | -5.54 | 114.27      | 120.14   |
| 1   | A     | 984  | VAL  | CA-C-N | 5.54  | 126.76      | 119.84   |
| 1   | A     | 984  | VAL  | C-N-CA | 5.54  | 126.76      | 119.84   |
| 1   | E     | 984  | VAL  | CA-C-N | 5.54  | 126.76      | 119.84   |
| 1   | E     | 984  | VAL  | C-N-CA | 5.54  | 126.76      | 119.84   |
| 1   | C     | 984  | VAL  | CA-C-N | 5.53  | 126.75      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | C     | 984  | VAL  | C-N-CA  | 5.53  | 126.75      | 119.84   |
| 1   | C     | 961  | LEU  | N-CA-C  | -5.52 | 99.82       | 109.48   |
| 2   | B     | 115  | ASN  | N-CA-C  | -5.51 | 106.44      | 112.72   |
| 1   | E     | 961  | LEU  | N-CA-C  | -5.48 | 99.89       | 109.48   |
| 2   | D     | 27   | LYS  | N-CA-C  | 5.43  | 122.36      | 110.80   |
| 2   | B     | 27   | LYS  | N-CA-C  | 5.42  | 122.34      | 110.80   |
| 2   | F     | 27   | LYS  | N-CA-C  | 5.41  | 122.32      | 110.80   |
| 2   | B     | 163  | ILE  | N-CA-C  | -5.41 | 105.26      | 110.72   |
| 1   | A     | 961  | LEU  | N-CA-C  | -5.40 | 100.03      | 109.48   |
| 2   | F     | 248  | ILE  | CB-CA-C | -5.31 | 105.02      | 111.87   |
| 2   | D     | 248  | ILE  | CB-CA-C | -5.30 | 105.03      | 111.87   |
| 1   | C     | 1134 | SER  | N-CA-C  | 5.29  | 118.85      | 109.96   |
| 2   | B     | 248  | ILE  | CB-CA-C | -5.29 | 105.04      | 111.87   |
| 1   | A     | 1134 | SER  | N-CA-C  | 5.28  | 118.83      | 109.96   |
| 1   | E     | 1134 | SER  | N-CA-C  | 5.28  | 118.82      | 109.96   |
| 2   | F     | 237  | VAL  | N-CA-C  | -5.28 | 104.37      | 111.44   |
| 1   | A     | 1093 | HIS  | N-CA-C  | -5.26 | 105.10      | 112.25   |
| 2   | B     | 237  | VAL  | N-CA-C  | -5.24 | 104.42      | 111.44   |
| 2   | D     | 237  | VAL  | N-CA-C  | -5.24 | 104.42      | 111.44   |
| 1   | C     | 1093 | HIS  | N-CA-C  | -5.23 | 105.14      | 112.25   |
| 2   | D     | 58   | LYS  | N-CA-C  | -5.23 | 105.64      | 112.23   |
| 1   | E     | 1093 | HIS  | N-CA-C  | -5.21 | 105.17      | 112.25   |
| 2   | F     | 58   | LYS  | N-CA-C  | -5.20 | 105.68      | 112.23   |
| 2   | B     | 58   | LYS  | N-CA-C  | -5.17 | 105.72      | 112.23   |
| 2   | D     | 85   | SER  | N-CA-C  | 5.10  | 116.92      | 109.84   |
| 2   | F     | 23   | GLU  | N-CA-C  | -5.09 | 105.86      | 111.71   |
| 2   | B     | 23   | GLU  | N-CA-C  | -5.08 | 105.87      | 111.71   |
| 2   | D     | 23   | GLU  | N-CA-C  | -5.06 | 105.89      | 111.71   |
| 2   | B     | 171  | ILE  | N-CA-C  | -5.05 | 105.67      | 110.42   |
| 2   | B     | 15   | PHE  | N-CA-C  | -5.02 | 105.99      | 111.82   |
| 2   | D     | 15   | PHE  | N-CA-C  | -5.02 | 106.00      | 111.82   |
| 2   | D     | 171  | ILE  | N-CA-C  | -5.01 | 105.71      | 110.42   |
| 2   | B     | 85   | SER  | N-CA-C  | 5.01  | 116.80      | 109.84   |

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     | 2388  | 0        | 2441     | 289     | 0            |
| 1   | C     | 2388  | 0        | 2441     | 256     | 0            |
| 1   | E     | 2388  | 0        | 2441     | 258     | 0            |
| 2   | B     | 2364  | 0        | 2319     | 232     | 0            |
| 2   | D     | 2364  | 0        | 2319     | 255     | 0            |
| 2   | F     | 2364  | 0        | 2319     | 234     | 0            |
| All | All   | 14256 | 0        | 14280    | 1443    | 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 51.

All (1443) 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:C:1090:MSE:HE2  | 1:C:1106:ALA:HA   | 1.30                     | 1.12              |
| 1:E:1090:MSE:HE2  | 1:E:1106:ALA:HA   | 1.29                     | 1.12              |
| 2:B:211:ARG:HH11  | 2:B:211:ARG:HB2   | 1.11                     | 1.10              |
| 1:C:1028:ALA:HB2  | 1:C:1200:ARG:CZ   | 1.80                     | 1.10              |
| 1:A:1090:MSE:HE2  | 1:A:1106:ALA:HA   | 1.30                     | 1.08              |
| 2:D:211:ARG:HH11  | 2:D:211:ARG:HB2   | 1.11                     | 1.08              |
| 1:A:1113:ILE:HG23 | 2:D:150:ASN:ND2   | 1.69                     | 1.06              |
| 2:F:211:ARG:HH11  | 2:F:211:ARG:HB2   | 1.11                     | 1.05              |
| 2:D:195:PRO:HG3   | 1:E:1079:PRO:HG3  | 1.40                     | 1.03              |
| 1:C:957:THR:HB    | 1:C:958:PRO:CD    | 1.93                     | 0.99              |
| 1:A:957:THR:HB    | 1:A:958:PRO:CD    | 1.92                     | 0.99              |
| 1:E:957:THR:HB    | 1:E:958:PRO:CD    | 1.94                     | 0.98              |
| 2:D:1:MSE:HG2     | 2:D:2:ASP:H       | 1.29                     | 0.97              |
| 1:C:1028:ALA:HB2  | 1:C:1200:ARG:NH1  | 1.78                     | 0.97              |
| 1:C:990:VAL:HG11  | 1:C:1020:ILE:HD11 | 1.46                     | 0.97              |
| 1:E:1097:LYS:HG3  | 1:E:1099:PHE:HE1  | 1.29                     | 0.97              |
| 2:B:1:MSE:HG2     | 2:B:2:ASP:H       | 1.29                     | 0.96              |
| 1:A:990:VAL:HG11  | 1:A:1020:ILE:HD11 | 1.46                     | 0.95              |
| 1:E:990:VAL:HG11  | 1:E:1020:ILE:HD11 | 1.45                     | 0.95              |
| 1:A:1083:THR:HG21 | 1:A:1118:ARG:NH1  | 1.84                     | 0.93              |
| 1:A:1097:LYS:HG3  | 1:A:1099:PHE:HE1  | 1.29                     | 0.93              |
| 1:C:1097:LYS:HG3  | 1:C:1099:PHE:HE1  | 1.29                     | 0.93              |
| 2:F:1:MSE:HG2     | 2:F:2:ASP:H       | 1.29                     | 0.92              |
| 1:C:1025:VAL:HG11 | 1:C:1030:ASP:HB2  | 1.51                     | 0.92              |
| 1:E:1025:VAL:HG11 | 1:E:1030:ASP:HB2  | 1.51                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1083:THR:HG21 | 1:E:1118:ARG:NH1  | 1.84                     | 0.92              |
| 1:A:1080:ILE:HG13 | 2:D:147:ASN:OD1   | 1.71                     | 0.91              |
| 1:C:1083:THR:HG21 | 1:C:1118:ARG:NH1  | 1.84                     | 0.91              |
| 2:B:6:ILE:HD12    | 2:B:6:ILE:H       | 1.36                     | 0.91              |
| 1:A:1003:LEU:HD21 | 2:D:110:VAL:HG21  | 1.53                     | 0.91              |
| 1:C:1079:PRO:HG3  | 2:F:195:PRO:HG3   | 1.54                     | 0.90              |
| 2:D:6:ILE:H       | 2:D:6:ILE:HD12    | 1.36                     | 0.90              |
| 2:F:6:ILE:HD12    | 2:F:6:ILE:H       | 1.36                     | 0.90              |
| 1:A:1025:VAL:HG11 | 1:A:1030:ASP:HB2  | 1.51                     | 0.90              |
| 1:C:994:MSE:HE3   | 1:C:1016:ALA:CB   | 2.02                     | 0.90              |
| 2:B:11:TYR:CE1    | 2:B:163:ILE:HD11  | 2.08                     | 0.88              |
| 2:B:211:ARG:HH11  | 2:B:211:ARG:CB    | 1.87                     | 0.88              |
| 1:A:994:MSE:HE3   | 1:A:1016:ALA:CB   | 2.02                     | 0.88              |
| 1:E:994:MSE:HE3   | 1:E:1016:ALA:CB   | 2.02                     | 0.88              |
| 2:D:211:ARG:HH11  | 2:D:211:ARG:CB    | 1.87                     | 0.88              |
| 2:F:211:ARG:HH11  | 2:F:211:ARG:CB    | 1.87                     | 0.88              |
| 1:E:1028:ALA:HB2  | 1:E:1200:ARG:CZ   | 2.02                     | 0.87              |
| 1:A:976:SER:C     | 1:A:978:ASP:H     | 1.82                     | 0.87              |
| 1:C:1025:VAL:HG23 | 1:C:1199:ILE:HG22 | 1.54                     | 0.87              |
| 1:E:1166:ASP:OD2  | 1:E:1169:THR:HB   | 1.76                     | 0.86              |
| 1:A:1028:ALA:HB2  | 1:A:1200:ARG:CZ   | 2.05                     | 0.86              |
| 1:A:1166:ASP:OD2  | 1:A:1169:THR:HB   | 1.76                     | 0.86              |
| 1:C:1166:ASP:OD2  | 1:C:1169:THR:HB   | 1.76                     | 0.85              |
| 1:C:976:SER:C     | 1:C:978:ASP:H     | 1.82                     | 0.85              |
| 2:F:11:TYR:CE1    | 2:F:163:ILE:HD11  | 2.10                     | 0.85              |
| 2:D:112:GLY:O     | 2:D:115:ASN:HB2   | 1.75                     | 0.84              |
| 1:C:1174:VAL:HG23 | 1:C:1176:THR:HB   | 1.58                     | 0.84              |
| 1:A:1174:VAL:HG23 | 1:A:1176:THR:HB   | 1.58                     | 0.84              |
| 1:E:1174:VAL:HG23 | 1:E:1176:THR:HB   | 1.58                     | 0.84              |
| 2:D:195:PRO:HG3   | 1:E:1079:PRO:CG   | 2.06                     | 0.84              |
| 1:E:976:SER:C     | 1:E:978:ASP:H     | 1.82                     | 0.84              |
| 1:A:1113:ILE:HG23 | 2:D:150:ASN:HD21  | 1.43                     | 0.83              |
| 2:D:87:TYR:HE1    | 2:D:119:GLU:HG2   | 1.42                     | 0.83              |
| 2:B:72:ILE:HD12   | 2:B:72:ILE:H      | 1.43                     | 0.83              |
| 1:E:1097:LYS:HG3  | 1:E:1099:PHE:CE1  | 2.14                     | 0.83              |
| 1:C:1097:LYS:HG3  | 1:C:1099:PHE:CE1  | 2.14                     | 0.83              |
| 2:F:211:ARG:HA    | 2:F:253:MSE:HE1   | 1.61                     | 0.83              |
| 2:B:211:ARG:HA    | 2:B:253:MSE:HE1   | 1.61                     | 0.82              |
| 1:A:0:MSE:HE1     | 2:B:138:VAL:HG11  | 1.60                     | 0.82              |
| 1:A:1097:LYS:HG3  | 1:A:1099:PHE:CE1  | 2.14                     | 0.82              |
| 1:A:1189:LYS:HE3  | 1:A:1192:ALA:HB2  | 1.61                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:72:ILE:H      | 2:F:72:ILE:HD12   | 1.43                     | 0.82              |
| 1:A:1045:ILE:HD12 | 1:A:1184:ILE:HG23 | 1.60                     | 0.82              |
| 1:C:1189:LYS:HE3  | 1:C:1192:ALA:HB2  | 1.61                     | 0.82              |
| 2:F:125:LEU:HD22  | 2:F:148:TYR:CD2   | 2.15                     | 0.82              |
| 2:B:125:LEU:HD22  | 2:B:148:TYR:CD2   | 2.15                     | 0.82              |
| 2:D:72:ILE:HD12   | 2:D:72:ILE:H      | 1.43                     | 0.82              |
| 2:D:211:ARG:HA    | 2:D:253:MSE:HE1   | 1.61                     | 0.82              |
| 2:B:20:GLN:HA     | 2:B:23:GLU:HG3    | 1.61                     | 0.81              |
| 2:B:264:GLN:OE1   | 2:B:264:GLN:HA    | 1.79                     | 0.81              |
| 2:F:20:GLN:HA     | 2:F:23:GLU:HG3    | 1.61                     | 0.81              |
| 2:D:264:GLN:HA    | 2:D:264:GLN:OE1   | 1.80                     | 0.81              |
| 1:E:1045:ILE:HD12 | 1:E:1184:ILE:HG23 | 1.60                     | 0.81              |
| 2:B:275:ILE:O     | 2:B:279:GLN:HG2   | 1.80                     | 0.81              |
| 2:D:20:GLN:HA     | 2:D:23:GLU:HG3    | 1.61                     | 0.81              |
| 2:F:264:GLN:HA    | 2:F:264:GLN:OE1   | 1.80                     | 0.81              |
| 2:D:94:THR:O      | 2:D:98:ILE:HG13   | 1.81                     | 0.80              |
| 2:F:94:THR:O      | 2:F:98:ILE:HG13   | 1.80                     | 0.80              |
| 2:D:35:PHE:CD1    | 2:D:87:TYR:HD2    | 1.99                     | 0.80              |
| 1:E:1189:LYS:HE3  | 1:E:1192:ALA:HB2  | 1.62                     | 0.80              |
| 2:F:211:ARG:HB2   | 2:F:211:ARG:NH1   | 1.96                     | 0.80              |
| 2:F:275:ILE:O     | 2:F:279:GLN:HG2   | 1.80                     | 0.80              |
| 2:D:125:LEU:HD22  | 2:D:148:TYR:CD2   | 2.15                     | 0.80              |
| 2:D:275:ILE:O     | 2:D:279:GLN:HG2   | 1.80                     | 0.80              |
| 2:B:94:THR:O      | 2:B:98:ILE:HG13   | 1.81                     | 0.79              |
| 1:C:1074:LYS:HE3  | 1:C:1147:PHE:CE1  | 2.17                     | 0.79              |
| 2:B:181:THR:HG22  | 2:B:182:SER:N     | 1.98                     | 0.79              |
| 2:B:211:ARG:HB2   | 2:B:211:ARG:NH1   | 1.95                     | 0.79              |
| 2:D:181:THR:HG22  | 2:D:182:SER:H     | 1.48                     | 0.79              |
| 1:C:1104:TYR:CE2  | 1:C:1143:PRO:HB3  | 2.17                     | 0.79              |
| 2:D:181:THR:HG22  | 2:D:182:SER:N     | 1.99                     | 0.78              |
| 2:B:181:THR:HG22  | 2:B:182:SER:H     | 1.48                     | 0.78              |
| 1:A:1099:PHE:HD1  | 1:A:1134:SER:HB3  | 1.47                     | 0.78              |
| 2:F:206:LEU:O     | 2:F:209:GLN:HB2   | 1.84                     | 0.78              |
| 2:B:71:ASN:HB2    | 2:B:73:GLU:CG     | 2.14                     | 0.78              |
| 2:F:71:ASN:HB2    | 2:F:73:GLU:HG2    | 1.65                     | 0.78              |
| 2:D:206:LEU:O     | 2:D:209:GLN:HB2   | 1.84                     | 0.78              |
| 2:D:71:ASN:HB2    | 2:D:73:GLU:HG2    | 1.65                     | 0.78              |
| 1:E:983:TYR:CE2   | 2:F:253:MSE:HG2   | 2.19                     | 0.78              |
| 1:A:983:TYR:CE2   | 2:B:253:MSE:HG2   | 2.19                     | 0.77              |
| 2:B:206:LEU:O     | 2:B:209:GLN:HB2   | 1.84                     | 0.77              |
| 2:D:71:ASN:HB2    | 2:D:73:GLU:CG     | 2.14                     | 0.77              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:181:THR:HG22 | 2:F:182:SER:H     | 1.48                     | 0.77              |
| 2:D:11:TYR:CE1   | 2:D:163:ILE:HD11  | 2.19                     | 0.77              |
| 2:D:211:ARG:HB2  | 2:D:211:ARG:NH1   | 1.95                     | 0.77              |
| 2:F:60:LEU:O     | 2:F:64:VAL:HG23   | 1.84                     | 0.77              |
| 2:F:181:THR:HG22 | 2:F:182:SER:N     | 1.99                     | 0.77              |
| 2:D:60:LEU:O     | 2:D:64:VAL:HG23   | 1.84                     | 0.77              |
| 2:B:71:ASN:HB2   | 2:B:73:GLU:HG2    | 1.65                     | 0.77              |
| 2:B:6:ILE:H      | 2:B:6:ILE:CD1     | 1.98                     | 0.76              |
| 1:E:1099:PHE:HD1 | 1:E:1134:SER:HB3  | 1.50                     | 0.76              |
| 1:A:957:THR:HB   | 1:A:958:PRO:HD2   | 1.68                     | 0.76              |
| 2:D:156:VAL:C    | 2:D:158:GLY:H     | 1.92                     | 0.76              |
| 2:F:71:ASN:HB2   | 2:F:73:GLU:CG     | 2.14                     | 0.76              |
| 2:D:6:ILE:HD12   | 2:D:6:ILE:N       | 2.01                     | 0.76              |
| 1:E:1002:LYS:NZ  | 1:E:1080:ILE:HD11 | 2.01                     | 0.76              |
| 1:C:994:MSE:HE3  | 1:C:1016:ALA:HB3  | 1.68                     | 0.75              |
| 2:B:60:LEU:O     | 2:B:64:VAL:HG23   | 1.84                     | 0.75              |
| 2:F:157:SER:HB2  | 2:F:161:GLU:HB2   | 1.67                     | 0.75              |
| 1:C:957:THR:HB   | 1:C:958:PRO:HD2   | 1.68                     | 0.75              |
| 2:D:6:ILE:H      | 2:D:6:ILE:CD1     | 1.98                     | 0.75              |
| 2:F:6:ILE:H      | 2:F:6:ILE:CD1     | 1.98                     | 0.75              |
| 2:D:87:TYR:CE1   | 2:D:119:GLU:HG2   | 2.22                     | 0.75              |
| 2:F:6:ILE:HD12   | 2:F:6:ILE:N       | 2.01                     | 0.74              |
| 1:A:1002:LYS:NZ  | 1:A:1080:ILE:HD11 | 2.01                     | 0.74              |
| 1:C:1002:LYS:NZ  | 1:C:1080:ILE:HD11 | 2.01                     | 0.74              |
| 1:E:994:MSE:HE3  | 1:E:1016:ALA:HB3  | 1.68                     | 0.74              |
| 1:A:994:MSE:HE3  | 1:A:1016:ALA:HB3  | 1.68                     | 0.74              |
| 1:A:1045:ILE:HB  | 1:A:1184:ILE:HD12 | 1.68                     | 0.74              |
| 1:E:957:THR:HB   | 1:E:958:PRO:HD2   | 1.68                     | 0.74              |
| 1:A:931:VAL:HG13 | 1:A:1168:LEU:HB2  | 1.67                     | 0.74              |
| 1:E:954:ILE:HD13 | 1:E:955:PRO:N     | 2.03                     | 0.74              |
| 1:C:1079:PRO:CG  | 2:F:195:PRO:HG3   | 2.18                     | 0.74              |
| 1:C:954:ILE:HD13 | 1:C:955:PRO:N     | 2.03                     | 0.73              |
| 2:F:35:PHE:CD1   | 2:F:87:TYR:HD2    | 2.05                     | 0.73              |
| 2:F:69:THR:HB    | 2:F:71:ASN:OD1    | 1.89                     | 0.73              |
| 1:A:954:ILE:HD13 | 1:A:955:PRO:N     | 2.03                     | 0.73              |
| 1:C:933:VAL:HG13 | 1:C:1187:ILE:HG23 | 1.69                     | 0.73              |
| 2:F:3:TYR:CB     | 2:F:6:ILE:HD13    | 2.19                     | 0.73              |
| 2:F:257:ASP:O    | 2:F:259:GLU:N     | 2.21                     | 0.73              |
| 2:F:63:TYR:O     | 2:F:66:PHE:HB3    | 1.89                     | 0.73              |
| 2:B:6:ILE:HD12   | 2:B:6:ILE:N       | 2.01                     | 0.73              |
| 2:B:3:TYR:CB     | 2:B:6:ILE:HD13    | 2.19                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:63:TYR:O      | 2:D:66:PHE:HB3    | 1.89                     | 0.73              |
| 2:B:257:ASP:O     | 2:B:259:GLU:N     | 2.21                     | 0.73              |
| 2:D:257:ASP:O     | 2:D:259:GLU:N     | 2.21                     | 0.72              |
| 1:E:1045:ILE:HB   | 1:E:1184:ILE:HD12 | 1.71                     | 0.72              |
| 2:D:3:TYR:CB      | 2:D:6:ILE:HD13    | 2.19                     | 0.72              |
| 2:F:159:ASP:O     | 2:F:162:MSE:HE2   | 1.89                     | 0.72              |
| 2:B:63:TYR:O      | 2:B:66:PHE:HB3    | 1.89                     | 0.72              |
| 2:B:125:LEU:O     | 2:B:129:ILE:HD13  | 1.90                     | 0.72              |
| 1:A:1113:ILE:HD12 | 2:D:150:ASN:HD22  | 1.52                     | 0.72              |
| 2:B:159:ASP:O     | 2:B:162:MSE:HE2   | 1.89                     | 0.72              |
| 2:D:125:LEU:O     | 2:D:129:ILE:HD13  | 1.90                     | 0.72              |
| 2:D:159:ASP:O     | 2:D:162:MSE:HE2   | 1.89                     | 0.71              |
| 1:A:1117:PRO:HB2  | 2:D:177:LYS:HZ3   | 1.56                     | 0.71              |
| 1:C:978:ASP:O     | 1:C:980:ILE:N     | 2.23                     | 0.71              |
| 2:F:156:VAL:C     | 2:F:158:GLY:H     | 1.99                     | 0.71              |
| 2:B:30:ASP:HB3    | 2:B:33:LEU:HD12   | 1.73                     | 0.71              |
| 1:E:978:ASP:O     | 1:E:980:ILE:N     | 2.23                     | 0.71              |
| 2:F:30:ASP:HB3    | 2:F:33:LEU:HD12   | 1.73                     | 0.71              |
| 1:E:1074:LYS:HE3  | 1:E:1147:PHE:CE1  | 2.25                     | 0.71              |
| 2:F:125:LEU:O     | 2:F:129:ILE:HD13  | 1.90                     | 0.71              |
| 1:A:1099:PHE:HA   | 1:A:1102:ALA:HB3  | 1.73                     | 0.71              |
| 2:F:258:THR:HG22  | 2:F:262:THR:OG1   | 1.91                     | 0.70              |
| 1:E:1174:VAL:CG2  | 1:E:1176:THR:HB   | 2.22                     | 0.70              |
| 2:D:30:ASP:HB3    | 2:D:33:LEU:HD12   | 1.73                     | 0.70              |
| 1:E:1099:PHE:HA   | 1:E:1102:ALA:HB3  | 1.73                     | 0.70              |
| 2:D:54:SER:C      | 2:D:56:LEU:H      | 2.00                     | 0.70              |
| 1:E:1185:ALA:O    | 1:E:1187:ILE:N    | 2.25                     | 0.70              |
| 2:B:57:GLY:HA2    | 2:B:60:LEU:HD12   | 1.73                     | 0.70              |
| 2:B:106:LEU:HD23  | 2:B:106:LEU:O     | 1.92                     | 0.70              |
| 1:A:1185:ALA:O    | 1:A:1187:ILE:N    | 2.25                     | 0.70              |
| 2:B:54:SER:C      | 2:B:56:LEU:H      | 1.99                     | 0.70              |
| 1:E:957:THR:CB    | 1:E:958:PRO:CD    | 2.70                     | 0.70              |
| 1:A:1074:LYS:HE3  | 1:A:1147:PHE:CE1  | 2.27                     | 0.70              |
| 2:B:258:THR:HG22  | 2:B:262:THR:OG1   | 1.92                     | 0.70              |
| 1:C:1174:VAL:CG2  | 1:C:1176:THR:HB   | 2.22                     | 0.70              |
| 2:D:106:LEU:O     | 2:D:106:LEU:HD23  | 1.92                     | 0.70              |
| 1:E:1023:LEU:HD23 | 1:E:1024:MSE:H    | 1.57                     | 0.70              |
| 1:A:957:THR:CB    | 1:A:958:PRO:CD    | 2.69                     | 0.70              |
| 1:A:978:ASP:O     | 1:A:980:ILE:N     | 2.23                     | 0.70              |
| 1:A:1174:VAL:CG2  | 1:A:1176:THR:HB   | 2.22                     | 0.70              |
| 1:A:1023:LEU:HD23 | 1:A:1024:MSE:H    | 1.56                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:957:THR:CB    | 1:C:958:PRO:CD    | 2.69                     | 0.69              |
| 1:C:1045:ILE:HD12 | 1:C:1184:ILE:HG23 | 1.74                     | 0.69              |
| 2:F:57:GLY:HA2    | 2:F:60:LEU:HD12   | 1.73                     | 0.69              |
| 1:A:1113:ILE:HD12 | 2:D:150:ASN:ND2   | 2.07                     | 0.69              |
| 1:E:1090:MSE:HG3  | 1:E:1106:ALA:HB2  | 1.75                     | 0.69              |
| 1:A:926:ALA:O     | 1:A:930:GLN:HG3   | 1.92                     | 0.69              |
| 2:B:222:LEU:O     | 2:B:222:LEU:HD23  | 1.92                     | 0.69              |
| 1:A:940:LYS:HB2   | 2:B:285:PHE:CE2   | 2.28                     | 0.69              |
| 1:A:961:LEU:HD21  | 2:B:134:LEU:HD11  | 1.72                     | 0.69              |
| 1:C:1185:ALA:O    | 1:C:1187:ILE:N    | 2.25                     | 0.69              |
| 1:E:926:ALA:O     | 1:E:930:GLN:HG3   | 1.92                     | 0.69              |
| 2:F:112:GLY:O     | 2:F:115:ASN:HB2   | 1.92                     | 0.69              |
| 1:C:1099:PHE:HA   | 1:C:1102:ALA:HB3  | 1.73                     | 0.69              |
| 1:A:1090:MSE:HG3  | 1:A:1106:ALA:HB2  | 1.75                     | 0.69              |
| 1:C:1023:LEU:HD23 | 1:C:1024:MSE:H    | 1.57                     | 0.69              |
| 1:C:1090:MSE:HG3  | 1:C:1106:ALA:HB2  | 1.74                     | 0.69              |
| 1:E:994:MSE:CE    | 1:E:1013:PHE:HD2  | 2.05                     | 0.69              |
| 1:A:1002:LYS:NZ   | 2:D:147:ASN:HB3   | 2.08                     | 0.69              |
| 2:D:57:GLY:HA2    | 2:D:60:LEU:HD12   | 1.73                     | 0.69              |
| 2:F:106:LEU:O     | 2:F:106:LEU:HD23  | 1.92                     | 0.69              |
| 1:A:933:VAL:HG13  | 1:A:1187:ILE:HG23 | 1.75                     | 0.69              |
| 1:C:926:ALA:O     | 1:C:930:GLN:HG3   | 1.92                     | 0.69              |
| 1:C:1181:ILE:HD12 | 1:C:1181:ILE:H    | 1.58                     | 0.69              |
| 2:D:222:LEU:HD23  | 2:D:222:LEU:O     | 1.92                     | 0.69              |
| 2:D:231:GLU:HB3   | 1:E:1113:ILE:HD12 | 1.74                     | 0.69              |
| 2:F:222:LEU:HD23  | 2:F:222:LEU:O     | 1.92                     | 0.69              |
| 1:E:1025:VAL:HG23 | 1:E:1199:ILE:HG22 | 1.74                     | 0.69              |
| 1:E:1181:ILE:H    | 1:E:1181:ILE:HD12 | 1.58                     | 0.69              |
| 1:A:1117:PRO:CA   | 2:D:177:LYS:HZ1   | 2.05                     | 0.69              |
| 2:B:175:THR:HG21  | 2:B:177:LYS:HD3   | 1.75                     | 0.68              |
| 2:F:175:THR:HG21  | 2:F:177:LYS:HD3   | 1.75                     | 0.68              |
| 1:A:1099:PHE:CD1  | 1:A:1134:SER:HB3  | 2.27                     | 0.68              |
| 2:D:227:TYR:O     | 2:D:231:GLU:HB2   | 1.94                     | 0.68              |
| 2:D:258:THR:HG22  | 2:D:262:THR:OG1   | 1.92                     | 0.68              |
| 2:F:54:SER:C      | 2:F:56:LEU:H      | 1.99                     | 0.68              |
| 2:B:162:MSE:HE3   | 2:B:163:ILE:CD1   | 2.24                     | 0.68              |
| 2:F:248:ILE:HD11  | 2:F:263:ASN:HB3   | 1.76                     | 0.68              |
| 1:E:931:VAL:HG13  | 1:E:1168:LEU:HB2  | 1.74                     | 0.68              |
| 2:D:162:MSE:HE3   | 2:D:163:ILE:CD1   | 2.24                     | 0.68              |
| 2:F:227:TYR:O     | 2:F:231:GLU:HB2   | 1.94                     | 0.68              |
| 1:C:994:MSE:CE    | 1:C:1013:PHE:HD2  | 2.05                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1153:THR:O    | 1:A:1154:TYR:HB2  | 1.94                     | 0.68              |
| 1:C:911:PRO:HB3   | 1:C:927:LEU:HD21  | 1.76                     | 0.67              |
| 2:D:175:THR:HG21  | 2:D:177:LYS:HD3   | 1.75                     | 0.67              |
| 1:C:1025:VAL:HG23 | 1:C:1199:ILE:CG2  | 2.24                     | 0.67              |
| 1:C:1033:LEU:HD23 | 1:C:1037:ILE:HG13 | 1.76                     | 0.67              |
| 2:D:248:ILE:HD11  | 2:D:263:ASN:HB3   | 1.76                     | 0.67              |
| 2:B:157:SER:HB2   | 2:B:161:GLU:HB2   | 1.77                     | 0.67              |
| 1:E:904:TRP:CH2   | 1:E:982:PRO:HB3   | 2.29                     | 0.67              |
| 1:E:1109:PHE:CZ   | 1:E:1118:ARG:HD3  | 2.30                     | 0.67              |
| 1:E:1153:THR:O    | 1:E:1154:TYR:HB2  | 1.95                     | 0.67              |
| 2:F:162:MSE:HE3   | 2:F:163:ILE:CD1   | 2.23                     | 0.67              |
| 2:B:227:TYR:O     | 2:B:231:GLU:HB2   | 1.93                     | 0.67              |
| 1:E:913:VAL:CG2   | 1:E:1024:MSE:HE3  | 2.24                     | 0.67              |
| 1:A:994:MSE:CE    | 1:A:1013:PHE:HD2  | 2.05                     | 0.67              |
| 1:A:1033:LEU:HD23 | 1:A:1037:ILE:HG13 | 1.76                     | 0.67              |
| 1:A:954:ILE:HD13  | 1:A:955:PRO:CD    | 2.25                     | 0.67              |
| 1:A:1104:TYR:CE2  | 1:A:1143:PRO:HB3  | 2.30                     | 0.67              |
| 1:A:1109:PHE:CZ   | 1:A:1118:ARG:HD3  | 2.30                     | 0.67              |
| 2:B:35:PHE:CD1    | 2:B:87:TYR:HD2    | 2.12                     | 0.67              |
| 1:E:911:PRO:HB3   | 1:E:927:LEU:HD21  | 1.76                     | 0.67              |
| 1:E:1002:LYS:HZ3  | 1:E:1080:ILE:HD11 | 1.60                     | 0.67              |
| 1:A:1181:ILE:HD12 | 1:A:1181:ILE:H    | 1.58                     | 0.67              |
| 2:B:186:TYR:CZ    | 2:B:190:LEU:HD11  | 2.30                     | 0.67              |
| 1:C:1109:PHE:CZ   | 1:C:1118:ARG:HD3  | 2.30                     | 0.67              |
| 2:D:186:TYR:CZ    | 2:D:190:LEU:HD11  | 2.30                     | 0.67              |
| 2:B:248:ILE:HD11  | 2:B:263:ASN:HB3   | 1.76                     | 0.67              |
| 1:A:911:PRO:HB3   | 1:A:927:LEU:HD21  | 1.76                     | 0.67              |
| 1:C:931:VAL:HG13  | 1:C:1168:LEU:HB2  | 1.77                     | 0.67              |
| 2:D:15:PHE:HB2    | 2:D:44:LEU:HD21   | 1.77                     | 0.67              |
| 1:E:1162:PRO:O    | 1:E:1175:ILE:HG12 | 1.95                     | 0.67              |
| 2:F:186:TYR:CZ    | 2:F:190:LEU:HD11  | 2.30                     | 0.67              |
| 2:F:15:PHE:HB2    | 2:F:44:LEU:HD21   | 1.77                     | 0.66              |
| 1:A:976:SER:O     | 1:A:978:ASP:N     | 2.29                     | 0.66              |
| 2:D:72:ILE:H      | 2:D:72:ILE:CD1    | 2.03                     | 0.66              |
| 1:E:1033:LEU:HD23 | 1:E:1037:ILE:HG13 | 1.76                     | 0.66              |
| 1:C:954:ILE:HD13  | 1:C:955:PRO:CD    | 2.26                     | 0.66              |
| 1:A:1147:PHE:HD1  | 1:A:1147:PHE:O    | 1.79                     | 0.66              |
| 1:E:1008:ILE:HD12 | 1:E:1008:ILE:H    | 1.61                     | 0.66              |
| 1:A:981:LEU:HD13  | 1:A:1024:MSE:HE2  | 1.78                     | 0.66              |
| 1:C:976:SER:C     | 1:C:978:ASP:N     | 2.51                     | 0.66              |
| 1:C:1008:ILE:HD12 | 1:C:1008:ILE:H    | 1.61                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:15:PHE:HB2    | 2:B:44:LEU:HD21   | 1.78                     | 0.66              |
| 1:C:1147:PHE:HD1  | 1:C:1147:PHE:O    | 1.79                     | 0.66              |
| 1:C:1153:THR:O    | 1:C:1154:TYR:HB2  | 1.94                     | 0.66              |
| 1:A:1162:PRO:O    | 1:A:1175:ILE:HG12 | 1.95                     | 0.65              |
| 1:C:1162:PRO:O    | 1:C:1175:ILE:HG12 | 1.95                     | 0.65              |
| 1:E:961:LEU:HD21  | 2:F:134:LEU:HD11  | 1.79                     | 0.65              |
| 2:D:19:LEU:O      | 2:D:23:GLU:HG2    | 1.97                     | 0.65              |
| 2:D:80:LYS:O      | 2:D:81:ASP:HB2    | 1.96                     | 0.65              |
| 1:E:976:SER:O     | 1:E:978:ASP:N     | 2.30                     | 0.65              |
| 1:A:957:THR:HB    | 1:A:958:PRO:HD3   | 1.78                     | 0.65              |
| 2:B:19:LEU:O      | 2:B:23:GLU:HG2    | 1.97                     | 0.65              |
| 1:C:976:SER:O     | 1:C:978:ASP:N     | 2.29                     | 0.65              |
| 1:E:954:ILE:HD13  | 1:E:955:PRO:CD    | 2.26                     | 0.65              |
| 1:E:1104:TYR:CE2  | 1:E:1143:PRO:HB3  | 2.32                     | 0.65              |
| 1:A:961:LEU:HD23  | 1:A:961:LEU:C     | 2.22                     | 0.65              |
| 1:A:1002:LYS:HZ3  | 1:A:1080:ILE:HD11 | 1.61                     | 0.64              |
| 1:A:1008:ILE:HD12 | 1:A:1008:ILE:H    | 1.61                     | 0.64              |
| 1:E:1147:PHE:HD1  | 1:E:1147:PHE:O    | 1.79                     | 0.64              |
| 2:F:87:TYR:HE1    | 2:F:119:GLU:HG2   | 1.62                     | 0.64              |
| 2:F:72:ILE:H      | 2:F:72:ILE:CD1    | 2.03                     | 0.64              |
| 2:F:80:LYS:O      | 2:F:81:ASP:HB2    | 1.97                     | 0.64              |
| 2:D:181:THR:CG2   | 2:D:182:SER:H     | 2.07                     | 0.64              |
| 2:F:19:LEU:O      | 2:F:23:GLU:HG2    | 1.97                     | 0.64              |
| 2:B:3:TYR:HB2     | 2:B:6:ILE:HD13    | 1.80                     | 0.64              |
| 1:C:1074:LYS:HE3  | 1:C:1147:PHE:HE1  | 1.62                     | 0.64              |
| 1:C:961:LEU:HD23  | 1:C:961:LEU:C     | 2.23                     | 0.64              |
| 1:C:1099:PHE:HD1  | 1:C:1134:SER:HB3  | 1.62                     | 0.64              |
| 1:E:1099:PHE:CD1  | 1:E:1134:SER:HB3  | 2.31                     | 0.64              |
| 1:A:0:MSE:HE2     | 2:B:138:VAL:HG21  | 1.79                     | 0.64              |
| 1:A:1084:ASN:HD21 | 2:D:143:THR:HG21  | 1.62                     | 0.63              |
| 1:A:1166:ASP:OD2  | 1:A:1169:THR:CB   | 2.46                     | 0.63              |
| 2:F:181:THR:CG2   | 2:F:182:SER:H     | 2.07                     | 0.63              |
| 1:A:1025:VAL:HG23 | 1:A:1199:ILE:HG22 | 1.79                     | 0.63              |
| 1:C:1181:ILE:H    | 1:C:1181:ILE:CD1  | 2.09                     | 0.63              |
| 1:E:957:THR:HB    | 1:E:958:PRO:HD3   | 1.79                     | 0.63              |
| 1:E:1166:ASP:OD2  | 1:E:1169:THR:CB   | 2.47                     | 0.63              |
| 2:F:63:TYR:HD1    | 2:F:91:LEU:HB3    | 1.64                     | 0.63              |
| 2:B:80:LYS:O      | 2:B:81:ASP:HB2    | 1.96                     | 0.63              |
| 2:D:157:SER:O     | 2:D:159:ASP:N     | 2.32                     | 0.63              |
| 1:E:1197:LEU:HD21 | 1:E:1199:ILE:HD11 | 1.80                     | 0.63              |
| 2:F:162:MSE:HE3   | 2:F:163:ILE:HD12  | 1.81                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1197:LEU:HD21 | 1:A:1199:ILE:HD11 | 1.80                     | 0.63              |
| 1:C:1002:LYS:HZ3  | 1:C:1080:ILE:HD11 | 1.63                     | 0.63              |
| 1:E:961:LEU:C     | 1:E:961:LEU:HD23  | 2.23                     | 0.63              |
| 1:A:1117:PRO:CB   | 2:D:177:LYS:NZ    | 2.62                     | 0.62              |
| 1:C:957:THR:HB    | 1:C:958:PRO:HD3   | 1.78                     | 0.62              |
| 1:E:1181:ILE:H    | 1:E:1181:ILE:CD1  | 2.09                     | 0.62              |
| 2:D:162:MSE:HE3   | 2:D:163:ILE:HD12  | 1.81                     | 0.62              |
| 1:C:1074:LYS:HE3  | 1:C:1147:PHE:CD1  | 2.34                     | 0.62              |
| 2:D:1:MSE:HG2     | 2:D:2:ASP:N       | 2.10                     | 0.62              |
| 2:D:157:SER:HB2   | 2:D:161:GLU:HB2   | 1.80                     | 0.62              |
| 2:D:208:LEU:HD21  | 2:D:250:LEU:HB2   | 1.81                     | 0.62              |
| 1:A:1117:PRO:HB2  | 2:D:177:LYS:NZ    | 2.14                     | 0.62              |
| 2:B:71:ASN:HB2    | 2:B:73:GLU:CD     | 2.25                     | 0.62              |
| 2:B:162:MSE:HE3   | 2:B:163:ILE:HD12  | 1.81                     | 0.62              |
| 2:F:1:MSE:HG2     | 2:F:2:ASP:N       | 2.10                     | 0.62              |
| 2:F:63:TYR:CD1    | 2:F:91:LEU:HB3    | 2.34                     | 0.62              |
| 1:C:1166:ASP:OD2  | 1:C:1169:THR:CB   | 2.47                     | 0.62              |
| 1:C:1197:LEU:HD21 | 1:C:1199:ILE:HD11 | 1.80                     | 0.62              |
| 2:D:3:TYR:HB2     | 2:D:6:ILE:HD13    | 1.80                     | 0.62              |
| 1:E:1042:ARG:HG3  | 1:E:1043:GLU:N    | 2.15                     | 0.62              |
| 2:B:20:GLN:HA     | 2:B:23:GLU:CG     | 2.30                     | 0.62              |
| 1:C:990:VAL:HG11  | 1:C:1020:ILE:CD1  | 2.27                     | 0.62              |
| 2:F:3:TYR:HB2     | 2:F:6:ILE:HD13    | 1.80                     | 0.61              |
| 2:F:20:GLN:HA     | 2:F:23:GLU:CG     | 2.30                     | 0.61              |
| 2:F:156:VAL:O     | 2:F:158:GLY:N     | 2.33                     | 0.61              |
| 1:A:1083:THR:HG21 | 1:A:1118:ARG:HH12 | 1.63                     | 0.61              |
| 2:F:248:ILE:CD1   | 2:F:263:ASN:HB3   | 2.30                     | 0.61              |
| 1:A:1042:ARG:HG3  | 1:A:1043:GLU:N    | 2.15                     | 0.61              |
| 1:A:1181:ILE:H    | 1:A:1181:ILE:CD1  | 2.09                     | 0.61              |
| 2:F:240:LYS:N     | 2:F:241:PRO:HD2   | 2.15                     | 0.61              |
| 2:B:208:LEU:HD21  | 2:B:250:LEU:HB2   | 1.81                     | 0.61              |
| 2:D:240:LYS:N     | 2:D:241:PRO:HD2   | 2.15                     | 0.61              |
| 1:C:1083:THR:HG21 | 1:C:1118:ARG:HH12 | 1.63                     | 0.61              |
| 2:D:71:ASN:HB2    | 2:D:73:GLU:CD     | 2.25                     | 0.61              |
| 2:F:197:TRP:CZ3   | 2:F:223:LEU:HD22  | 2.36                     | 0.61              |
| 2:F:208:LEU:HD21  | 2:F:250:LEU:HB2   | 1.81                     | 0.61              |
| 1:E:957:THR:O     | 1:E:959:CYS:N     | 2.34                     | 0.61              |
| 1:E:994:MSE:HE1   | 1:E:1013:PHE:HD2  | 1.66                     | 0.61              |
| 1:A:971:TYR:CA    | 2:B:211:ARG:HH21  | 2.13                     | 0.61              |
| 1:C:1042:ARG:HG3  | 1:C:1043:GLU:N    | 2.15                     | 0.61              |
| 1:E:930:GLN:C     | 1:E:1194:ALA:HB1  | 2.26                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:961:LEU:HD23  | 1:A:962:PRO:CD    | 2.31                     | 0.61              |
| 1:E:1083:THR:HG21 | 1:E:1118:ARG:HH12 | 1.63                     | 0.61              |
| 2:F:71:ASN:HB2    | 2:F:73:GLU:CD     | 2.25                     | 0.61              |
| 1:C:957:THR:O     | 1:C:959:CYS:N     | 2.34                     | 0.61              |
| 2:B:79:LEU:HD23   | 2:B:84:ASN:OD1    | 2.01                     | 0.60              |
| 1:C:954:ILE:HA    | 2:D:205:ASN:ND2   | 2.15                     | 0.60              |
| 1:C:1025:VAL:O    | 1:C:1201:VAL:HG23 | 2.01                     | 0.60              |
| 2:D:248:ILE:CD1   | 2:D:263:ASN:HB3   | 2.30                     | 0.60              |
| 2:F:204:LEU:O     | 2:F:204:LEU:HD12  | 2.01                     | 0.60              |
| 2:B:248:ILE:CD1   | 2:B:263:ASN:HB3   | 2.30                     | 0.60              |
| 2:D:197:TRP:CZ3   | 2:D:223:LEU:HD22  | 2.36                     | 0.60              |
| 2:B:240:LYS:N     | 2:B:241:PRO:HD2   | 2.15                     | 0.60              |
| 1:C:961:LEU:HG    | 1:C:962:PRO:HD2   | 1.83                     | 0.60              |
| 2:D:72:ILE:HG13   | 2:D:99:LEU:HD11   | 1.82                     | 0.60              |
| 1:E:915:VAL:HG11  | 1:E:943:PHE:HA    | 1.84                     | 0.60              |
| 1:A:957:THR:O     | 1:A:959:CYS:N     | 2.34                     | 0.60              |
| 1:C:915:VAL:HG11  | 1:C:943:PHE:HA    | 1.84                     | 0.60              |
| 1:E:961:LEU:HD23  | 1:E:962:PRO:CD    | 2.31                     | 0.60              |
| 2:F:79:LEU:HD23   | 2:F:84:ASN:OD1    | 2.01                     | 0.60              |
| 1:C:910:LEU:HB2   | 1:C:911:PRO:HD2   | 1.84                     | 0.60              |
| 1:C:1005:LYS:HB3  | 1:C:1008:ILE:HD13 | 1.84                     | 0.60              |
| 2:F:149:THR:C     | 2:F:151:ALA:H     | 2.09                     | 0.60              |
| 1:C:1023:LEU:HD23 | 1:C:1024:MSE:N    | 2.17                     | 0.60              |
| 2:D:79:LEU:HD23   | 2:D:84:ASN:OD1    | 2.01                     | 0.60              |
| 1:E:1023:LEU:HD23 | 1:E:1024:MSE:N    | 2.17                     | 0.60              |
| 2:D:149:THR:C     | 2:D:151:ALA:H     | 2.09                     | 0.60              |
| 1:C:994:MSE:HE1   | 1:C:1013:PHE:HD2  | 1.66                     | 0.59              |
| 1:C:1045:ILE:HB   | 1:C:1184:ILE:HD12 | 1.84                     | 0.59              |
| 2:D:195:PRO:CG    | 1:E:1079:PRO:HG3  | 2.25                     | 0.59              |
| 1:E:910:LEU:HB2   | 1:E:911:PRO:HD2   | 1.84                     | 0.59              |
| 1:E:961:LEU:HG    | 1:E:962:PRO:HD2   | 1.84                     | 0.59              |
| 1:E:1071:TYR:HE2  | 1:E:1141:PHE:HB2  | 1.67                     | 0.59              |
| 2:D:20:GLN:HA     | 2:D:23:GLU:CG     | 2.30                     | 0.59              |
| 2:F:15:PHE:HB3    | 2:F:40:THR:HG23   | 1.83                     | 0.59              |
| 2:B:197:TRP:CZ3   | 2:B:223:LEU:HD22  | 2.36                     | 0.59              |
| 2:B:204:LEU:HD12  | 2:B:204:LEU:O     | 2.02                     | 0.59              |
| 1:A:1005:LYS:HB3  | 1:A:1008:ILE:HD13 | 1.84                     | 0.59              |
| 2:D:149:THR:C     | 2:D:151:ALA:N     | 2.59                     | 0.59              |
| 1:E:1094:PHE:C    | 1:E:1096:HIS:H    | 2.10                     | 0.59              |
| 1:A:915:VAL:HG11  | 1:A:943:PHE:HA    | 1.84                     | 0.59              |
| 2:B:15:PHE:HB3    | 2:B:40:THR:HG23   | 1.83                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:990:VAL:HG11  | 1:E:1020:ILE:CD1  | 2.27                     | 0.59              |
| 1:A:994:MSE:HE1   | 1:A:1013:PHE:HD2  | 1.66                     | 0.59              |
| 1:A:1002:LYS:HZ2  | 2:D:147:ASN:HB3   | 1.68                     | 0.59              |
| 1:A:1018:TYR:HE2  | 1:A:1187:ILE:CG1  | 2.15                     | 0.59              |
| 1:A:1132:MSE:O    | 1:A:1134:SER:N    | 2.35                     | 0.59              |
| 1:A:961:LEU:HG    | 1:A:962:PRO:HD2   | 1.84                     | 0.59              |
| 2:B:63:TYR:CD1    | 2:B:91:LEU:HB3    | 2.38                     | 0.59              |
| 1:C:1094:PHE:C    | 1:C:1096:HIS:H    | 2.10                     | 0.59              |
| 1:C:1162:PRO:HB2  | 1:C:1175:ILE:HG13 | 1.85                     | 0.59              |
| 1:E:1162:PRO:HB2  | 1:E:1175:ILE:HG13 | 1.85                     | 0.59              |
| 1:A:910:LEU:HB2   | 1:A:911:PRO:HD2   | 1.84                     | 0.59              |
| 1:A:1023:LEU:HD23 | 1:A:1024:MSE:N    | 2.17                     | 0.59              |
| 1:A:1117:PRO:HA   | 2:D:177:LYS:HZ1   | 1.68                     | 0.59              |
| 1:C:975:VAL:O     | 1:C:976:SER:C     | 2.46                     | 0.59              |
| 1:C:1084:ASN:O    | 1:C:1088:VAL:HG23 | 2.03                     | 0.59              |
| 1:E:1005:LYS:HB3  | 1:E:1008:ILE:HD13 | 1.84                     | 0.59              |
| 2:B:193:THR:HB    | 2:B:194:PHE:CD1   | 2.38                     | 0.59              |
| 1:C:961:LEU:HD21  | 2:D:134:LEU:HD11  | 1.84                     | 0.59              |
| 1:A:1084:ASN:O    | 1:A:1088:VAL:HG23 | 2.03                     | 0.58              |
| 2:D:193:THR:HB    | 2:D:194:PHE:CD1   | 2.38                     | 0.58              |
| 2:D:216:ALA:O     | 2:D:220:VAL:HG23  | 2.03                     | 0.58              |
| 2:D:204:LEU:HD12  | 2:D:204:LEU:O     | 2.02                     | 0.58              |
| 1:A:1162:PRO:HB2  | 1:A:1175:ILE:HG13 | 1.85                     | 0.58              |
| 2:D:15:PHE:HB3    | 2:D:40:THR:HG23   | 1.83                     | 0.58              |
| 2:F:193:THR:HB    | 2:F:194:PHE:CD1   | 2.37                     | 0.58              |
| 1:A:981:LEU:HB3   | 1:A:1024:MSE:HE1  | 1.84                     | 0.58              |
| 1:C:961:LEU:CG    | 1:C:962:PRO:HD2   | 2.34                     | 0.58              |
| 1:A:1136:ALA:C    | 1:A:1137:ILE:HG13 | 2.28                     | 0.58              |
| 1:C:1025:VAL:CG1  | 1:C:1030:ASP:HB2  | 2.31                     | 0.58              |
| 2:B:69:THR:HB     | 2:B:71:ASN:OD1    | 2.04                     | 0.58              |
| 1:C:961:LEU:HD23  | 1:C:962:PRO:CD    | 2.32                     | 0.58              |
| 1:E:975:VAL:O     | 1:E:976:SER:C     | 2.45                     | 0.58              |
| 1:A:1033:LEU:HD23 | 1:A:1033:LEU:O    | 2.04                     | 0.58              |
| 2:D:35:PHE:CG     | 2:D:87:TYR:CD2    | 2.92                     | 0.58              |
| 2:F:149:THR:C     | 2:F:151:ALA:N     | 2.60                     | 0.58              |
| 1:A:1094:PHE:C    | 1:A:1096:HIS:H    | 2.10                     | 0.58              |
| 1:C:1028:ALA:CB   | 1:C:1200:ARG:CZ   | 2.70                     | 0.58              |
| 2:D:44:LEU:O      | 2:D:45:GLY:C      | 2.46                     | 0.58              |
| 1:E:1136:ALA:C    | 1:E:1137:ILE:HG13 | 2.28                     | 0.58              |
| 2:D:149:THR:O     | 2:D:151:ALA:N     | 2.37                     | 0.58              |
| 1:A:1003:LEU:CD2  | 2:D:106:LEU:HD22  | 2.34                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1033:LEU:HD23 | 1:E:1033:LEU:O    | 2.04                     | 0.57              |
| 2:D:72:ILE:HD12   | 2:D:72:ILE:N      | 2.18                     | 0.57              |
| 2:D:157:SER:C     | 2:D:159:ASP:H     | 2.13                     | 0.57              |
| 1:E:1025:VAL:CG1  | 1:E:1030:ASP:HB2  | 2.31                     | 0.57              |
| 2:F:149:THR:O     | 2:F:151:ALA:N     | 2.38                     | 0.57              |
| 1:A:975:VAL:O     | 1:A:976:SER:C     | 2.45                     | 0.57              |
| 2:B:149:THR:C     | 2:B:151:ALA:N     | 2.60                     | 0.57              |
| 2:B:149:THR:C     | 2:B:151:ALA:H     | 2.09                     | 0.57              |
| 2:F:59:VAL:O      | 2:F:62:LEU:HB2    | 2.05                     | 0.57              |
| 1:C:1033:LEU:HD23 | 1:C:1033:LEU:O    | 2.04                     | 0.57              |
| 2:F:72:ILE:HD12   | 2:F:72:ILE:N      | 2.18                     | 0.57              |
| 2:B:92:LEU:HD22   | 2:B:96:GLN:HG3    | 1.87                     | 0.57              |
| 2:B:222:LEU:HD21  | 2:B:228:TYR:HE1   | 1.68                     | 0.57              |
| 1:C:1147:PHE:CD1  | 1:C:1147:PHE:C    | 2.82                     | 0.57              |
| 1:E:1084:ASN:O    | 1:E:1088:VAL:HG23 | 2.03                     | 0.57              |
| 2:F:216:ALA:O     | 2:F:220:VAL:HG23  | 2.03                     | 0.57              |
| 2:B:149:THR:O     | 2:B:151:ALA:N     | 2.38                     | 0.57              |
| 1:C:1136:ALA:C    | 1:C:1137:ILE:HG13 | 2.28                     | 0.57              |
| 1:E:921:ASP:OD2   | 2:F:288:LEU:HD22  | 2.04                     | 0.57              |
| 1:E:1123:ARG:HH11 | 1:E:1123:ARG:HG2  | 1.70                     | 0.57              |
| 1:A:940:LYS:HA    | 2:B:285:PHE:CZ    | 2.40                     | 0.57              |
| 1:A:954:ILE:HD13  | 1:A:955:PRO:HD2   | 1.87                     | 0.57              |
| 2:B:59:VAL:O      | 2:B:62:LEU:HB2    | 2.05                     | 0.57              |
| 1:C:1147:PHE:HD1  | 1:C:1147:PHE:C    | 2.13                     | 0.57              |
| 1:E:961:LEU:CG    | 1:E:962:PRO:HD2   | 2.34                     | 0.57              |
| 1:E:1110:LEU:HD11 | 1:E:1123:ARG:HA   | 1.87                     | 0.57              |
| 1:C:1110:LEU:HD11 | 1:C:1123:ARG:HA   | 1.87                     | 0.57              |
| 1:C:1131:SER:OG   | 1:C:1132:MSE:HE2  | 2.05                     | 0.57              |
| 2:D:92:LEU:HD22   | 2:D:96:GLN:HG3    | 1.87                     | 0.57              |
| 2:D:157:SER:C     | 2:D:159:ASP:N     | 2.63                     | 0.57              |
| 1:E:1001:PHE:CE1  | 1:E:1048:LEU:HD21 | 2.40                     | 0.57              |
| 1:E:1147:PHE:CD1  | 1:E:1147:PHE:C    | 2.83                     | 0.57              |
| 2:B:230:VAL:O     | 2:B:233:LYS:HG3   | 2.05                     | 0.57              |
| 2:D:59:VAL:O      | 2:D:62:LEU:HB2    | 2.05                     | 0.57              |
| 1:E:974:THR:HG22  | 1:E:974:THR:O     | 2.04                     | 0.57              |
| 1:A:990:VAL:HG11  | 1:A:1020:ILE:CD1  | 2.27                     | 0.56              |
| 2:D:222:LEU:HD21  | 2:D:228:TYR:HE1   | 1.68                     | 0.56              |
| 2:D:230:VAL:O     | 2:D:233:LYS:HG3   | 2.05                     | 0.56              |
| 1:E:1074:LYS:HE3  | 1:E:1147:PHE:HE1  | 1.67                     | 0.56              |
| 1:A:930:GLN:HB3   | 1:A:1196:GLY:O    | 2.05                     | 0.56              |
| 1:A:961:LEU:CG    | 1:A:962:PRO:HD2   | 2.35                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1147:PHE:CD1  | 1:A:1147:PHE:C    | 2.82                     | 0.56              |
| 2:B:216:ALA:O     | 2:B:220:VAL:HG23  | 2.03                     | 0.56              |
| 1:E:1065:MSE:HG3  | 1:E:1066:LEU:N    | 2.19                     | 0.56              |
| 1:E:1131:SER:OG   | 1:E:1132:MSE:HE2  | 2.05                     | 0.56              |
| 1:A:989:VAL:O     | 1:A:990:VAL:C     | 2.48                     | 0.56              |
| 1:A:1001:PHE:CE1  | 1:A:1048:LEU:HD21 | 2.40                     | 0.56              |
| 1:A:1074:LYS:HE3  | 1:A:1147:PHE:HE1  | 1.70                     | 0.56              |
| 2:B:1:MSE:HG2     | 2:B:2:ASP:N       | 2.10                     | 0.56              |
| 2:B:72:ILE:HD12   | 2:B:72:ILE:N      | 2.18                     | 0.56              |
| 2:D:106:LEU:O     | 2:D:110:VAL:HG23  | 2.06                     | 0.56              |
| 2:D:252:LEU:HD21  | 2:D:259:GLU:HG3   | 1.87                     | 0.56              |
| 2:F:35:PHE:CG     | 2:F:87:TYR:CD2    | 2.94                     | 0.56              |
| 2:F:92:LEU:HD22   | 2:F:96:GLN:HG3    | 1.87                     | 0.56              |
| 2:F:252:LEU:HD21  | 2:F:259:GLU:HG3   | 1.87                     | 0.56              |
| 1:C:1123:ARG:HG2  | 1:C:1123:ARG:HH11 | 1.70                     | 0.56              |
| 2:B:252:LEU:HD21  | 2:B:259:GLU:HG3   | 1.87                     | 0.56              |
| 1:C:983:TYR:CE2   | 2:D:253:MSE:HG2   | 2.40                     | 0.56              |
| 1:C:1099:PHE:CD1  | 1:C:1134:SER:HB3  | 2.40                     | 0.56              |
| 2:F:230:VAL:O     | 2:F:233:LYS:HG3   | 2.05                     | 0.56              |
| 2:D:181:THR:CG2   | 2:D:182:SER:N     | 2.64                     | 0.56              |
| 1:E:1083:THR:HG23 | 1:E:1109:PHE:CE1  | 2.41                     | 0.56              |
| 1:A:1123:ARG:HG2  | 1:A:1123:ARG:HH11 | 1.70                     | 0.56              |
| 1:C:1001:PHE:CE1  | 1:C:1048:LEU:HD21 | 2.40                     | 0.56              |
| 2:D:156:VAL:O     | 2:D:158:GLY:N     | 2.38                     | 0.56              |
| 2:F:222:LEU:HD21  | 2:F:228:TYR:HE1   | 1.69                     | 0.56              |
| 1:A:981:LEU:HD13  | 1:A:1024:MSE:CE   | 2.36                     | 0.56              |
| 1:A:1083:THR:HG23 | 1:A:1109:PHE:CE1  | 2.41                     | 0.56              |
| 1:C:974:THR:O     | 1:C:974:THR:HG22  | 2.04                     | 0.56              |
| 1:C:1083:THR:HG23 | 1:C:1109:PHE:CE1  | 2.41                     | 0.56              |
| 1:E:1018:TYR:HE2  | 1:E:1187:ILE:CG1  | 2.18                     | 0.56              |
| 1:A:1131:SER:OG   | 1:A:1132:MSE:HE2  | 2.05                     | 0.56              |
| 2:B:54:SER:C      | 2:B:56:LEU:N      | 2.64                     | 0.56              |
| 1:C:1113:ILE:HD12 | 2:F:231:GLU:HB3   | 1.88                     | 0.56              |
| 2:F:37:LYS:HE2    | 2:F:50:GLN:HE22   | 1.71                     | 0.56              |
| 1:A:974:THR:HG22  | 1:A:974:THR:O     | 2.04                     | 0.56              |
| 2:B:63:TYR:HD1    | 2:B:91:LEU:HB3    | 1.70                     | 0.56              |
| 2:B:106:LEU:O     | 2:B:110:VAL:HG23  | 2.05                     | 0.56              |
| 2:B:222:LEU:HD23  | 2:B:222:LEU:C     | 2.30                     | 0.56              |
| 2:B:270:HIS:CD2   | 2:B:272:HIS:HB3   | 2.41                     | 0.56              |
| 1:C:954:ILE:HD13  | 1:C:955:PRO:HD2   | 1.88                     | 0.56              |
| 1:C:1151:ALA:HB3  | 1:C:1173:TYR:CE2  | 2.41                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:222:LEU:HD23  | 2:D:222:LEU:C     | 2.31                     | 0.56              |
| 1:E:1147:PHE:HD1  | 1:E:1147:PHE:C    | 2.13                     | 0.56              |
| 1:A:932:GLY:O     | 1:A:1188:SER:HB2  | 2.06                     | 0.55              |
| 1:C:1002:LYS:HZ1  | 1:C:1080:ILE:HD11 | 1.71                     | 0.55              |
| 2:F:222:LEU:HD23  | 2:F:222:LEU:C     | 2.31                     | 0.55              |
| 2:D:270:HIS:CD2   | 2:D:272:HIS:HB3   | 2.41                     | 0.55              |
| 2:D:25:PHE:O      | 2:D:26:SER:C      | 2.50                     | 0.55              |
| 1:E:989:VAL:O     | 1:E:990:VAL:C     | 2.48                     | 0.55              |
| 1:E:1151:ALA:HB3  | 1:E:1173:TYR:CE2  | 2.41                     | 0.55              |
| 1:A:1147:PHE:HD1  | 1:A:1147:PHE:C    | 2.13                     | 0.55              |
| 1:C:987:LEU:O     | 1:C:988:ASP:C     | 2.49                     | 0.55              |
| 2:B:148:TYR:O     | 2:B:151:ALA:HB3   | 2.07                     | 0.55              |
| 1:C:1065:MSE:HG3  | 1:C:1066:LEU:N    | 2.19                     | 0.55              |
| 1:E:954:ILE:HD13  | 1:E:955:PRO:HD2   | 1.88                     | 0.55              |
| 2:F:106:LEU:O     | 2:F:110:VAL:HG23  | 2.06                     | 0.55              |
| 2:B:1:MSE:CG      | 2:B:2:ASP:H       | 2.10                     | 0.55              |
| 1:C:989:VAL:O     | 1:C:990:VAL:C     | 2.48                     | 0.55              |
| 2:D:35:PHE:CG     | 2:D:87:TYR:HD2    | 2.23                     | 0.55              |
| 1:E:930:GLN:O     | 1:E:1194:ALA:HB1  | 2.07                     | 0.55              |
| 1:A:1065:MSE:HG3  | 1:A:1066:LEU:N    | 2.20                     | 0.55              |
| 1:E:946:ILE:HD11  | 1:E:1022:LEU:HB3  | 1.88                     | 0.55              |
| 1:A:1110:LEU:HD11 | 1:A:1123:ARG:HA   | 1.87                     | 0.55              |
| 2:B:270:HIS:CG    | 2:B:271:GLU:H     | 2.25                     | 0.55              |
| 1:A:954:ILE:HA    | 2:B:205:ASN:ND2   | 2.22                     | 0.55              |
| 1:A:987:LEU:O     | 1:A:988:ASP:C     | 2.49                     | 0.55              |
| 1:A:1153:THR:O    | 1:A:1154:TYR:CB   | 2.55                     | 0.55              |
| 2:B:6:ILE:CD1     | 2:B:6:ILE:N       | 2.67                     | 0.55              |
| 2:B:35:PHE:CG     | 2:B:87:TYR:HD2    | 2.24                     | 0.55              |
| 1:C:1028:ALA:HA   | 1:C:1200:ARG:HD2  | 1.88                     | 0.55              |
| 1:A:931:VAL:HG11  | 1:A:1168:LEU:HD13 | 1.89                     | 0.54              |
| 1:A:961:LEU:HD23  | 1:A:962:PRO:N     | 2.22                     | 0.54              |
| 1:E:987:LEU:O     | 1:E:988:ASP:C     | 2.49                     | 0.54              |
| 2:F:270:HIS:CG    | 2:F:271:GLU:H     | 2.25                     | 0.54              |
| 2:F:270:HIS:CD2   | 2:F:272:HIS:HB3   | 2.41                     | 0.54              |
| 2:B:263:ASN:C     | 2:B:263:ASN:OD1   | 2.50                     | 0.54              |
| 1:E:976:SER:C     | 1:E:978:ASP:N     | 2.51                     | 0.54              |
| 1:E:1153:THR:O    | 1:E:1154:TYR:CB   | 2.55                     | 0.54              |
| 2:F:148:TYR:O     | 2:F:151:ALA:HB3   | 2.07                     | 0.54              |
| 2:F:258:THR:O     | 2:F:259:GLU:C     | 2.50                     | 0.54              |
| 1:A:1151:ALA:HB3  | 1:A:1173:TYR:CE2  | 2.41                     | 0.54              |
| 2:D:148:TYR:O     | 2:D:151:ALA:HB3   | 2.07                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:162:MSE:HE3   | 2:F:163:ILE:HD13  | 1.90                     | 0.54              |
| 1:A:1117:PRO:CB   | 2:D:177:LYS:HZ1   | 2.18                     | 0.54              |
| 2:B:25:PHE:O      | 2:B:26:SER:C      | 2.50                     | 0.54              |
| 1:A:1066:LEU:HB3  | 1:A:1093:HIS:CE1  | 2.43                     | 0.54              |
| 2:B:4:PHE:HD1     | 2:B:159:ASP:HB2   | 1.71                     | 0.54              |
| 1:C:981:LEU:HD13  | 1:C:1024:MSE:CE   | 2.38                     | 0.54              |
| 2:D:76:GLU:OE2    | 2:D:104:LYS:NZ    | 2.40                     | 0.54              |
| 1:E:930:GLN:HB3   | 1:E:1196:GLY:O    | 2.07                     | 0.54              |
| 1:E:933:VAL:HG13  | 1:E:1187:ILE:HG23 | 1.90                     | 0.54              |
| 1:E:1181:ILE:HD12 | 1:E:1181:ILE:N    | 2.22                     | 0.54              |
| 2:F:54:SER:C      | 2:F:56:LEU:N      | 2.64                     | 0.54              |
| 1:C:1153:THR:O    | 1:C:1154:TYR:CB   | 2.55                     | 0.54              |
| 2:D:270:HIS:CG    | 2:D:271:GLU:H     | 2.25                     | 0.54              |
| 2:D:291:LYS:O     | 2:D:291:LYS:HG2   | 2.08                     | 0.54              |
| 2:D:291:LYS:HD2   | 2:D:292:TYR:CE1   | 2.43                     | 0.54              |
| 1:E:938:PRO:HG2   | 1:E:1187:ILE:HD11 | 1.89                     | 0.54              |
| 1:E:1006:PRO:HG2  | 1:E:1007:ASP:H    | 1.73                     | 0.54              |
| 1:E:1066:LEU:HB3  | 1:E:1093:HIS:CE1  | 2.43                     | 0.54              |
| 1:A:1003:LEU:HD21 | 2:D:110:VAL:CG2   | 2.33                     | 0.54              |
| 1:A:1006:PRO:HG2  | 1:A:1007:ASP:H    | 1.73                     | 0.54              |
| 1:A:1065:MSE:SE   | 1:A:1066:LEU:HD23 | 2.58                     | 0.54              |
| 2:B:291:LYS:O     | 2:B:291:LYS:HG2   | 2.07                     | 0.54              |
| 1:C:1071:TYR:HE2  | 1:C:1141:PHE:HB2  | 1.71                     | 0.54              |
| 1:C:1181:ILE:HD12 | 1:C:1181:ILE:N    | 2.22                     | 0.54              |
| 2:D:263:ASN:C     | 2:D:263:ASN:OD1   | 2.51                     | 0.54              |
| 1:E:952:THR:HA    | 2:F:249:THR:HG21  | 1.89                     | 0.54              |
| 1:E:1035:HIS:O    | 1:E:1039:GLU:HG2  | 2.08                     | 0.54              |
| 1:E:1060:GLY:C    | 1:E:1062:THR:H    | 2.16                     | 0.54              |
| 2:F:263:ASN:OD1   | 2:F:263:ASN:C     | 2.51                     | 0.54              |
| 1:A:981:LEU:HB3   | 1:A:982:PRO:HD2   | 1.90                     | 0.54              |
| 2:B:30:ASP:CB     | 2:B:33:LEU:HD12   | 2.38                     | 0.54              |
| 2:F:69:THR:CB     | 2:F:71:ASN:OD1    | 2.56                     | 0.54              |
| 1:A:1060:GLY:C    | 1:A:1062:THR:H    | 2.16                     | 0.54              |
| 1:C:1035:HIS:O    | 1:C:1039:GLU:HG2  | 2.08                     | 0.54              |
| 2:D:30:ASP:CB     | 2:D:33:LEU:HD12   | 2.37                     | 0.54              |
| 2:D:37:LYS:HE2    | 2:D:50:GLN:HE22   | 1.73                     | 0.54              |
| 2:D:166:LEU:O     | 2:D:169:SER:HB3   | 2.08                     | 0.54              |
| 1:A:1025:VAL:CG1  | 1:A:1030:ASP:HB2  | 2.31                     | 0.53              |
| 1:A:1071:TYR:HE2  | 1:A:1141:PHE:HB2  | 1.73                     | 0.53              |
| 1:C:1066:LEU:HB3  | 1:C:1093:HIS:CE1  | 2.43                     | 0.53              |
| 1:C:1113:ILE:HD11 | 2:F:227:TYR:CD1   | 2.43                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:981:LEU:HB3   | 1:E:982:PRO:HD2   | 1.90                     | 0.53              |
| 2:F:35:PHE:CG     | 2:F:87:TYR:HD2    | 2.24                     | 0.53              |
| 2:B:162:MSE:HE3   | 2:B:163:ILE:HD13  | 1.90                     | 0.53              |
| 2:B:258:THR:O     | 2:B:259:GLU:C     | 2.50                     | 0.53              |
| 1:C:1006:PRO:HG2  | 1:C:1007:ASP:H    | 1.73                     | 0.53              |
| 1:E:1025:VAL:HG23 | 1:E:1199:ILE:CG2  | 2.39                     | 0.53              |
| 1:E:1189:LYS:CE   | 1:E:1192:ALA:HB2  | 2.36                     | 0.53              |
| 2:F:166:LEU:O     | 2:F:169:SER:HB3   | 2.08                     | 0.53              |
| 1:A:966:GLY:HA3   | 2:B:173:PHE:CZ    | 2.43                     | 0.53              |
| 1:A:1035:HIS:O    | 1:A:1039:GLU:HG2  | 2.08                     | 0.53              |
| 2:D:162:MSE:HE3   | 2:D:163:ILE:HD13  | 1.90                     | 0.53              |
| 2:D:222:LEU:CD2   | 2:D:228:TYR:CE1   | 2.92                     | 0.53              |
| 2:B:222:LEU:CD2   | 2:B:228:TYR:CE1   | 2.92                     | 0.53              |
| 2:B:272:HIS:O     | 2:B:273:ALA:C     | 2.52                     | 0.53              |
| 2:D:4:PHE:HD1     | 2:D:159:ASP:HB2   | 1.73                     | 0.53              |
| 2:D:102:LEU:HD13  | 2:D:135:ASN:HB2   | 1.91                     | 0.53              |
| 1:E:961:LEU:HD23  | 1:E:962:PRO:N     | 2.23                     | 0.53              |
| 1:E:974:THR:O     | 1:E:975:VAL:HG23  | 2.08                     | 0.53              |
| 1:E:994:MSE:HE2   | 1:E:1013:PHE:HD2  | 1.73                     | 0.53              |
| 1:E:1018:TYR:HE2  | 1:E:1187:ILE:HG12 | 1.73                     | 0.53              |
| 1:E:1065:MSE:SE   | 1:E:1066:LEU:HD23 | 2.58                     | 0.53              |
| 1:A:962:PRO:HG2   | 2:B:134:LEU:CD1   | 2.38                     | 0.53              |
| 1:A:974:THR:O     | 1:A:975:VAL:HG23  | 2.08                     | 0.53              |
| 1:C:974:THR:O     | 1:C:975:VAL:HG23  | 2.08                     | 0.53              |
| 1:C:998:TYR:HD1   | 1:C:998:TYR:N     | 2.07                     | 0.53              |
| 1:C:1123:ARG:HG2  | 1:C:1123:ARG:NH1  | 2.24                     | 0.53              |
| 1:E:1099:PHE:HB3  | 1:E:1129:ALA:HB1  | 1.91                     | 0.53              |
| 1:A:962:PRO:HG2   | 2:B:134:LEU:HD11  | 1.89                     | 0.53              |
| 1:A:971:TYR:HA    | 2:B:211:ARG:HH21  | 1.71                     | 0.53              |
| 1:A:1189:LYS:CE   | 1:A:1192:ALA:HB2  | 2.36                     | 0.53              |
| 1:C:961:LEU:HD23  | 1:C:962:PRO:N     | 2.23                     | 0.53              |
| 2:D:258:THR:O     | 2:D:259:GLU:C     | 2.50                     | 0.53              |
| 2:F:14:ASN:O      | 2:F:14:ASN:ND2    | 2.37                     | 0.53              |
| 2:F:25:PHE:O      | 2:F:26:SER:C      | 2.50                     | 0.53              |
| 2:F:272:HIS:O     | 2:F:273:ALA:C     | 2.52                     | 0.53              |
| 2:F:291:LYS:O     | 2:F:291:LYS:HG2   | 2.08                     | 0.53              |
| 2:B:227:TYR:HA    | 2:B:231:GLU:HG3   | 1.91                     | 0.53              |
| 1:C:1004:ASN:CG   | 1:C:1004:ASN:O    | 2.52                     | 0.53              |
| 1:C:1099:PHE:HB3  | 1:C:1129:ALA:HB1  | 1.91                     | 0.53              |
| 2:D:269:ASP:OD1   | 2:D:269:ASP:C     | 2.52                     | 0.53              |
| 1:E:998:TYR:N     | 1:E:998:TYR:HD1   | 2.07                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1045:ILE:CD1  | 1:E:1184:ILE:HG23 | 2.37                     | 0.53              |
| 1:A:904:TRP:CH2   | 1:A:982:PRO:HB3   | 2.44                     | 0.53              |
| 2:F:227:TYR:HA    | 2:F:231:GLU:HG3   | 1.91                     | 0.53              |
| 1:A:1025:VAL:HG12 | 1:A:1026:ASP:N    | 2.24                     | 0.53              |
| 1:A:1090:MSE:CE   | 1:A:1106:ALA:HA   | 2.21                     | 0.53              |
| 2:F:269:ASP:OD1   | 2:F:269:ASP:C     | 2.52                     | 0.53              |
| 1:A:931:VAL:HG12  | 1:A:933:VAL:HG23  | 1.91                     | 0.52              |
| 1:A:998:TYR:N     | 1:A:998:TYR:CD1   | 2.77                     | 0.52              |
| 1:A:1181:ILE:HD12 | 1:A:1181:ILE:N    | 2.22                     | 0.52              |
| 1:E:1002:LYS:HZ1  | 1:E:1080:ILE:HD11 | 1.73                     | 0.52              |
| 1:E:1132:MSE:O    | 1:E:1134:SER:N    | 2.42                     | 0.52              |
| 2:F:135:ASN:O     | 2:F:136:ASN:HB2   | 2.09                     | 0.52              |
| 2:B:35:PHE:CG     | 2:B:87:TYR:CD2    | 2.97                     | 0.52              |
| 1:C:1065:MSE:SE   | 1:C:1066:LEU:HD23 | 2.59                     | 0.52              |
| 1:C:1109:PHE:C    | 1:C:1109:PHE:CD2  | 2.87                     | 0.52              |
| 2:D:231:GLU:HB3   | 1:E:1113:ILE:CD1  | 2.38                     | 0.52              |
| 2:D:272:HIS:O     | 2:D:273:ALA:C     | 2.52                     | 0.52              |
| 1:E:1075:ALA:O    | 1:E:1077:LEU:HG   | 2.09                     | 0.52              |
| 1:E:1109:PHE:C    | 1:E:1109:PHE:CD2  | 2.87                     | 0.52              |
| 1:A:998:TYR:N     | 1:A:998:TYR:HD1   | 2.07                     | 0.52              |
| 1:A:1101:GLN:O    | 1:A:1104:TYR:HB3  | 2.09                     | 0.52              |
| 1:C:1025:VAL:HG12 | 1:C:1026:ASP:N    | 2.24                     | 0.52              |
| 1:C:1101:GLN:O    | 1:C:1104:TYR:HB3  | 2.10                     | 0.52              |
| 2:D:178:GLU:OE1   | 2:D:182:SER:HB3   | 2.10                     | 0.52              |
| 1:E:961:LEU:CD2   | 1:E:962:PRO:HD2   | 2.39                     | 0.52              |
| 1:A:961:LEU:CD2   | 1:A:962:PRO:HD2   | 2.39                     | 0.52              |
| 1:A:1002:LYS:HZ1  | 1:A:1080:ILE:HD11 | 1.72                     | 0.52              |
| 1:C:1042:ARG:HD3  | 1:C:1169:THR:HG22 | 1.90                     | 0.52              |
| 1:E:1029:GLU:O    | 1:E:1032:LYS:HB3  | 2.10                     | 0.52              |
| 1:A:1075:ALA:O    | 1:A:1077:LEU:HG   | 2.10                     | 0.52              |
| 1:A:1109:PHE:C    | 1:A:1109:PHE:CD2  | 2.87                     | 0.52              |
| 1:C:961:LEU:CD2   | 1:C:962:PRO:HD2   | 2.39                     | 0.52              |
| 1:C:998:TYR:N     | 1:C:998:TYR:CD1   | 2.77                     | 0.52              |
| 2:D:222:LEU:CD2   | 2:D:228:TYR:HE1   | 2.22                     | 0.52              |
| 1:E:1008:ILE:HD12 | 1:E:1008:ILE:N    | 2.25                     | 0.52              |
| 2:F:222:LEU:CD2   | 2:F:228:TYR:HE1   | 2.23                     | 0.52              |
| 1:A:1004:ASN:CG   | 1:A:1004:ASN:O    | 2.51                     | 0.52              |
| 1:A:1073:THR:HG23 | 1:A:1086:LEU:CD2  | 2.40                     | 0.52              |
| 1:C:1073:THR:HG23 | 1:C:1086:LEU:CD2  | 2.40                     | 0.52              |
| 2:F:178:GLU:OE1   | 2:F:182:SER:HB3   | 2.10                     | 0.52              |
| 2:F:187:TYR:O     | 2:F:188:GLU:C     | 2.53                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:938:PRO:HG2   | 1:A:1187:ILE:HD11 | 1.92                     | 0.52              |
| 2:B:166:LEU:O     | 2:B:169:SER:HB3   | 2.08                     | 0.52              |
| 2:B:181:THR:CG2   | 2:B:182:SER:H     | 2.07                     | 0.52              |
| 2:B:260:ASP:O     | 2:B:262:THR:N     | 2.43                     | 0.52              |
| 1:C:974:THR:O     | 1:C:975:VAL:CG2   | 2.58                     | 0.52              |
| 1:C:1075:ALA:O    | 1:C:1077:LEU:HG   | 2.09                     | 0.52              |
| 2:D:87:TYR:CE1    | 2:D:120:GLY:CA    | 2.92                     | 0.52              |
| 2:D:112:GLY:HA2   | 2:D:115:ASN:OD1   | 2.09                     | 0.52              |
| 2:D:135:ASN:O     | 2:D:136:ASN:HB2   | 2.10                     | 0.52              |
| 2:D:158:GLY:O     | 2:D:159:ASP:HB3   | 2.10                     | 0.52              |
| 1:E:920:PHE:CD2   | 2:F:285:PHE:HD1   | 2.28                     | 0.52              |
| 2:F:222:LEU:CD2   | 2:F:228:TYR:CE1   | 2.92                     | 0.52              |
| 1:A:994:MSE:HE2   | 1:A:1013:PHE:HD2  | 1.73                     | 0.52              |
| 1:A:1118:ARG:NH2  | 2:D:143:THR:HA    | 2.25                     | 0.52              |
| 1:A:1123:ARG:HG2  | 1:A:1123:ARG:NH1  | 2.24                     | 0.52              |
| 2:D:227:TYR:CE2   | 1:E:1080:ILE:HB   | 2.45                     | 0.52              |
| 1:E:1094:PHE:HE1  | 1:E:1129:ALA:HB2  | 1.75                     | 0.52              |
| 2:F:158:GLY:O     | 2:F:159:ASP:HB3   | 2.10                     | 0.52              |
| 1:A:974:THR:O     | 1:A:975:VAL:CG2   | 2.58                     | 0.52              |
| 1:C:1132:MSE:O    | 1:C:1134:SER:N    | 2.43                     | 0.52              |
| 2:D:227:TYR:HA    | 2:D:231:GLU:HG3   | 1.91                     | 0.52              |
| 1:E:974:THR:O     | 1:E:975:VAL:CG2   | 2.58                     | 0.52              |
| 1:E:1109:PHE:HZ   | 1:E:1118:ARG:HD3  | 1.75                     | 0.52              |
| 2:F:56:LEU:O      | 2:F:59:VAL:HB     | 2.10                     | 0.52              |
| 2:B:135:ASN:O     | 2:B:136:ASN:HB2   | 2.09                     | 0.52              |
| 1:C:981:LEU:HB3   | 1:C:982:PRO:HD2   | 1.90                     | 0.52              |
| 2:F:30:ASP:CB     | 2:F:33:LEU:HD12   | 2.38                     | 0.52              |
| 1:A:1094:PHE:HE1  | 1:A:1129:ALA:HB2  | 1.75                     | 0.51              |
| 1:A:1099:PHE:HB3  | 1:A:1129:ALA:HB1  | 1.91                     | 0.51              |
| 1:C:987:LEU:HD23  | 1:C:1033:LEU:HD22 | 1.92                     | 0.51              |
| 1:C:1094:PHE:HE1  | 1:C:1129:ALA:HB2  | 1.75                     | 0.51              |
| 2:D:260:ASP:O     | 2:D:262:THR:N     | 2.43                     | 0.51              |
| 1:A:1018:TYR:HE2  | 1:A:1187:ILE:HG12 | 1.74                     | 0.51              |
| 1:A:1029:GLU:O    | 1:A:1032:LYS:HB3  | 2.10                     | 0.51              |
| 2:B:222:LEU:CD2   | 2:B:228:TYR:HE1   | 2.23                     | 0.51              |
| 2:B:241:PRO:HG2   | 2:B:242:THR:H     | 1.75                     | 0.51              |
| 2:B:269:ASP:C     | 2:B:269:ASP:OD1   | 2.52                     | 0.51              |
| 1:C:931:VAL:HG12  | 1:C:933:VAL:HG23  | 1.91                     | 0.51              |
| 2:D:56:LEU:O      | 2:D:59:VAL:HB     | 2.10                     | 0.51              |
| 1:E:904:TRP:CZ2   | 1:E:982:PRO:HB3   | 2.45                     | 0.51              |
| 1:E:1073:THR:HG23 | 1:E:1086:LEU:CD2  | 2.39                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:54:SER:O      | 2:D:56:LEU:N      | 2.37                     | 0.51              |
| 1:A:987:LEU:HD23  | 1:A:1033:LEU:HD22 | 1.92                     | 0.51              |
| 1:A:994:MSE:HE1   | 1:A:1013:PHE:CD2  | 2.45                     | 0.51              |
| 1:A:1097:LYS:O    | 1:A:1097:LYS:HG2  | 2.10                     | 0.51              |
| 2:B:96:GLN:O      | 2:B:99:LEU:HB2    | 2.10                     | 0.51              |
| 2:B:178:GLU:OE1   | 2:B:182:SER:HB3   | 2.10                     | 0.51              |
| 2:B:187:TYR:O     | 2:B:188:GLU:C     | 2.53                     | 0.51              |
| 1:C:994:MSE:HE2   | 1:C:1013:PHE:HD2  | 1.74                     | 0.51              |
| 1:C:1060:GLY:C    | 1:C:1062:THR:H    | 2.16                     | 0.51              |
| 1:C:1097:LYS:O    | 1:C:1097:LYS:HG2  | 2.10                     | 0.51              |
| 2:D:54:SER:C      | 2:D:56:LEU:N      | 2.65                     | 0.51              |
| 2:D:187:TYR:O     | 2:D:188:GLU:C     | 2.53                     | 0.51              |
| 1:E:998:TYR:N     | 1:E:998:TYR:CD1   | 2.77                     | 0.51              |
| 1:E:1097:LYS:O    | 1:E:1097:LYS:HG2  | 2.10                     | 0.51              |
| 2:F:241:PRO:HG2   | 2:F:242:THR:H     | 1.75                     | 0.51              |
| 1:A:1008:ILE:HD12 | 1:A:1008:ILE:N    | 2.25                     | 0.51              |
| 2:F:157:SER:C     | 2:F:159:ASP:H     | 2.19                     | 0.51              |
| 1:A:1045:ILE:CD1  | 1:A:1184:ILE:HG23 | 2.36                     | 0.51              |
| 1:A:1109:PHE:HZ   | 1:A:1118:ARG:HD3  | 1.75                     | 0.51              |
| 2:D:96:GLN:O      | 2:D:99:LEU:HB2    | 2.11                     | 0.51              |
| 1:E:1020:ILE:O    | 1:E:1023:LEU:HB2  | 2.11                     | 0.51              |
| 1:E:1025:VAL:HG12 | 1:E:1026:ASP:N    | 2.25                     | 0.51              |
| 2:F:1:MSE:CG      | 2:F:2:ASP:H       | 2.10                     | 0.51              |
| 2:F:260:ASP:O     | 2:F:262:THR:N     | 2.43                     | 0.51              |
| 2:B:117:GLU:C     | 2:B:119:GLU:H     | 2.17                     | 0.51              |
| 2:B:291:LYS:HD2   | 2:B:292:TYR:CE1   | 2.46                     | 0.51              |
| 1:C:911:PRO:O     | 1:C:912:ALA:C     | 2.54                     | 0.51              |
| 2:D:76:GLU:CD     | 2:D:104:LYS:NZ    | 2.68                     | 0.51              |
| 2:D:86:PRO:HG2    | 2:D:119:GLU:O     | 2.10                     | 0.51              |
| 1:E:1101:GLN:O    | 1:E:1104:TYR:HB3  | 2.09                     | 0.51              |
| 1:A:911:PRO:O     | 1:A:912:ALA:C     | 2.54                     | 0.51              |
| 1:A:983:TYR:HE2   | 2:B:253:MSE:HG2   | 1.72                     | 0.51              |
| 2:B:156:VAL:C     | 2:B:158:GLY:H     | 2.19                     | 0.51              |
| 1:C:928:SER:O     | 1:C:932:GLY:HA2   | 2.11                     | 0.51              |
| 1:C:950:CYS:O     | 1:C:968:VAL:HG23  | 2.11                     | 0.51              |
| 1:C:994:MSE:HE1   | 1:C:1013:PHE:CD2  | 2.45                     | 0.51              |
| 2:D:156:VAL:C     | 2:D:158:GLY:N     | 2.64                     | 0.51              |
| 2:D:231:GLU:OE2   | 1:E:1118:ARG:NH1  | 2.44                     | 0.51              |
| 1:E:1004:ASN:O    | 1:E:1004:ASN:CG   | 2.52                     | 0.51              |
| 1:A:1020:ILE:HD13 | 1:A:1023:LEU:HD12 | 1.93                     | 0.51              |
| 1:A:1113:ILE:CD1  | 2:D:150:ASN:ND2   | 2.73                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:48:GLN:O      | 2:B:49:SER:C      | 2.54                     | 0.51              |
| 2:B:56:LEU:O      | 2:B:59:VAL:HB     | 2.10                     | 0.51              |
| 1:E:928:SER:O     | 1:E:932:GLY:HA2   | 2.11                     | 0.51              |
| 1:E:931:VAL:HG12  | 1:E:933:VAL:HG23  | 1.91                     | 0.51              |
| 1:E:987:LEU:HD23  | 1:E:1033:LEU:HD22 | 1.92                     | 0.51              |
| 1:E:993:LYS:HG2   | 1:E:1015:GLU:HG2  | 1.93                     | 0.51              |
| 1:A:947:TYR:CE1   | 1:A:951:ARG:NH2   | 2.79                     | 0.50              |
| 1:A:993:LYS:HG2   | 1:A:1015:GLU:HG2  | 1.93                     | 0.50              |
| 1:C:1020:ILE:O    | 1:C:1023:LEU:HB2  | 2.12                     | 0.50              |
| 1:C:1020:ILE:HD13 | 1:C:1023:LEU:HD12 | 1.94                     | 0.50              |
| 1:E:1123:ARG:HG2  | 1:E:1123:ARG:NH1  | 2.24                     | 0.50              |
| 2:F:197:TRP:O     | 2:F:201:LEU:HB2   | 2.10                     | 0.50              |
| 1:A:928:SER:O     | 1:A:932:GLY:HA2   | 2.11                     | 0.50              |
| 2:B:197:TRP:O     | 2:B:201:LEU:HB2   | 2.10                     | 0.50              |
| 2:B:260:ASP:C     | 2:B:262:THR:N     | 2.70                     | 0.50              |
| 2:D:97:ALA:HB2    | 2:D:105:SER:OG    | 2.11                     | 0.50              |
| 2:D:241:PRO:HG2   | 2:D:242:THR:H     | 1.75                     | 0.50              |
| 2:F:41:LEU:HD13   | 2:F:46:GLN:O      | 2.11                     | 0.50              |
| 2:F:48:GLN:O      | 2:F:49:SER:C      | 2.54                     | 0.50              |
| 1:A:0:MSE:CE      | 2:B:138:VAL:HG21  | 2.41                     | 0.50              |
| 1:A:950:CYS:O     | 1:A:968:VAL:HG23  | 2.11                     | 0.50              |
| 1:A:952:THR:HA    | 2:B:249:THR:HG21  | 1.94                     | 0.50              |
| 1:A:971:TYR:HA    | 2:B:211:ARG:NH2   | 2.25                     | 0.50              |
| 1:C:932:GLY:O     | 1:C:1188:SER:HB2  | 2.10                     | 0.50              |
| 1:E:950:CYS:O     | 1:E:968:VAL:HG23  | 2.11                     | 0.50              |
| 1:E:994:MSE:HE1   | 1:E:1013:PHE:CD2  | 2.45                     | 0.50              |
| 2:F:42:LEU:HD21   | 2:F:64:VAL:HG13   | 1.94                     | 0.50              |
| 1:C:1180:LYS:O    | 1:C:1190:ILE:HG13 | 2.11                     | 0.50              |
| 1:E:983:TYR:HE2   | 2:F:253:MSE:HG2   | 1.70                     | 0.50              |
| 1:E:1191:GLY:O    | 1:E:1192:ALA:C    | 2.55                     | 0.50              |
| 2:F:159:ASP:OD1   | 2:F:160:ASN:N     | 2.45                     | 0.50              |
| 1:A:930:GLN:C     | 1:A:1194:ALA:HB1  | 2.36                     | 0.50              |
| 1:A:1191:GLY:O    | 1:A:1192:ALA:C    | 2.55                     | 0.50              |
| 1:C:1029:GLU:O    | 1:C:1032:LYS:HB3  | 2.10                     | 0.50              |
| 1:C:1079:PRO:O    | 1:C:1082:ARG:N    | 2.45                     | 0.50              |
| 2:D:197:TRP:O     | 2:D:201:LEU:HB2   | 2.11                     | 0.50              |
| 1:E:961:LEU:HD23  | 1:E:962:PRO:HD2   | 1.94                     | 0.50              |
| 1:A:1003:LEU:HD21 | 2:D:106:LEU:HD22  | 1.94                     | 0.50              |
| 2:B:158:GLY:O     | 2:B:159:ASP:HB3   | 2.10                     | 0.50              |
| 1:C:931:VAL:HG11  | 1:C:1168:LEU:HD13 | 1.94                     | 0.50              |
| 2:F:96:GLN:O      | 2:F:99:LEU:HB2    | 2.11                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:157:SER:C     | 2:F:159:ASP:N     | 2.70                     | 0.50              |
| 2:F:157:SER:O     | 2:F:159:ASP:N     | 2.45                     | 0.50              |
| 1:A:961:LEU:HD23  | 1:A:962:PRO:HD2   | 1.94                     | 0.50              |
| 1:A:974:THR:C     | 1:A:975:VAL:HG23  | 2.37                     | 0.50              |
| 2:B:72:ILE:H      | 2:B:72:ILE:CD1    | 2.03                     | 0.50              |
| 1:C:993:LYS:HG2   | 1:C:1015:GLU:HG2  | 1.93                     | 0.50              |
| 2:D:227:TYR:CD1   | 1:E:1113:ILE:HD11 | 2.47                     | 0.50              |
| 2:D:244:LEU:O     | 2:D:245:ALA:C     | 2.55                     | 0.50              |
| 1:A:1079:PRO:O    | 1:A:1082:ARG:N    | 2.45                     | 0.50              |
| 1:A:1126:LYS:O    | 1:A:1130:ASP:HB2  | 2.12                     | 0.50              |
| 1:C:1008:ILE:HD12 | 1:C:1008:ILE:N    | 2.25                     | 0.50              |
| 1:C:1083:THR:CG2  | 1:C:1118:ARG:NH1  | 2.67                     | 0.50              |
| 1:C:1109:PHE:HZ   | 1:C:1118:ARG:HD3  | 1.75                     | 0.50              |
| 2:D:184:PHE:CE2   | 2:D:188:GLU:HG3   | 2.47                     | 0.50              |
| 2:D:213:ILE:HG13  | 2:D:214:ALA:N     | 2.26                     | 0.50              |
| 2:F:213:ILE:HG13  | 2:F:214:ALA:N     | 2.27                     | 0.50              |
| 2:B:44:LEU:O      | 2:B:45:GLY:C      | 2.55                     | 0.49              |
| 2:B:97:ALA:HB2    | 2:B:105:SER:OG    | 2.11                     | 0.49              |
| 1:C:939:LEU:HD13  | 1:C:1187:ILE:CD1  | 2.41                     | 0.49              |
| 1:C:1090:MSE:CE   | 1:C:1106:ALA:HA   | 2.21                     | 0.49              |
| 1:E:1126:LYS:O    | 1:E:1130:ASP:HB2  | 2.12                     | 0.49              |
| 2:F:97:ALA:HB2    | 2:F:105:SER:OG    | 2.11                     | 0.49              |
| 1:A:1045:ILE:HB   | 1:A:1184:ILE:CD1  | 2.41                     | 0.49              |
| 1:A:1094:PHE:C    | 1:A:1096:HIS:N    | 2.70                     | 0.49              |
| 2:D:48:GLN:O      | 2:D:49:SER:C      | 2.54                     | 0.49              |
| 2:D:159:ASP:OD1   | 2:D:160:ASN:N     | 2.45                     | 0.49              |
| 2:D:277:HIS:O     | 2:D:281:ILE:HG22  | 2.13                     | 0.49              |
| 1:A:1020:ILE:O    | 1:A:1023:LEU:HB2  | 2.11                     | 0.49              |
| 1:A:1180:LYS:O    | 1:A:1190:ILE:HG13 | 2.12                     | 0.49              |
| 2:B:156:VAL:HG12  | 2:B:156:VAL:O     | 2.13                     | 0.49              |
| 1:C:938:PRO:HG2   | 1:C:1187:ILE:HD11 | 1.93                     | 0.49              |
| 1:C:1126:LYS:O    | 1:C:1130:ASP:HB2  | 2.12                     | 0.49              |
| 2:D:260:ASP:C     | 2:D:262:THR:N     | 2.70                     | 0.49              |
| 1:E:1079:PRO:O    | 1:E:1082:ARG:N    | 2.45                     | 0.49              |
| 2:F:184:PHE:CE2   | 2:F:188:GLU:HG3   | 2.47                     | 0.49              |
| 2:F:242:THR:O     | 2:F:245:ALA:HB3   | 2.12                     | 0.49              |
| 2:B:102:LEU:HD13  | 2:B:135:ASN:HB2   | 1.95                     | 0.49              |
| 1:C:947:TYR:CE1   | 1:C:951:ARG:CZ    | 2.96                     | 0.49              |
| 1:C:1093:HIS:O    | 1:C:1102:ALA:HB2  | 2.13                     | 0.49              |
| 1:E:911:PRO:O     | 1:E:912:ALA:C     | 2.54                     | 0.49              |
| 1:E:1180:LYS:O    | 1:E:1190:ILE:HG13 | 2.12                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:156:VAL:C     | 2:F:158:GLY:N     | 2.66                     | 0.49              |
| 1:C:1191:GLY:O    | 1:C:1192:ALA:C    | 2.55                     | 0.49              |
| 1:E:1051:GLU:O    | 1:E:1055:ARG:HG3  | 2.13                     | 0.49              |
| 2:F:222:LEU:C     | 2:F:222:LEU:CD2   | 2.86                     | 0.49              |
| 2:F:260:ASP:C     | 2:F:262:THR:N     | 2.70                     | 0.49              |
| 1:A:1074:LYS:HE3  | 1:A:1147:PHE:CD1  | 2.48                     | 0.49              |
| 2:B:37:LYS:HE2    | 2:B:50:GLN:HE22   | 1.77                     | 0.49              |
| 2:B:184:PHE:CE2   | 2:B:188:GLU:HG3   | 2.47                     | 0.49              |
| 2:B:184:PHE:HD2   | 2:B:184:PHE:O     | 1.95                     | 0.49              |
| 2:B:277:HIS:O     | 2:B:281:ILE:HG22  | 2.13                     | 0.49              |
| 2:D:72:ILE:CG1    | 2:D:99:LEU:HD11   | 2.43                     | 0.49              |
| 2:D:156:VAL:O     | 2:D:156:VAL:HG12  | 2.13                     | 0.49              |
| 1:E:974:THR:C     | 1:E:975:VAL:HG23  | 2.37                     | 0.49              |
| 1:E:1020:ILE:HD13 | 1:E:1023:LEU:HD12 | 1.93                     | 0.49              |
| 1:E:1025:VAL:O    | 1:E:1201:VAL:HG23 | 2.12                     | 0.49              |
| 1:A:947:TYR:CE1   | 1:A:951:ARG:CZ    | 2.96                     | 0.49              |
| 2:B:159:ASP:OD1   | 2:B:160:ASN:N     | 2.46                     | 0.49              |
| 2:B:213:ILE:HG13  | 2:B:214:ALA:N     | 2.26                     | 0.49              |
| 1:C:974:THR:C     | 1:C:975:VAL:HG23  | 2.37                     | 0.49              |
| 2:D:222:LEU:C     | 2:D:222:LEU:CD2   | 2.86                     | 0.49              |
| 1:E:956:SER:O     | 1:E:957:THR:C     | 2.56                     | 0.49              |
| 1:E:1071:TYR:CE2  | 1:E:1141:PHE:HB2  | 2.47                     | 0.49              |
| 1:E:1083:THR:HG22 | 1:E:1084:ASN:N    | 2.28                     | 0.49              |
| 1:A:954:ILE:HA    | 2:B:205:ASN:HD21  | 1.78                     | 0.49              |
| 1:A:1051:GLU:O    | 1:A:1055:ARG:HG3  | 2.13                     | 0.49              |
| 1:A:1109:PHE:HZ   | 1:A:1118:ARG:CD   | 2.26                     | 0.49              |
| 1:C:954:ILE:HA    | 2:D:205:ASN:HD21  | 1.76                     | 0.49              |
| 1:C:1094:PHE:C    | 1:C:1096:HIS:N    | 2.70                     | 0.49              |
| 1:C:1189:LYS:CE   | 1:C:1192:ALA:HB2  | 2.36                     | 0.49              |
| 1:E:1028:ALA:HB2  | 1:E:1200:ARG:NH1  | 2.26                     | 0.49              |
| 1:A:1161:THR:HG23 | 1:A:1162:PRO:HD2  | 1.95                     | 0.48              |
| 1:C:1161:THR:HG23 | 1:C:1162:PRO:HD2  | 1.95                     | 0.48              |
| 2:F:54:SER:O      | 2:F:56:LEU:N      | 2.37                     | 0.48              |
| 2:F:184:PHE:HD2   | 2:F:184:PHE:O     | 1.95                     | 0.48              |
| 1:A:1083:THR:HG22 | 1:A:1084:ASN:N    | 2.28                     | 0.48              |
| 2:B:117:GLU:O     | 2:B:119:GLU:N     | 2.33                     | 0.48              |
| 2:B:184:PHE:C     | 2:B:184:PHE:CD2   | 2.90                     | 0.48              |
| 2:B:242:THR:O     | 2:B:245:ALA:HB3   | 2.13                     | 0.48              |
| 1:C:904:TRP:CH2   | 1:C:982:PRO:HB3   | 2.48                     | 0.48              |
| 2:D:184:PHE:HD2   | 2:D:184:PHE:O     | 1.95                     | 0.48              |
| 1:E:1074:LYS:HE3  | 1:E:1147:PHE:CD1  | 2.48                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1093:HIS:O    | 1:E:1102:ALA:HB2  | 2.12                     | 0.48              |
| 2:F:15:PHE:HB3    | 2:F:40:THR:CG2    | 2.43                     | 0.48              |
| 2:F:102:LEU:HD13  | 2:F:135:ASN:HB2   | 1.94                     | 0.48              |
| 2:B:15:PHE:HB3    | 2:B:40:THR:CG2    | 2.43                     | 0.48              |
| 2:B:18:CYS:O      | 2:B:22:ILE:HG13   | 2.13                     | 0.48              |
| 2:D:242:THR:O     | 2:D:245:ALA:HB3   | 2.12                     | 0.48              |
| 1:E:920:PHE:HB3   | 2:F:288:LEU:HD12  | 1.95                     | 0.48              |
| 1:A:940:LYS:CB    | 2:B:285:PHE:CE2   | 2.96                     | 0.48              |
| 1:C:1028:ALA:CB   | 1:C:1200:ARG:NH1  | 2.65                     | 0.48              |
| 2:F:184:PHE:C     | 2:F:184:PHE:CD2   | 2.90                     | 0.48              |
| 2:F:277:HIS:O     | 2:F:281:ILE:HG22  | 2.13                     | 0.48              |
| 2:B:284:LYS:O     | 2:B:287:GLU:HB3   | 2.14                     | 0.48              |
| 1:C:947:TYR:CE1   | 1:C:951:ARG:NH2   | 2.81                     | 0.48              |
| 2:D:184:PHE:C     | 2:D:184:PHE:CD2   | 2.90                     | 0.48              |
| 1:E:1073:THR:HG23 | 1:E:1086:LEU:HD23 | 1.95                     | 0.48              |
| 1:E:1109:PHE:HZ   | 1:E:1118:ARG:CD   | 2.26                     | 0.48              |
| 1:E:1164:VAL:HG22 | 1:E:1175:ILE:HD13 | 1.96                     | 0.48              |
| 2:F:244:LEU:O     | 2:F:245:ALA:C     | 2.56                     | 0.48              |
| 2:D:15:PHE:HB3    | 2:D:40:THR:CG2    | 2.43                     | 0.48              |
| 1:A:956:SER:O     | 1:A:957:THR:C     | 2.56                     | 0.48              |
| 2:B:72:ILE:HG13   | 2:B:99:LEU:HD11   | 1.94                     | 0.48              |
| 2:B:256:LEU:O     | 2:B:257:ASP:C     | 2.56                     | 0.48              |
| 2:D:14:ASN:O      | 2:D:14:ASN:ND2    | 2.37                     | 0.48              |
| 2:D:85:SER:HB3    | 2:D:88:GLU:OE2    | 2.14                     | 0.48              |
| 1:A:1093:HIS:O    | 1:A:1102:ALA:HB2  | 2.13                     | 0.48              |
| 2:B:73:GLU:HB2    | 2:B:74:GLU:H      | 1.56                     | 0.48              |
| 2:B:222:LEU:C     | 2:B:222:LEU:CD2   | 2.85                     | 0.48              |
| 1:C:952:THR:HA    | 2:D:249:THR:HG21  | 1.96                     | 0.48              |
| 2:B:244:LEU:O     | 2:B:245:ALA:C     | 2.55                     | 0.48              |
| 1:C:1109:PHE:HZ   | 1:C:1118:ARG:CD   | 2.26                     | 0.48              |
| 2:F:72:ILE:HG13   | 2:F:99:LEU:HD11   | 1.96                     | 0.48              |
| 1:A:1164:VAL:HG22 | 1:A:1175:ILE:HD13 | 1.96                     | 0.47              |
| 1:C:1104:TYR:CZ   | 1:C:1143:PRO:HB3  | 2.48                     | 0.47              |
| 2:F:18:CYS:O      | 2:F:22:ILE:HG13   | 2.13                     | 0.47              |
| 1:A:1070:ALA:O    | 1:A:1073:THR:HB   | 2.14                     | 0.47              |
| 2:B:232:GLN:O     | 2:B:234:GLU:N     | 2.47                     | 0.47              |
| 1:C:1067:GLU:HG2  | 1:C:1071:TYR:CE1  | 2.50                     | 0.47              |
| 1:C:1073:THR:HG23 | 1:C:1086:LEU:HD23 | 1.95                     | 0.47              |
| 1:C:1164:VAL:HG22 | 1:C:1175:ILE:HD13 | 1.96                     | 0.47              |
| 1:E:970:ALA:HB2   | 1:E:982:PRO:O     | 2.14                     | 0.47              |
| 2:F:232:GLN:O     | 2:F:234:GLU:N     | 2.47                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1067:GLU:HG2  | 1:A:1071:TYR:CE1  | 2.49                     | 0.47              |
| 1:C:1051:GLU:O    | 1:C:1055:ARG:HG3  | 2.13                     | 0.47              |
| 2:D:197:TRP:O     | 2:D:198:LYS:C     | 2.58                     | 0.47              |
| 1:E:904:TRP:CD2   | 1:E:982:PRO:HD3   | 2.50                     | 0.47              |
| 1:E:946:ILE:CD1   | 1:E:1022:LEU:HB3  | 2.44                     | 0.47              |
| 2:F:206:LEU:HD13  | 2:F:206:LEU:HA    | 1.67                     | 0.47              |
| 2:F:256:LEU:O     | 2:F:257:ASP:C     | 2.57                     | 0.47              |
| 1:A:1083:THR:CG2  | 1:A:1118:ARG:NH1  | 2.68                     | 0.47              |
| 2:B:106:LEU:HD23  | 2:B:106:LEU:C     | 2.39                     | 0.47              |
| 2:F:106:LEU:HD23  | 2:F:106:LEU:C     | 2.39                     | 0.47              |
| 2:F:284:LYS:O     | 2:F:287:GLU:HB3   | 2.14                     | 0.47              |
| 1:A:1018:TYR:CE2  | 1:A:1187:ILE:CG1  | 2.95                     | 0.47              |
| 1:A:1142:ASP:O    | 1:A:1142:ASP:CG   | 2.58                     | 0.47              |
| 2:B:54:SER:O      | 2:B:56:LEU:N      | 2.36                     | 0.47              |
| 2:D:49:SER:HB2    | 2:D:61:ASP:CG     | 2.40                     | 0.47              |
| 2:D:106:LEU:HD23  | 2:D:106:LEU:C     | 2.39                     | 0.47              |
| 2:F:288:LEU:O     | 2:F:292:TYR:HD1   | 1.98                     | 0.47              |
| 1:A:969:ARG:O     | 2:B:211:ARG:NE    | 2.42                     | 0.47              |
| 1:A:1113:ILE:CG2  | 1:A:1119:ALA:HB2  | 2.45                     | 0.47              |
| 1:A:1127:ASN:C    | 1:A:1129:ALA:N    | 2.73                     | 0.47              |
| 1:C:1087:GLN:OE1  | 1:C:1118:ARG:HG3  | 2.15                     | 0.47              |
| 1:C:1109:PHE:CE1  | 1:C:1118:ARG:HD3  | 2.49                     | 0.47              |
| 1:E:1070:ALA:O    | 1:E:1073:THR:HB   | 2.14                     | 0.47              |
| 1:E:1087:GLN:OE1  | 1:E:1118:ARG:HG3  | 2.15                     | 0.47              |
| 2:F:156:VAL:O     | 2:F:156:VAL:HG12  | 2.13                     | 0.47              |
| 2:F:267:LYS:O     | 2:F:269:ASP:N     | 2.45                     | 0.47              |
| 1:A:954:ILE:HG22  | 1:A:964:GLN:HB2   | 1.97                     | 0.47              |
| 1:A:970:ALA:HB2   | 1:A:982:PRO:O     | 2.14                     | 0.47              |
| 1:A:1025:VAL:O    | 1:A:1201:VAL:HG23 | 2.15                     | 0.47              |
| 1:A:1127:ASN:C    | 1:A:1129:ALA:H    | 2.23                     | 0.47              |
| 2:B:12:THR:C      | 2:B:198:LYS:HD3   | 2.39                     | 0.47              |
| 2:B:66:PHE:CE1    | 2:B:72:ILE:HG23   | 2.50                     | 0.47              |
| 1:C:910:LEU:HB2   | 1:C:911:PRO:CD    | 2.45                     | 0.47              |
| 1:C:956:SER:O     | 1:C:957:THR:C     | 2.56                     | 0.47              |
| 1:C:970:ALA:HB2   | 1:C:982:PRO:O     | 2.14                     | 0.47              |
| 1:C:994:MSE:CE    | 1:C:1013:PHE:HA   | 2.45                     | 0.47              |
| 1:C:1070:ALA:O    | 1:C:1073:THR:HB   | 2.14                     | 0.47              |
| 2:D:87:TYR:CE1    | 2:D:120:GLY:HA3   | 2.50                     | 0.47              |
| 2:D:267:LYS:O     | 2:D:269:ASP:N     | 2.45                     | 0.47              |
| 1:E:1161:THR:HG23 | 1:E:1162:PRO:HD2  | 1.95                     | 0.47              |
| 2:F:159:ASP:O     | 2:F:162:MSE:CE    | 2.62                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1109:PHE:CE1  | 1:A:1118:ARG:HD3  | 2.50                     | 0.47              |
| 2:B:49:SER:HB2    | 2:B:61:ASP:CG     | 2.40                     | 0.47              |
| 2:B:154:ASP:O     | 2:B:155:THR:C     | 2.58                     | 0.47              |
| 2:D:256:LEU:O     | 2:D:257:ASP:C     | 2.57                     | 0.47              |
| 1:E:1127:ASN:C    | 1:E:1129:ALA:H    | 2.23                     | 0.47              |
| 1:E:1142:ASP:O    | 1:E:1142:ASP:CG   | 2.57                     | 0.47              |
| 2:F:262:THR:C     | 2:F:264:GLN:H     | 2.23                     | 0.47              |
| 1:C:954:ILE:HG22  | 1:C:964:GLN:HB2   | 1.96                     | 0.47              |
| 2:D:232:GLN:O     | 2:D:234:GLU:N     | 2.47                     | 0.47              |
| 2:D:284:LYS:O     | 2:D:287:GLU:HB3   | 2.14                     | 0.47              |
| 1:E:1067:GLU:HG2  | 1:E:1071:TYR:CE1  | 2.49                     | 0.47              |
| 1:E:1109:PHE:CE1  | 1:E:1118:ARG:HD3  | 2.50                     | 0.47              |
| 1:A:994:MSE:CE    | 1:A:1013:PHE:HA   | 2.45                     | 0.47              |
| 1:E:994:MSE:CE    | 1:E:1013:PHE:HA   | 2.45                     | 0.47              |
| 1:E:1018:TYR:CE2  | 1:E:1187:ILE:CG1  | 2.98                     | 0.47              |
| 2:F:154:ASP:O     | 2:F:155:THR:C     | 2.58                     | 0.47              |
| 1:A:1100:LEU:HD11 | 1:A:1133:ALA:HB1  | 1.97                     | 0.46              |
| 2:D:18:CYS:O      | 2:D:22:ILE:HG13   | 2.13                     | 0.46              |
| 2:D:154:ASP:O     | 2:D:155:THR:C     | 2.58                     | 0.46              |
| 1:A:1073:THR:HG23 | 1:A:1086:LEU:HD23 | 1.95                     | 0.46              |
| 1:C:911:PRO:O     | 1:C:915:VAL:HG23  | 2.15                     | 0.46              |
| 1:C:1128:LYS:O    | 1:C:1132:MSE:HE3  | 2.16                     | 0.46              |
| 1:C:1142:ASP:O    | 1:C:1142:ASP:CG   | 2.57                     | 0.46              |
| 1:E:921:ASP:HA    | 2:F:288:LEU:HD13  | 1.97                     | 0.46              |
| 1:A:1087:GLN:OE1  | 1:A:1118:ARG:HG3  | 2.15                     | 0.46              |
| 2:B:14:ASN:O      | 2:B:14:ASN:ND2    | 2.37                     | 0.46              |
| 2:D:262:THR:C     | 2:D:264:GLN:H     | 2.23                     | 0.46              |
| 1:E:1121:GLN:O    | 1:E:1125:ILE:HG12 | 2.15                     | 0.46              |
| 1:A:904:TRP:CZ3   | 1:A:982:PRO:HB3   | 2.50                     | 0.46              |
| 1:A:1002:LYS:HZ2  | 2:D:147:ASN:CB    | 2.28                     | 0.46              |
| 1:C:1113:ILE:HD11 | 2:F:227:TYR:HD1   | 1.81                     | 0.46              |
| 1:C:1113:ILE:CG2  | 1:C:1119:ALA:HB2  | 2.45                     | 0.46              |
| 2:D:49:SER:HB2    | 2:D:61:ASP:OD2    | 2.15                     | 0.46              |
| 2:D:234:GLU:C     | 2:D:236:ALA:H     | 2.23                     | 0.46              |
| 1:E:1042:ARG:HB3  | 1:E:1169:THR:HG23 | 1.98                     | 0.46              |
| 1:A:911:PRO:O     | 1:A:915:VAL:HG23  | 2.15                     | 0.46              |
| 1:C:991:ASN:O     | 1:C:992:GLU:C     | 2.59                     | 0.46              |
| 1:C:1127:ASN:C    | 1:C:1129:ALA:H    | 2.23                     | 0.46              |
| 1:E:987:LEU:HA    | 1:E:990:VAL:HG23  | 1.98                     | 0.46              |
| 1:E:1113:ILE:CG2  | 1:E:1119:ALA:HB2  | 2.45                     | 0.46              |
| 1:E:1128:LYS:O    | 1:E:1132:MSE:HE3  | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:991:ASN:O     | 1:A:992:GLU:C     | 2.59                     | 0.46              |
| 2:B:211:ARG:HH11  | 2:B:211:ARG:CG    | 2.29                     | 0.46              |
| 2:B:267:LYS:O     | 2:B:269:ASP:N     | 2.45                     | 0.46              |
| 1:C:981:LEU:HD13  | 1:C:1024:MSE:HE2  | 1.98                     | 0.46              |
| 1:C:1127:ASN:C    | 1:C:1129:ALA:N    | 2.73                     | 0.46              |
| 1:E:911:PRO:O     | 1:E:915:VAL:HG23  | 2.15                     | 0.46              |
| 1:E:1045:ILE:HB   | 1:E:1184:ILE:CD1  | 2.42                     | 0.46              |
| 2:F:49:SER:HB2    | 2:F:61:ASP:CG     | 2.40                     | 0.46              |
| 1:A:1050:ILE:HD11 | 1:A:1149:ILE:HG21 | 1.97                     | 0.46              |
| 2:D:69:THR:HB     | 2:D:71:ASN:OD1    | 2.15                     | 0.46              |
| 2:D:260:ASP:O     | 2:D:261:LEU:C     | 2.59                     | 0.46              |
| 1:E:959:CYS:C     | 1:E:961:LEU:H     | 2.24                     | 0.46              |
| 1:E:1083:THR:CG2  | 1:E:1118:ARG:NH1  | 2.67                     | 0.46              |
| 1:A:1128:LYS:O    | 1:A:1132:MSE:HE3  | 2.16                     | 0.46              |
| 1:C:1121:GLN:O    | 1:C:1125:ILE:HG12 | 2.16                     | 0.46              |
| 1:E:991:ASN:O     | 1:E:992:GLU:C     | 2.58                     | 0.46              |
| 1:E:1033:LEU:CD2  | 1:E:1037:ILE:HG13 | 2.44                     | 0.46              |
| 1:E:1100:LEU:HD11 | 1:E:1133:ALA:HB1  | 1.97                     | 0.46              |
| 1:E:1127:ASN:C    | 1:E:1129:ALA:N    | 2.73                     | 0.46              |
| 1:A:959:CYS:C     | 1:A:961:LEU:H     | 2.24                     | 0.46              |
| 1:A:987:LEU:HA    | 1:A:990:VAL:HG23  | 1.98                     | 0.46              |
| 1:A:1025:VAL:HG23 | 1:A:1199:ILE:CG2  | 2.45                     | 0.46              |
| 1:A:1162:PRO:HB2  | 1:A:1175:ILE:CG1  | 2.45                     | 0.46              |
| 2:B:49:SER:HB2    | 2:B:61:ASP:OD2    | 2.16                     | 0.46              |
| 1:C:903:ILE:O     | 1:C:907:ASN:HB2   | 2.16                     | 0.46              |
| 1:C:1042:ARG:HB3  | 1:C:1169:THR:HG23 | 1.98                     | 0.46              |
| 1:C:1142:ASP:OD1  | 1:C:1145:ALA:HB3  | 2.16                     | 0.46              |
| 1:C:1162:PRO:HB2  | 1:C:1175:ILE:CG1  | 2.45                     | 0.46              |
| 2:D:124:LEU:HA    | 2:D:124:LEU:HD23  | 1.77                     | 0.46              |
| 1:E:903:ILE:O     | 1:E:907:ASN:HB2   | 2.16                     | 0.46              |
| 1:A:1084:ASN:HD21 | 2:D:143:THR:CG2   | 2.28                     | 0.46              |
| 1:C:1033:LEU:CD2  | 1:C:1037:ILE:HG13 | 2.44                     | 0.46              |
| 2:F:234:GLU:C     | 2:F:236:ALA:H     | 2.23                     | 0.46              |
| 1:A:903:ILE:O     | 1:A:907:ASN:HB2   | 2.16                     | 0.45              |
| 1:A:1142:ASP:OD1  | 1:A:1145:ALA:HB3  | 2.16                     | 0.45              |
| 2:D:12:THR:C      | 2:D:198:LYS:HD3   | 2.41                     | 0.45              |
| 2:D:106:LEU:C     | 2:D:106:LEU:CD2   | 2.89                     | 0.45              |
| 1:E:954:ILE:HG22  | 1:E:964:GLN:HB2   | 1.97                     | 0.45              |
| 2:D:197:TRP:CH2   | 2:D:223:LEU:HD22  | 2.52                     | 0.45              |
| 1:E:1166:ASP:HA   | 1:E:1167:PRO:HD2  | 1.78                     | 0.45              |
| 2:F:106:LEU:C     | 2:F:106:LEU:CD2   | 2.90                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:197:TRP:CH2   | 2:F:223:LEU:HD22  | 2.51                     | 0.45              |
| 2:B:106:LEU:C     | 2:B:106:LEU:CD2   | 2.89                     | 0.45              |
| 2:B:262:THR:C     | 2:B:264:GLN:H     | 2.23                     | 0.45              |
| 1:C:0:MSE:O       | 1:C:900:GLU:C     | 2.59                     | 0.45              |
| 1:C:1113:ILE:CD1  | 2:F:231:GLU:HB3   | 2.47                     | 0.45              |
| 2:D:1:MSE:O       | 2:D:2:ASP:HB2     | 2.17                     | 0.45              |
| 1:E:910:LEU:HB2   | 1:E:911:PRO:CD    | 2.45                     | 0.45              |
| 1:E:1142:ASP:OD1  | 1:E:1145:ALA:HB3  | 2.16                     | 0.45              |
| 2:F:109:CYS:O     | 2:F:124:LEU:HD13  | 2.17                     | 0.45              |
| 2:F:260:ASP:O     | 2:F:261:LEU:C     | 2.59                     | 0.45              |
| 1:A:1042:ARG:HB3  | 1:A:1169:THR:HG23 | 1.97                     | 0.45              |
| 1:A:1121:GLN:O    | 1:A:1125:ILE:HG12 | 2.15                     | 0.45              |
| 2:B:234:GLU:C     | 2:B:236:ALA:H     | 2.23                     | 0.45              |
| 2:D:140:THR:O     | 2:D:141:ALA:C     | 2.59                     | 0.45              |
| 2:F:62:LEU:HB3    | 2:F:75:LEU:HG     | 1.98                     | 0.45              |
| 2:F:129:ILE:HD12  | 2:F:129:ILE:N     | 2.32                     | 0.45              |
| 2:F:260:ASP:O     | 2:F:264:GLN:HG2   | 2.17                     | 0.45              |
| 2:B:117:GLU:OE2   | 2:B:152:ILE:CD1   | 2.65                     | 0.45              |
| 2:B:129:ILE:HD12  | 2:B:129:ILE:N     | 2.31                     | 0.45              |
| 2:B:260:ASP:O     | 2:B:261:LEU:C     | 2.59                     | 0.45              |
| 1:C:959:CYS:C     | 1:C:961:LEU:H     | 2.24                     | 0.45              |
| 1:C:961:LEU:HD23  | 1:C:962:PRO:HD2   | 1.94                     | 0.45              |
| 2:D:1:MSE:CG      | 2:D:2:ASP:H       | 2.11                     | 0.45              |
| 2:D:204:LEU:HD12  | 2:D:204:LEU:C     | 2.42                     | 0.45              |
| 1:E:1075:ALA:O    | 1:E:1077:LEU:N    | 2.50                     | 0.45              |
| 2:F:62:LEU:HD13   | 2:F:75:LEU:HA     | 1.99                     | 0.45              |
| 1:A:910:LEU:HB2   | 1:A:911:PRO:CD    | 2.45                     | 0.45              |
| 1:A:1002:LYS:NZ   | 2:D:147:ASN:CB    | 2.79                     | 0.45              |
| 1:A:1028:ALA:HB2  | 1:A:1200:ARG:NH1  | 2.31                     | 0.45              |
| 2:B:159:ASP:O     | 2:B:162:MSE:CE    | 2.62                     | 0.45              |
| 1:C:1100:LEU:HD11 | 1:C:1133:ALA:HB1  | 1.98                     | 0.45              |
| 2:D:63:TYR:CD2    | 2:D:63:TYR:C      | 2.95                     | 0.45              |
| 1:A:1028:ALA:HB2  | 1:A:1200:ARG:NH2  | 2.28                     | 0.45              |
| 2:B:140:THR:O     | 2:B:141:ALA:C     | 2.59                     | 0.45              |
| 2:B:197:TRP:O     | 2:B:198:LYS:C     | 2.57                     | 0.45              |
| 1:C:972:ASP:O     | 1:C:974:THR:N     | 2.50                     | 0.45              |
| 1:C:1075:ALA:O    | 1:C:1077:LEU:N    | 2.50                     | 0.45              |
| 1:C:1184:ILE:HG22 | 1:C:1185:ALA:N    | 2.32                     | 0.45              |
| 2:D:211:ARG:HH11  | 2:D:211:ARG:CG    | 2.29                     | 0.45              |
| 2:B:44:LEU:O      | 2:B:46:GLN:N      | 2.50                     | 0.45              |
| 2:D:129:ILE:HD12  | 2:D:129:ILE:N     | 2.31                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:954:ILE:HA    | 2:F:205:ASN:ND2   | 2.31                     | 0.45              |
| 1:E:1094:PHE:C    | 1:E:1096:HIS:N    | 2.70                     | 0.45              |
| 1:E:1131:SER:C    | 1:E:1132:MSE:HG2  | 2.42                     | 0.45              |
| 1:E:1162:PRO:HB2  | 1:E:1175:ILE:CG1  | 2.45                     | 0.45              |
| 2:F:11:TYR:CZ     | 2:F:163:ILE:HD11  | 2.48                     | 0.45              |
| 2:F:49:SER:HB2    | 2:F:61:ASP:OD2    | 2.16                     | 0.45              |
| 2:F:140:THR:O     | 2:F:141:ALA:C     | 2.59                     | 0.45              |
| 1:A:1184:ILE:HG22 | 1:A:1185:ALA:N    | 2.32                     | 0.45              |
| 2:B:54:SER:HB2    | 2:B:57:GLY:H      | 1.82                     | 0.45              |
| 1:C:1083:THR:HG22 | 1:C:1084:ASN:N    | 2.28                     | 0.45              |
| 1:E:979:GLN:O     | 1:E:979:GLN:HG2   | 2.17                     | 0.45              |
| 2:F:197:TRP:O     | 2:F:198:LYS:C     | 2.58                     | 0.45              |
| 1:A:0:MSE:SE      | 2:B:138:VAL:HB    | 2.67                     | 0.45              |
| 1:C:1016:ALA:O    | 1:C:1020:ILE:HG12 | 2.17                     | 0.45              |
| 1:C:1161:THR:CG2  | 1:C:1162:PRO:HD2  | 2.47                     | 0.45              |
| 2:D:34:LEU:HD22   | 2:D:34:LEU:C      | 2.42                     | 0.45              |
| 2:D:56:LEU:HG     | 2:D:57:GLY:N      | 2.32                     | 0.45              |
| 2:D:206:LEU:C     | 2:D:209:GLN:HB2   | 2.42                     | 0.45              |
| 2:F:34:LEU:C      | 2:F:34:LEU:HD22   | 2.42                     | 0.45              |
| 1:A:972:ASP:O     | 1:A:974:THR:N     | 2.50                     | 0.44              |
| 2:B:66:PHE:HE2    | 2:B:98:ILE:HD12   | 1.83                     | 0.44              |
| 2:D:244:LEU:HB2   | 2:D:266:VAL:HG23  | 1.99                     | 0.44              |
| 2:F:120:GLY:HA2   | 2:F:123:GLU:OE1   | 2.17                     | 0.44              |
| 2:F:244:LEU:HB2   | 2:F:266:VAL:HG23  | 2.00                     | 0.44              |
| 1:A:1161:THR:CG2  | 1:A:1162:PRO:HD2  | 2.47                     | 0.44              |
| 1:C:954:ILE:HB    | 2:D:173:PHE:CE2   | 2.52                     | 0.44              |
| 1:E:1050:ILE:HD11 | 1:E:1149:ILE:HG21 | 1.99                     | 0.44              |
| 2:F:63:TYR:C      | 2:F:63:TYR:CD2    | 2.95                     | 0.44              |
| 2:F:211:ARG:HH11  | 2:F:211:ARG:CG    | 2.30                     | 0.44              |
| 1:A:913:VAL:CG2   | 1:A:1024:MSE:HE3  | 2.48                     | 0.44              |
| 1:A:1018:TYR:CE2  | 1:A:1187:ILE:HG13 | 2.53                     | 0.44              |
| 2:B:117:GLU:C     | 2:B:119:GLU:N     | 2.75                     | 0.44              |
| 2:B:125:LEU:O     | 2:B:129:ILE:CD1   | 2.63                     | 0.44              |
| 2:B:197:TRP:CH2   | 2:B:223:LEU:HD22  | 2.51                     | 0.44              |
| 2:B:206:LEU:C     | 2:B:209:GLN:HB2   | 2.42                     | 0.44              |
| 1:C:1131:SER:C    | 1:C:1132:MSE:HG2  | 2.42                     | 0.44              |
| 1:E:1016:ALA:O    | 1:E:1020:ILE:HG12 | 2.17                     | 0.44              |
| 2:F:73:GLU:HB2    | 2:F:74:GLU:H      | 1.57                     | 0.44              |
| 1:A:946:ILE:HD11  | 1:A:1022:LEU:HB3  | 1.99                     | 0.44              |
| 1:A:1033:LEU:CD2  | 1:A:1037:ILE:HG13 | 2.45                     | 0.44              |
| 1:A:1074:LYS:HG3  | 1:A:1147:PHE:HE1  | 1.83                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:979:GLN:O    | 1:C:979:GLN:HG2   | 2.18                     | 0.44              |
| 2:F:54:SER:HB2   | 2:F:57:GLY:H      | 1.82                     | 0.44              |
| 2:F:56:LEU:HG    | 2:F:57:GLY:N      | 2.32                     | 0.44              |
| 2:B:63:TYR:CD2   | 2:B:63:TYR:C      | 2.95                     | 0.44              |
| 2:B:210:GLN:C    | 2:B:212:ASN:H     | 2.26                     | 0.44              |
| 1:C:987:LEU:HA   | 1:C:990:VAL:HG23  | 1.99                     | 0.44              |
| 2:D:260:ASP:O    | 2:D:264:GLN:HG2   | 2.16                     | 0.44              |
| 1:E:972:ASP:O    | 1:E:974:THR:N     | 2.50                     | 0.44              |
| 1:A:997:GLY:HA3  | 1:A:1013:PHE:CE2  | 2.53                     | 0.44              |
| 2:B:1:MSE:O      | 2:B:2:ASP:HB2     | 2.16                     | 0.44              |
| 2:B:34:LEU:C     | 2:B:34:LEU:HD22   | 2.42                     | 0.44              |
| 2:F:6:ILE:CG2    | 2:F:22:ILE:HG12   | 2.48                     | 0.44              |
| 2:F:41:LEU:HB3   | 2:F:47:TYR:HA     | 1.99                     | 0.44              |
| 2:F:85:SER:HB3   | 2:F:88:GLU:OE2    | 2.18                     | 0.44              |
| 1:A:907:ASN:ND2  | 1:A:978:ASP:O     | 2.50                     | 0.44              |
| 2:B:96:GLN:OE1   | 2:B:105:SER:HA    | 2.18                     | 0.44              |
| 2:B:184:PHE:O    | 2:B:188:GLU:HB2   | 2.18                     | 0.44              |
| 2:B:260:ASP:O    | 2:B:264:GLN:HG2   | 2.17                     | 0.44              |
| 1:E:1042:ARG:HD3 | 1:E:1169:THR:HG22 | 2.00                     | 0.44              |
| 1:A:1018:TYR:HE2 | 1:A:1187:ILE:HG13 | 1.81                     | 0.44              |
| 1:C:933:VAL:HG13 | 1:C:1187:ILE:CG2  | 2.43                     | 0.44              |
| 2:D:193:THR:HG22 | 2:D:193:THR:O     | 2.18                     | 0.44              |
| 2:F:1:MSE:O      | 2:F:2:ASP:HB2     | 2.16                     | 0.44              |
| 2:F:96:GLN:OE1   | 2:F:105:SER:HA    | 2.18                     | 0.44              |
| 2:F:204:LEU:HD12 | 2:F:204:LEU:C     | 2.41                     | 0.44              |
| 2:F:248:ILE:HD11 | 2:F:263:ASN:CB    | 2.46                     | 0.44              |
| 1:E:997:GLY:HA3  | 1:E:1013:PHE:CE2  | 2.53                     | 0.44              |
| 1:E:1074:LYS:HG3 | 1:E:1147:PHE:HE1  | 1.83                     | 0.44              |
| 1:A:1131:SER:C   | 1:A:1132:MSE:HG2  | 2.42                     | 0.43              |
| 2:B:257:ASP:C    | 2:B:259:GLU:N     | 2.76                     | 0.43              |
| 2:B:270:HIS:CG   | 2:B:271:GLU:N     | 2.86                     | 0.43              |
| 2:D:35:PHE:CD1   | 2:D:87:TYR:CD2    | 2.91                     | 0.43              |
| 1:A:1071:TYR:CE2 | 1:A:1141:PHE:HB2  | 2.51                     | 0.43              |
| 1:A:1075:ALA:O   | 1:A:1077:LEU:N    | 2.50                     | 0.43              |
| 1:C:939:LEU:HD13 | 1:C:1187:ILE:HD12 | 2.00                     | 0.43              |
| 1:C:997:GLY:HA3  | 1:C:1013:PHE:CE2  | 2.54                     | 0.43              |
| 1:E:1090:MSE:CE  | 1:E:1106:ALA:HA   | 2.21                     | 0.43              |
| 1:E:1161:THR:CG2 | 1:E:1162:PRO:HD2  | 2.47                     | 0.43              |
| 1:A:979:GLN:O    | 1:A:979:GLN:HG2   | 2.18                     | 0.43              |
| 2:D:96:GLN:OE1   | 2:D:105:SER:HA    | 2.18                     | 0.43              |
| 2:D:159:ASP:O    | 2:D:162:MSE:CE    | 2.62                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:184:PHE:O     | 2:D:188:GLU:HB2   | 2.18                     | 0.43              |
| 2:D:248:ILE:HD11  | 2:D:263:ASN:CB    | 2.47                     | 0.43              |
| 2:D:210:GLN:C     | 2:D:212:ASN:H     | 2.26                     | 0.43              |
| 2:F:12:THR:C      | 2:F:198:LYS:HD3   | 2.43                     | 0.43              |
| 2:F:112:GLY:O     | 2:F:115:ASN:N     | 2.51                     | 0.43              |
| 1:A:1097:LYS:O    | 1:A:1136:ALA:CB   | 2.67                     | 0.43              |
| 2:B:6:ILE:CG2     | 2:B:22:ILE:HG12   | 2.48                     | 0.43              |
| 2:B:248:ILE:HD11  | 2:B:263:ASN:CB    | 2.47                     | 0.43              |
| 2:D:54:SER:HB2    | 2:D:57:GLY:H      | 1.82                     | 0.43              |
| 1:E:1009:ALA:O    | 1:E:1012:CYS:HB2  | 2.18                     | 0.43              |
| 1:E:1184:ILE:HG22 | 1:E:1185:ALA:N    | 2.32                     | 0.43              |
| 2:F:184:PHE:O     | 2:F:188:GLU:HB2   | 2.18                     | 0.43              |
| 2:F:187:TYR:CD1   | 2:F:206:LEU:HD21  | 2.54                     | 0.43              |
| 2:F:206:LEU:C     | 2:F:209:GLN:HB2   | 2.42                     | 0.43              |
| 1:A:1016:ALA:O    | 1:A:1020:ILE:HG12 | 2.18                     | 0.43              |
| 1:A:1186:MSE:H    | 1:A:1186:MSE:HG3  | 1.64                     | 0.43              |
| 2:B:117:GLU:HA    | 2:B:121:THR:HB    | 1.99                     | 0.43              |
| 2:B:175:THR:O     | 2:B:176:ASN:CB    | 2.67                     | 0.43              |
| 2:D:270:HIS:CG    | 2:D:271:GLU:N     | 2.86                     | 0.43              |
| 2:F:142:SER:O     | 2:F:143:THR:C     | 2.62                     | 0.43              |
| 2:F:193:THR:O     | 2:F:193:THR:HG22  | 2.18                     | 0.43              |
| 2:F:244:LEU:O     | 2:F:247:GLN:HB2   | 2.19                     | 0.43              |
| 2:B:66:PHE:CE2    | 2:B:95:ALA:HA     | 2.53                     | 0.43              |
| 2:B:187:TYR:CD1   | 2:B:206:LEU:HD21  | 2.54                     | 0.43              |
| 2:B:193:THR:O     | 2:B:193:THR:HG22  | 2.17                     | 0.43              |
| 1:C:1009:ALA:O    | 1:C:1012:CYS:HB2  | 2.18                     | 0.43              |
| 2:D:125:LEU:O     | 2:D:129:ILE:CD1   | 2.63                     | 0.43              |
| 1:E:908:SER:OG    | 1:E:910:LEU:HD23  | 2.19                     | 0.43              |
| 2:F:66:PHE:HE2    | 2:F:98:ILE:HD12   | 1.82                     | 0.43              |
| 2:B:94:THR:HG22   | 2:B:98:ILE:HD11   | 2.01                     | 0.43              |
| 2:B:156:VAL:O     | 2:B:158:GLY:N     | 2.43                     | 0.43              |
| 1:C:908:SER:OG    | 1:C:910:LEU:HD23  | 2.18                     | 0.43              |
| 1:C:981:LEU:HD22  | 1:C:1024:MSE:HE1  | 2.00                     | 0.43              |
| 1:C:1008:ILE:H    | 1:C:1008:ILE:CD1  | 2.31                     | 0.43              |
| 2:D:197:TRP:CE3   | 2:D:223:LEU:HD22  | 2.54                     | 0.43              |
| 1:E:994:MSE:HE2   | 1:E:994:MSE:HA    | 2.01                     | 0.43              |
| 2:F:257:ASP:C     | 2:F:259:GLU:N     | 2.77                     | 0.43              |
| 2:F:262:THR:C     | 2:F:264:GLN:N     | 2.77                     | 0.43              |
| 1:A:931:VAL:O     | 1:A:931:VAL:CG1   | 2.67                     | 0.43              |
| 1:C:980:ILE:C     | 1:C:981:LEU:HG    | 2.44                     | 0.43              |
| 1:C:1079:PRO:HG2  | 1:C:1080:ILE:H    | 1.84                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:D:244:LEU:O     | 2:D:247:GLN:HB2  | 2.19                     | 0.43              |
| 1:E:1028:ALA:HB2  | 1:E:1200:ARG:NH2 | 2.31                     | 0.43              |
| 1:A:908:SER:OG    | 1:A:910:LEU:HD23 | 2.18                     | 0.43              |
| 2:D:17:GLN:O      | 2:D:18:CYS:C     | 2.62                     | 0.43              |
| 2:D:94:THR:HG22   | 2:D:98:ILE:HD11  | 2.01                     | 0.43              |
| 2:D:257:ASP:C     | 2:D:259:GLU:N    | 2.76                     | 0.43              |
| 1:E:931:VAL:O     | 1:E:931:VAL:CG1  | 2.67                     | 0.43              |
| 1:A:994:MSE:HE2   | 1:A:994:MSE:HA   | 2.01                     | 0.42              |
| 2:D:142:SER:O     | 2:D:143:THR:C    | 2.62                     | 0.42              |
| 1:E:921:ASP:N     | 2:F:288:LEU:HD11 | 2.34                     | 0.42              |
| 1:E:987:LEU:HA    | 1:E:990:VAL:CG2  | 2.49                     | 0.42              |
| 1:E:1157:ILE:HG23 | 1:E:1161:THR:HB  | 2.01                     | 0.42              |
| 2:F:44:LEU:HA     | 2:F:234:GLU:OE1  | 2.19                     | 0.42              |
| 2:F:71:ASN:HB2    | 2:F:73:GLU:OE1   | 2.19                     | 0.42              |
| 1:A:1009:ALA:O    | 1:A:1012:CYS:HB2 | 2.18                     | 0.42              |
| 2:B:244:LEU:HB2   | 2:B:266:VAL:HG23 | 2.00                     | 0.42              |
| 1:C:994:MSE:CE    | 1:C:1013:PHE:CD2 | 2.96                     | 0.42              |
| 2:D:187:TYR:CD1   | 2:D:206:LEU:HD21 | 2.54                     | 0.42              |
| 1:E:993:LYS:HE3   | 1:E:1015:GLU:CD  | 2.44                     | 0.42              |
| 1:A:1157:ILE:HG23 | 1:A:1161:THR:HB  | 2.01                     | 0.42              |
| 1:E:913:VAL:HG22  | 1:E:1024:MSE:HE3 | 2.00                     | 0.42              |
| 2:F:197:TRP:CE3   | 2:F:223:LEU:HD22 | 2.54                     | 0.42              |
| 2:F:270:HIS:CG    | 2:F:271:GLU:N    | 2.86                     | 0.42              |
| 2:B:56:LEU:HG     | 2:B:57:GLY:N     | 2.32                     | 0.42              |
| 2:B:244:LEU:O     | 2:B:247:GLN:HB2  | 2.19                     | 0.42              |
| 2:B:245:ALA:O     | 2:B:248:ILE:HB   | 2.20                     | 0.42              |
| 2:B:262:THR:C     | 2:B:264:GLN:N    | 2.77                     | 0.42              |
| 1:C:931:VAL:O     | 1:C:931:VAL:CG1  | 2.67                     | 0.42              |
| 1:C:981:LEU:HD13  | 1:C:1024:MSE:HE1 | 2.00                     | 0.42              |
| 2:D:134:LEU:HD23  | 2:D:134:LEU:HA   | 1.90                     | 0.42              |
| 2:D:235:ASN:O     | 2:D:235:ASN:ND2  | 2.46                     | 0.42              |
| 2:D:274:PHE:CD2   | 2:D:274:PHE:C    | 2.97                     | 0.42              |
| 1:E:1079:PRO:HG2  | 1:E:1080:ILE:H   | 1.84                     | 0.42              |
| 1:E:1100:LEU:HD12 | 1:E:1100:LEU:HA  | 1.72                     | 0.42              |
| 1:E:1186:MSE:H    | 1:E:1186:MSE:HG3 | 1.63                     | 0.42              |
| 2:F:17:GLN:O      | 2:F:18:CYS:C     | 2.62                     | 0.42              |
| 2:F:274:PHE:CD2   | 2:F:274:PHE:C    | 2.97                     | 0.42              |
| 2:B:116:ASP:O     | 2:B:117:GLU:HB2  | 2.19                     | 0.42              |
| 2:B:204:LEU:HD12  | 2:B:204:LEU:C    | 2.41                     | 0.42              |
| 2:B:258:THR:O     | 2:B:260:ASP:N    | 2.53                     | 0.42              |
| 1:C:987:LEU:HA    | 1:C:990:VAL:CG2  | 2.49                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:993:LYS:HE3   | 1:C:1015:GLU:CD   | 2.44                     | 0.42              |
| 1:C:1100:LEU:HD12 | 1:C:1100:LEU:HA   | 1.72                     | 0.42              |
| 2:D:6:ILE:CG2     | 2:D:22:ILE:HG12   | 2.48                     | 0.42              |
| 2:D:92:LEU:O      | 2:D:96:GLN:HG3    | 2.20                     | 0.42              |
| 2:D:238:LEU:HD23  | 2:D:239:TYR:CE1   | 2.55                     | 0.42              |
| 1:A:937:GLU:C     | 1:A:939:LEU:H     | 2.27                     | 0.42              |
| 1:A:1166:ASP:HA   | 1:A:1167:PRO:HD2  | 1.78                     | 0.42              |
| 2:B:124:LEU:HD23  | 2:B:124:LEU:HA    | 1.76                     | 0.42              |
| 2:B:142:SER:O     | 2:B:143:THR:C     | 2.62                     | 0.42              |
| 2:B:197:TRP:CE3   | 2:B:223:LEU:HD22  | 2.54                     | 0.42              |
| 1:C:1028:ALA:O    | 1:C:1031:GLU:HB3  | 2.19                     | 0.42              |
| 2:D:109:CYS:HB3   | 2:D:128:ALA:HB2   | 2.01                     | 0.42              |
| 2:D:175:THR:O     | 2:D:176:ASN:CB    | 2.67                     | 0.42              |
| 2:D:245:ALA:O     | 2:D:248:ILE:HB    | 2.20                     | 0.42              |
| 2:F:175:THR:O     | 2:F:176:ASN:CB    | 2.67                     | 0.42              |
| 2:F:210:GLN:C     | 2:F:212:ASN:H     | 2.26                     | 0.42              |
| 1:A:987:LEU:HA    | 1:A:990:VAL:CG2   | 2.49                     | 0.42              |
| 1:C:946:ILE:HD11  | 1:C:1022:LEU:HB3  | 2.02                     | 0.42              |
| 1:C:1071:TYR:CE2  | 1:C:1141:PHE:HB2  | 2.53                     | 0.42              |
| 1:C:1074:LYS:HG3  | 1:C:1147:PHE:HE1  | 1.83                     | 0.42              |
| 2:D:62:LEU:HD23   | 2:D:62:LEU:HA     | 1.82                     | 0.42              |
| 2:D:257:ASP:O     | 2:D:258:THR:C     | 2.62                     | 0.42              |
| 1:E:1028:ALA:O    | 1:E:1031:GLU:HB3  | 2.19                     | 0.42              |
| 1:E:1060:GLY:C    | 1:E:1062:THR:N    | 2.78                     | 0.42              |
| 2:F:45:GLY:HA2    | 2:F:234:GLU:OE2   | 2.20                     | 0.42              |
| 1:A:910:LEU:O     | 1:A:911:PRO:C     | 2.63                     | 0.42              |
| 1:A:993:LYS:HE3   | 1:A:1015:GLU:CD   | 2.44                     | 0.42              |
| 2:B:17:GLN:O      | 2:B:18:CYS:C      | 2.62                     | 0.42              |
| 2:B:238:LEU:HD23  | 2:B:239:TYR:CE1   | 2.55                     | 0.42              |
| 1:C:1157:ILE:HG23 | 1:C:1161:THR:HB   | 2.01                     | 0.42              |
| 2:D:44:LEU:HA     | 2:D:234:GLU:OE1   | 2.19                     | 0.42              |
| 2:D:63:TYR:CD1    | 2:D:91:LEU:HB3    | 2.55                     | 0.42              |
| 1:A:1042:ARG:HD3  | 1:A:1169:THR:HG22 | 2.00                     | 0.42              |
| 1:A:1131:SER:O    | 1:A:1132:MSE:CB   | 2.68                     | 0.42              |
| 1:C:1114:SER:HB3  | 2:F:232:GLN:HA    | 2.01                     | 0.42              |
| 2:F:94:THR:HG22   | 2:F:98:ILE:HD11   | 2.01                     | 0.42              |
| 2:F:238:LEU:HD23  | 2:F:239:TYR:CE1   | 2.55                     | 0.42              |
| 2:F:257:ASP:O     | 2:F:258:THR:C     | 2.62                     | 0.42              |
| 1:A:1033:LEU:HD23 | 1:A:1033:LEU:C    | 2.45                     | 0.42              |
| 2:B:157:SER:O     | 2:B:159:ASP:N     | 2.53                     | 0.42              |
| 2:B:275:ILE:HD13  | 2:B:275:ILE:HA    | 1.95                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:994:MSE:HE2   | 1:C:994:MSE:HA   | 2.01                     | 0.42              |
| 2:D:62:LEU:HB3    | 2:D:75:LEU:HG    | 2.02                     | 0.42              |
| 1:E:980:ILE:C     | 1:E:981:LEU:HG   | 2.45                     | 0.42              |
| 1:A:1079:PRO:HG2  | 1:A:1080:ILE:H   | 1.84                     | 0.41              |
| 1:C:921:ASP:O     | 1:C:925:GLN:HG3  | 2.20                     | 0.41              |
| 1:C:1022:LEU:HD23 | 1:C:1022:LEU:HA  | 1.83                     | 0.41              |
| 1:C:1033:LEU:HD23 | 1:C:1033:LEU:C   | 2.45                     | 0.41              |
| 1:C:1060:GLY:C    | 1:C:1062:THR:N   | 2.78                     | 0.41              |
| 1:C:1113:ILE:HG22 | 1:C:1119:ALA:HB2 | 2.01                     | 0.41              |
| 2:D:71:ASN:HB2    | 2:D:73:GLU:OE1   | 2.19                     | 0.41              |
| 1:E:1113:ILE:HG22 | 1:E:1119:ALA:HB2 | 2.01                     | 0.41              |
| 1:E:1158:TYR:N    | 1:E:1158:TYR:CD1 | 2.88                     | 0.41              |
| 1:A:980:ILE:C     | 1:A:981:LEU:HG   | 2.45                     | 0.41              |
| 2:B:15:PHE:HB2    | 2:B:44:LEU:CD2   | 2.47                     | 0.41              |
| 2:B:71:ASN:HB2    | 2:B:73:GLU:OE1   | 2.19                     | 0.41              |
| 2:B:274:PHE:CD2   | 2:B:274:PHE:C    | 2.97                     | 0.41              |
| 1:C:989:VAL:O     | 1:C:992:GLU:N    | 2.54                     | 0.41              |
| 2:D:244:LEU:HD12  | 2:D:266:VAL:HG23 | 2.01                     | 0.41              |
| 2:D:262:THR:C     | 2:D:264:GLN:N    | 2.77                     | 0.41              |
| 2:F:156:VAL:O     | 2:F:156:VAL:CG1  | 2.69                     | 0.41              |
| 2:F:244:LEU:HD12  | 2:F:266:VAL:HG23 | 2.01                     | 0.41              |
| 2:F:283:ALA:O     | 2:F:284:LYS:C    | 2.64                     | 0.41              |
| 1:A:1028:ALA:O    | 1:A:1031:GLU:HB3 | 2.19                     | 0.41              |
| 1:C:910:LEU:O     | 1:C:911:PRO:C    | 2.64                     | 0.41              |
| 1:C:937:GLU:C     | 1:C:939:LEU:H    | 2.28                     | 0.41              |
| 1:C:1158:TYR:CD1  | 1:C:1158:TYR:N   | 2.88                     | 0.41              |
| 2:D:15:PHE:HB2    | 2:D:44:LEU:CD2   | 2.47                     | 0.41              |
| 2:D:193:THR:CG2   | 2:D:194:PHE:CE1  | 3.03                     | 0.41              |
| 2:D:258:THR:O     | 2:D:260:ASP:N    | 2.53                     | 0.41              |
| 1:E:989:VAL:O     | 1:E:992:GLU:N    | 2.53                     | 0.41              |
| 1:E:1071:TYR:O    | 1:E:1074:LYS:HB2 | 2.20                     | 0.41              |
| 2:F:4:PHE:HD1     | 2:F:159:ASP:HB2  | 1.85                     | 0.41              |
| 2:F:87:TYR:CE1    | 2:F:119:GLU:HG2  | 2.49                     | 0.41              |
| 2:F:245:ALA:O     | 2:F:248:ILE:HB   | 2.20                     | 0.41              |
| 1:A:1071:TYR:O    | 1:A:1074:LYS:HB2 | 2.20                     | 0.41              |
| 1:A:1158:TYR:CD1  | 1:A:1158:TYR:N   | 2.88                     | 0.41              |
| 1:A:1178:LYS:HE3  | 1:A:1191:GLY:HA3 | 2.02                     | 0.41              |
| 2:B:1:MSE:O       | 2:B:2:ASP:CB     | 2.68                     | 0.41              |
| 2:B:166:LEU:HA    | 2:B:166:LEU:HD12 | 1.60                     | 0.41              |
| 2:B:283:ALA:O     | 2:B:284:LYS:C    | 2.63                     | 0.41              |
| 2:D:206:LEU:HA    | 2:D:206:LEU:HD13 | 1.67                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:1018:TYR:O   | 1:E:1021:THR:HB   | 2.20                     | 0.41              |
| 1:A:1018:TYR:O   | 1:A:1021:THR:HB   | 2.21                     | 0.41              |
| 1:A:1142:ASP:HA  | 1:A:1143:PRO:HD2  | 1.91                     | 0.41              |
| 2:B:117:GLU:OE2  | 2:B:152:ILE:HD12  | 2.20                     | 0.41              |
| 2:B:240:LYS:O    | 2:B:241:PRO:C     | 2.62                     | 0.41              |
| 1:C:1027:ASP:O   | 1:C:1028:ALA:C    | 2.64                     | 0.41              |
| 1:C:1131:SER:O   | 1:C:1132:MSE:CB   | 2.68                     | 0.41              |
| 2:D:1:MSE:O      | 2:D:2:ASP:CB      | 2.68                     | 0.41              |
| 2:D:156:VAL:O    | 2:D:156:VAL:CG1   | 2.68                     | 0.41              |
| 1:E:937:GLU:C    | 1:E:939:LEU:H     | 2.28                     | 0.41              |
| 2:F:41:LEU:CD1   | 2:F:46:GLN:O      | 2.67                     | 0.41              |
| 1:A:900:GLU:O    | 1:A:901:THR:C     | 2.64                     | 0.41              |
| 2:B:41:LEU:HD13  | 2:B:46:GLN:O      | 2.21                     | 0.41              |
| 2:D:7:LYS:HE2    | 2:D:123:GLU:OE2   | 2.20                     | 0.41              |
| 2:D:145:PHE:O    | 2:D:146:ASP:C     | 2.64                     | 0.41              |
| 2:D:283:ALA:O    | 2:D:284:LYS:C     | 2.63                     | 0.41              |
| 1:E:1117:PRO:HG2 | 1:E:1118:ARG:H    | 1.86                     | 0.41              |
| 2:F:1:MSE:O      | 2:F:2:ASP:CB      | 2.68                     | 0.41              |
| 2:F:92:LEU:O     | 2:F:96:GLN:HG3    | 2.20                     | 0.41              |
| 1:A:1129:ALA:C   | 1:A:1131:SER:H    | 2.29                     | 0.41              |
| 1:A:1182:ASP:HA  | 1:A:1190:ILE:HD11 | 2.02                     | 0.41              |
| 2:B:145:PHE:O    | 2:B:146:ASP:C     | 2.63                     | 0.41              |
| 2:B:244:LEU:HD12 | 2:B:266:VAL:HG23  | 2.01                     | 0.41              |
| 2:D:34:LEU:C     | 2:D:34:LEU:CD2    | 2.93                     | 0.41              |
| 2:D:159:ASP:C    | 2:D:161:GLU:N     | 2.78                     | 0.41              |
| 1:E:987:LEU:N    | 1:E:987:LEU:HD12  | 2.35                     | 0.41              |
| 1:E:1178:LYS:HE3 | 1:E:1191:GLY:HA3  | 2.02                     | 0.41              |
| 2:F:11:TYR:CD1   | 2:F:163:ILE:HD11  | 2.55                     | 0.41              |
| 2:F:240:LYS:O    | 2:F:241:PRO:C     | 2.62                     | 0.41              |
| 1:A:921:ASP:O    | 1:A:925:GLN:HG3   | 2.20                     | 0.41              |
| 1:A:987:LEU:N    | 1:A:987:LEU:HD12  | 2.36                     | 0.41              |
| 1:C:1071:TYR:O   | 1:C:1074:LYS:HB2  | 2.20                     | 0.41              |
| 1:C:1166:ASP:HA  | 1:C:1167:PRO:HD2  | 1.78                     | 0.41              |
| 1:C:1182:ASP:HA  | 1:C:1190:ILE:HD11 | 2.02                     | 0.41              |
| 2:F:124:LEU:O    | 2:F:125:LEU:C     | 2.64                     | 0.41              |
| 2:F:258:THR:O    | 2:F:260:ASP:N     | 2.53                     | 0.41              |
| 1:A:989:VAL:O    | 1:A:992:GLU:N     | 2.53                     | 0.41              |
| 1:A:1003:LEU:CD2 | 2:D:110:VAL:HG21  | 2.38                     | 0.41              |
| 2:B:112:GLY:C    | 2:B:114:ASP:N     | 2.76                     | 0.41              |
| 1:C:1080:ILE:HB  | 2:F:227:TYR:CE2   | 2.56                     | 0.41              |
| 1:C:1096:HIS:O   | 1:C:1097:LYS:C    | 2.64                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1109:PHE:CZ   | 1:C:1118:ARG:CD   | 3.01                     | 0.41              |
| 1:C:1129:ALA:C    | 1:C:1131:SER:H    | 2.29                     | 0.41              |
| 1:C:1178:LYS:HE3  | 1:C:1191:GLY:HA3  | 2.02                     | 0.41              |
| 2:D:266:VAL:CG1   | 2:D:275:ILE:HG12  | 2.51                     | 0.41              |
| 1:E:910:LEU:O     | 1:E:911:PRO:C     | 2.64                     | 0.41              |
| 1:E:1100:LEU:CD1  | 1:E:1133:ALA:HB1  | 2.51                     | 0.41              |
| 1:E:1131:SER:O    | 1:E:1132:MSE:CB   | 2.68                     | 0.41              |
| 1:A:904:TRP:CD2   | 1:A:982:PRO:HD3   | 2.56                     | 0.41              |
| 1:A:1100:LEU:HB3  | 1:A:1101:GLN:NE2  | 2.36                     | 0.41              |
| 2:B:266:VAL:CG1   | 2:B:275:ILE:HG12  | 2.51                     | 0.41              |
| 1:C:1100:LEU:CD1  | 1:C:1133:ALA:HB1  | 2.51                     | 0.41              |
| 1:C:1117:PRO:HG2  | 1:C:1118:ARG:H    | 1.86                     | 0.41              |
| 1:E:900:GLU:O     | 1:E:901:THR:C     | 2.64                     | 0.41              |
| 1:E:904:TRP:CG    | 1:E:982:PRO:HD3   | 2.56                     | 0.41              |
| 1:E:921:ASP:O     | 1:E:925:GLN:HG3   | 2.20                     | 0.41              |
| 1:E:931:VAL:HG11  | 1:E:1168:LEU:HD13 | 2.02                     | 0.41              |
| 2:F:34:LEU:C      | 2:F:34:LEU:CD2    | 2.94                     | 0.41              |
| 2:F:159:ASP:C     | 2:F:161:GLU:N     | 2.78                     | 0.41              |
| 2:F:266:VAL:CG1   | 2:F:275:ILE:HG12  | 2.51                     | 0.41              |
| 1:A:901:THR:HG22  | 1:A:902:ALA:N     | 2.35                     | 0.40              |
| 1:A:940:LYS:HA    | 2:B:285:PHE:CE2   | 2.55                     | 0.40              |
| 1:A:1113:ILE:HG22 | 1:A:1119:ALA:HB2  | 2.01                     | 0.40              |
| 2:B:34:LEU:C      | 2:B:34:LEU:CD2    | 2.93                     | 0.40              |
| 2:B:92:LEU:O      | 2:B:96:GLN:HG3    | 2.21                     | 0.40              |
| 2:B:134:LEU:HD23  | 2:B:134:LEU:HA    | 1.90                     | 0.40              |
| 2:B:193:THR:CG2   | 2:B:194:PHE:CE1   | 3.04                     | 0.40              |
| 1:C:900:GLU:O     | 1:C:901:THR:C     | 2.64                     | 0.40              |
| 1:C:901:THR:O     | 1:C:904:TRP:HB2   | 2.21                     | 0.40              |
| 1:E:954:ILE:HD12  | 2:F:170:TYR:HE2   | 1.87                     | 0.40              |
| 1:E:1045:ILE:HD12 | 1:E:1184:ILE:CG2  | 2.43                     | 0.40              |
| 1:E:1100:LEU:HD13 | 1:E:1133:ALA:CA   | 2.52                     | 0.40              |
| 1:E:1129:ALA:C    | 1:E:1131:SER:H    | 2.29                     | 0.40              |
| 2:F:193:THR:CG2   | 2:F:194:PHE:CE1   | 3.04                     | 0.40              |
| 1:A:904:TRP:CG    | 1:A:982:PRO:HD3   | 2.56                     | 0.40              |
| 2:B:87:TYR:CE1    | 2:B:120:GLY:CA    | 3.04                     | 0.40              |
| 2:B:257:ASP:O     | 2:B:258:THR:C     | 2.62                     | 0.40              |
| 1:C:957:THR:CB    | 1:C:958:PRO:HD3   | 2.48                     | 0.40              |
| 1:C:983:TYR:HE2   | 2:D:253:MSE:HG2   | 1.86                     | 0.40              |
| 1:C:1018:TYR:O    | 1:C:1021:THR:HB   | 2.20                     | 0.40              |
| 2:D:240:LYS:O     | 2:D:241:PRO:C     | 2.62                     | 0.40              |
| 1:A:901:THR:O     | 1:A:904:TRP:HB2   | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:954:ILE:CG2   | 1:A:964:GLN:HB2   | 2.51                     | 0.40              |
| 1:C:941:LYS:HE2   | 1:C:942:TYR:CZ    | 2.56                     | 0.40              |
| 1:C:954:ILE:CG2   | 1:C:964:GLN:HB2   | 2.51                     | 0.40              |
| 2:D:35:PHE:CG     | 2:D:87:TYR:CE2    | 3.09                     | 0.40              |
| 1:E:941:LYS:HE2   | 1:E:942:TYR:CZ    | 2.56                     | 0.40              |
| 2:F:15:PHE:HB2    | 2:F:44:LEU:CD2    | 2.47                     | 0.40              |
| 1:A:1080:ILE:CG1  | 2:D:147:ASN:OD1   | 2.55                     | 0.40              |
| 1:A:1097:LYS:O    | 1:A:1136:ALA:HB3  | 2.21                     | 0.40              |
| 1:A:1117:PRO:HG2  | 1:A:1118:ARG:H    | 1.86                     | 0.40              |
| 2:B:15:PHE:HA     | 2:B:18:CYS:HB3    | 2.03                     | 0.40              |
| 2:B:125:LEU:HD22  | 2:B:148:TYR:CE2   | 2.56                     | 0.40              |
| 2:B:156:VAL:O     | 2:B:156:VAL:CG1   | 2.68                     | 0.40              |
| 1:C:904:TRP:CG    | 1:C:982:PRO:HD3   | 2.57                     | 0.40              |
| 1:E:954:ILE:HA    | 2:F:205:ASN:HD21  | 1.86                     | 0.40              |
| 1:E:1027:ASP:O    | 1:E:1028:ALA:C    | 2.64                     | 0.40              |
| 1:E:1033:LEU:HD23 | 1:E:1033:LEU:C    | 2.45                     | 0.40              |
| 2:F:15:PHE:HA     | 2:F:18:CYS:HB3    | 2.04                     | 0.40              |
| 2:F:201:LEU:O     | 2:F:204:LEU:HB3   | 2.22                     | 0.40              |
| 1:A:1096:HIS:O    | 1:A:1097:LYS:C    | 2.64                     | 0.40              |
| 2:B:147:ASN:O     | 2:B:151:ALA:HB2   | 2.22                     | 0.40              |
| 2:D:241:PRO:O     | 2:D:242:THR:C     | 2.64                     | 0.40              |
| 1:E:901:THR:HG22  | 1:E:902:ALA:N     | 2.35                     | 0.40              |
| 1:E:1182:ASP:HA   | 1:E:1190:ILE:HD11 | 2.02                     | 0.40              |
| 2:F:147:ASN:O     | 2:F:151:ALA:HB2   | 2.22                     | 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     | 301/325 (93%) | 233 (77%) | 53 (18%) | 15 (5%)  | <b>1</b> <b>10</b> |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | C     | 301/325 (93%)   | 232 (77%)  | 53 (18%)  | 16 (5%)  | 1           | 9  |
| 1   | E     | 301/325 (93%)   | 233 (77%)  | 53 (18%)  | 15 (5%)  | 1           | 10 |
| 2   | B     | 291/310 (94%)   | 211 (72%)  | 59 (20%)  | 21 (7%)  | 1           | 6  |
| 2   | D     | 291/310 (94%)   | 215 (74%)  | 56 (19%)  | 20 (7%)  | 1           | 6  |
| 2   | F     | 291/310 (94%)   | 212 (73%)  | 61 (21%)  | 18 (6%)  | 1           | 7  |
| All | All   | 1776/1905 (93%) | 1336 (75%) | 335 (19%) | 105 (6%) | 1           | 8  |

All (105) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 957  | THR  |
| 1   | A     | 973  | ASP  |
| 1   | A     | 977  | GLU  |
| 1   | A     | 979  | GLN  |
| 1   | A     | 985  | PRO  |
| 1   | A     | 1132 | MSE  |
| 1   | A     | 1133 | ALA  |
| 1   | A     | 1186 | MSE  |
| 2   | B     | 2    | ASP  |
| 2   | B     | 73   | GLU  |
| 2   | B     | 159  | ASP  |
| 2   | B     | 181  | THR  |
| 2   | B     | 258  | THR  |
| 2   | B     | 273  | ALA  |
| 1   | C     | 957  | THR  |
| 1   | C     | 973  | ASP  |
| 1   | C     | 977  | GLU  |
| 1   | C     | 979  | GLN  |
| 1   | C     | 985  | PRO  |
| 1   | C     | 1132 | MSE  |
| 1   | C     | 1133 | ALA  |
| 1   | C     | 1186 | MSE  |
| 2   | D     | 2    | ASP  |
| 2   | D     | 73   | GLU  |
| 2   | D     | 159  | ASP  |
| 2   | D     | 181  | THR  |
| 2   | D     | 258  | THR  |
| 2   | D     | 273  | ALA  |
| 1   | E     | 957  | THR  |
| 1   | E     | 973  | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 977  | GLU  |
| 1   | E     | 979  | GLN  |
| 1   | E     | 985  | PRO  |
| 1   | E     | 1132 | MSE  |
| 1   | E     | 1133 | ALA  |
| 1   | E     | 1186 | MSE  |
| 2   | F     | 2    | ASP  |
| 2   | F     | 73   | GLU  |
| 2   | F     | 159  | ASP  |
| 2   | F     | 181  | THR  |
| 2   | F     | 258  | THR  |
| 2   | F     | 273  | ALA  |
| 1   | A     | 1076 | LYS  |
| 1   | A     | 1154 | TYR  |
| 2   | B     | 119  | GLU  |
| 2   | B     | 157  | SER  |
| 2   | B     | 233  | LYS  |
| 2   | B     | 234  | GLU  |
| 2   | B     | 261  | LEU  |
| 1   | C     | 900  | GLU  |
| 1   | C     | 1076 | LYS  |
| 1   | C     | 1154 | TYR  |
| 2   | D     | 157  | SER  |
| 2   | D     | 158  | GLY  |
| 2   | D     | 233  | LYS  |
| 2   | D     | 234  | GLU  |
| 2   | D     | 261  | LEU  |
| 1   | E     | 1076 | LYS  |
| 1   | E     | 1154 | TYR  |
| 2   | F     | 157  | SER  |
| 2   | F     | 158  | GLY  |
| 2   | F     | 233  | LYS  |
| 2   | F     | 234  | GLU  |
| 2   | F     | 261  | LEU  |
| 1   | A     | 901  | THR  |
| 1   | A     | 959  | CYS  |
| 1   | A     | 1062 | THR  |
| 2   | B     | 26   | SER  |
| 2   | B     | 27   | LYS  |
| 2   | B     | 45   | GLY  |
| 2   | B     | 116  | ASP  |
| 2   | B     | 118  | ALA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 149  | THR  |
| 2   | B     | 150  | ASN  |
| 2   | B     | 269  | ASP  |
| 1   | C     | 901  | THR  |
| 1   | C     | 959  | CYS  |
| 1   | C     | 1062 | THR  |
| 2   | D     | 26   | SER  |
| 2   | D     | 27   | LYS  |
| 2   | D     | 149  | THR  |
| 2   | D     | 150  | ASN  |
| 2   | D     | 269  | ASP  |
| 1   | E     | 901  | THR  |
| 1   | E     | 959  | CYS  |
| 1   | E     | 1062 | THR  |
| 2   | F     | 26   | SER  |
| 2   | F     | 27   | LYS  |
| 2   | F     | 149  | THR  |
| 2   | F     | 150  | ASN  |
| 2   | F     | 269  | ASP  |
| 1   | A     | 1039 | GLU  |
| 2   | B     | 241  | PRO  |
| 2   | B     | 259  | GLU  |
| 1   | C     | 1039 | GLU  |
| 2   | D     | 69   | THR  |
| 2   | D     | 241  | PRO  |
| 1   | E     | 1039 | GLU  |
| 2   | F     | 241  | PRO  |
| 1   | A     | 911  | PRO  |
| 1   | C     | 911  | PRO  |
| 2   | D     | 259  | GLU  |
| 1   | E     | 911  | PRO  |
| 2   | F     | 259  | GLU  |
| 2   | D     | 45   | GLY  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 257/268 (96%)   | 224 (87%)  | 33 (13%)  | 4           | 18 |
| 1   | C     | 257/268 (96%)   | 224 (87%)  | 33 (13%)  | 4           | 18 |
| 1   | E     | 257/268 (96%)   | 224 (87%)  | 33 (13%)  | 4           | 18 |
| 2   | B     | 263/275 (96%)   | 217 (82%)  | 46 (18%)  | 2           | 8  |
| 2   | D     | 263/275 (96%)   | 216 (82%)  | 47 (18%)  | 2           | 7  |
| 2   | F     | 263/275 (96%)   | 216 (82%)  | 47 (18%)  | 2           | 7  |
| All | All   | 1560/1629 (96%) | 1321 (85%) | 239 (15%) | 3           | 12 |

All (239) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 901  | THR  |
| 1   | A     | 909  | LYS  |
| 1   | A     | 910  | LEU  |
| 1   | A     | 931  | VAL  |
| 1   | A     | 939  | LEU  |
| 1   | A     | 952  | THR  |
| 1   | A     | 954  | ILE  |
| 1   | A     | 956  | SER  |
| 1   | A     | 960  | GLU  |
| 1   | A     | 969  | ARG  |
| 1   | A     | 984  | VAL  |
| 1   | A     | 985  | PRO  |
| 1   | A     | 993  | LYS  |
| 1   | A     | 1046 | LEU  |
| 1   | A     | 1052 | LEU  |
| 1   | A     | 1059 | GLU  |
| 1   | A     | 1062 | THR  |
| 1   | A     | 1063 | VAL  |
| 1   | A     | 1065 | MSE  |
| 1   | A     | 1080 | ILE  |
| 1   | A     | 1083 | THR  |
| 1   | A     | 1091 | SER  |
| 1   | A     | 1098 | ASN  |
| 1   | A     | 1099 | PHE  |
| 1   | A     | 1130 | ASP  |
| 1   | A     | 1132 | MSE  |
| 1   | A     | 1142 | ASP  |
| 1   | A     | 1147 | PHE  |
| 1   | A     | 1153 | THR  |
| 1   | A     | 1164 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1166 | ASP  |
| 1   | A     | 1171 | SER  |
| 1   | A     | 1181 | ILE  |
| 2   | B     | 2    | ASP  |
| 2   | B     | 3    | TYR  |
| 2   | B     | 6    | ILE  |
| 2   | B     | 14   | ASN  |
| 2   | B     | 16   | VAL  |
| 2   | B     | 34   | LEU  |
| 2   | B     | 39   | LYS  |
| 2   | B     | 41   | LEU  |
| 2   | B     | 56   | LEU  |
| 2   | B     | 64   | VAL  |
| 2   | B     | 68   | ASP  |
| 2   | B     | 69   | THR  |
| 2   | B     | 72   | ILE  |
| 2   | B     | 73   | GLU  |
| 2   | B     | 75   | LEU  |
| 2   | B     | 79   | LEU  |
| 2   | B     | 84   | ASN  |
| 2   | B     | 92   | LEU  |
| 2   | B     | 106  | LEU  |
| 2   | B     | 122  | THR  |
| 2   | B     | 131  | VAL  |
| 2   | B     | 138  | VAL  |
| 2   | B     | 139  | SER  |
| 2   | B     | 153  | GLU  |
| 2   | B     | 154  | ASP  |
| 2   | B     | 162  | MSE  |
| 2   | B     | 163  | ILE  |
| 2   | B     | 188  | GLU  |
| 2   | B     | 196  | THR  |
| 2   | B     | 199  | THR  |
| 2   | B     | 201  | LEU  |
| 2   | B     | 206  | LEU  |
| 2   | B     | 211  | ARG  |
| 2   | B     | 220  | VAL  |
| 2   | B     | 223  | LEU  |
| 2   | B     | 235  | ASN  |
| 2   | B     | 237  | VAL  |
| 2   | B     | 249  | THR  |
| 2   | B     | 250  | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 257  | ASP  |
| 2   | B     | 259  | GLU  |
| 2   | B     | 260  | ASP  |
| 2   | B     | 266  | VAL  |
| 2   | B     | 271  | GLU  |
| 2   | B     | 272  | HIS  |
| 2   | B     | 281  | ILE  |
| 1   | C     | 901  | THR  |
| 1   | C     | 909  | LYS  |
| 1   | C     | 910  | LEU  |
| 1   | C     | 931  | VAL  |
| 1   | C     | 939  | LEU  |
| 1   | C     | 952  | THR  |
| 1   | C     | 954  | ILE  |
| 1   | C     | 956  | SER  |
| 1   | C     | 960  | GLU  |
| 1   | C     | 969  | ARG  |
| 1   | C     | 984  | VAL  |
| 1   | C     | 985  | PRO  |
| 1   | C     | 993  | LYS  |
| 1   | C     | 1046 | LEU  |
| 1   | C     | 1052 | LEU  |
| 1   | C     | 1059 | GLU  |
| 1   | C     | 1062 | THR  |
| 1   | C     | 1063 | VAL  |
| 1   | C     | 1065 | MSE  |
| 1   | C     | 1080 | ILE  |
| 1   | C     | 1083 | THR  |
| 1   | C     | 1091 | SER  |
| 1   | C     | 1098 | ASN  |
| 1   | C     | 1099 | PHE  |
| 1   | C     | 1130 | ASP  |
| 1   | C     | 1132 | MSE  |
| 1   | C     | 1142 | ASP  |
| 1   | C     | 1147 | PHE  |
| 1   | C     | 1153 | THR  |
| 1   | C     | 1164 | VAL  |
| 1   | C     | 1166 | ASP  |
| 1   | C     | 1171 | SER  |
| 1   | C     | 1181 | ILE  |
| 2   | D     | 2    | ASP  |
| 2   | D     | 3    | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 6   | ILE  |
| 2   | D     | 14  | ASN  |
| 2   | D     | 16  | VAL  |
| 2   | D     | 34  | LEU  |
| 2   | D     | 39  | LYS  |
| 2   | D     | 41  | LEU  |
| 2   | D     | 56  | LEU  |
| 2   | D     | 64  | VAL  |
| 2   | D     | 68  | ASP  |
| 2   | D     | 69  | THR  |
| 2   | D     | 72  | ILE  |
| 2   | D     | 73  | GLU  |
| 2   | D     | 75  | LEU  |
| 2   | D     | 79  | LEU  |
| 2   | D     | 84  | ASN  |
| 2   | D     | 92  | LEU  |
| 2   | D     | 106 | LEU  |
| 2   | D     | 115 | ASN  |
| 2   | D     | 122 | THR  |
| 2   | D     | 131 | VAL  |
| 2   | D     | 138 | VAL  |
| 2   | D     | 139 | SER  |
| 2   | D     | 153 | GLU  |
| 2   | D     | 154 | ASP  |
| 2   | D     | 162 | MSE  |
| 2   | D     | 163 | ILE  |
| 2   | D     | 188 | GLU  |
| 2   | D     | 196 | THR  |
| 2   | D     | 199 | THR  |
| 2   | D     | 201 | LEU  |
| 2   | D     | 206 | LEU  |
| 2   | D     | 211 | ARG  |
| 2   | D     | 220 | VAL  |
| 2   | D     | 223 | LEU  |
| 2   | D     | 235 | ASN  |
| 2   | D     | 237 | VAL  |
| 2   | D     | 249 | THR  |
| 2   | D     | 250 | LEU  |
| 2   | D     | 257 | ASP  |
| 2   | D     | 259 | GLU  |
| 2   | D     | 260 | ASP  |
| 2   | D     | 266 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | D     | 271  | GLU  |
| 2   | D     | 272  | HIS  |
| 2   | D     | 281  | ILE  |
| 1   | E     | 901  | THR  |
| 1   | E     | 909  | LYS  |
| 1   | E     | 910  | LEU  |
| 1   | E     | 931  | VAL  |
| 1   | E     | 939  | LEU  |
| 1   | E     | 952  | THR  |
| 1   | E     | 954  | ILE  |
| 1   | E     | 956  | SER  |
| 1   | E     | 960  | GLU  |
| 1   | E     | 969  | ARG  |
| 1   | E     | 984  | VAL  |
| 1   | E     | 985  | PRO  |
| 1   | E     | 993  | LYS  |
| 1   | E     | 1046 | LEU  |
| 1   | E     | 1052 | LEU  |
| 1   | E     | 1059 | GLU  |
| 1   | E     | 1062 | THR  |
| 1   | E     | 1063 | VAL  |
| 1   | E     | 1065 | MSE  |
| 1   | E     | 1080 | ILE  |
| 1   | E     | 1083 | THR  |
| 1   | E     | 1091 | SER  |
| 1   | E     | 1098 | ASN  |
| 1   | E     | 1099 | PHE  |
| 1   | E     | 1130 | ASP  |
| 1   | E     | 1132 | MSE  |
| 1   | E     | 1142 | ASP  |
| 1   | E     | 1147 | PHE  |
| 1   | E     | 1153 | THR  |
| 1   | E     | 1164 | VAL  |
| 1   | E     | 1166 | ASP  |
| 1   | E     | 1171 | SER  |
| 1   | E     | 1181 | ILE  |
| 2   | F     | 2    | ASP  |
| 2   | F     | 3    | TYR  |
| 2   | F     | 6    | ILE  |
| 2   | F     | 14   | ASN  |
| 2   | F     | 16   | VAL  |
| 2   | F     | 34   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 39  | LYS  |
| 2   | F     | 41  | LEU  |
| 2   | F     | 56  | LEU  |
| 2   | F     | 64  | VAL  |
| 2   | F     | 68  | ASP  |
| 2   | F     | 69  | THR  |
| 2   | F     | 72  | ILE  |
| 2   | F     | 73  | GLU  |
| 2   | F     | 75  | LEU  |
| 2   | F     | 79  | LEU  |
| 2   | F     | 84  | ASN  |
| 2   | F     | 92  | LEU  |
| 2   | F     | 106 | LEU  |
| 2   | F     | 115 | ASN  |
| 2   | F     | 122 | THR  |
| 2   | F     | 131 | VAL  |
| 2   | F     | 138 | VAL  |
| 2   | F     | 139 | SER  |
| 2   | F     | 153 | GLU  |
| 2   | F     | 154 | ASP  |
| 2   | F     | 162 | MSE  |
| 2   | F     | 163 | ILE  |
| 2   | F     | 188 | GLU  |
| 2   | F     | 196 | THR  |
| 2   | F     | 199 | THR  |
| 2   | F     | 201 | LEU  |
| 2   | F     | 206 | LEU  |
| 2   | F     | 211 | ARG  |
| 2   | F     | 220 | VAL  |
| 2   | F     | 223 | LEU  |
| 2   | F     | 235 | ASN  |
| 2   | F     | 237 | VAL  |
| 2   | F     | 249 | THR  |
| 2   | F     | 250 | LEU  |
| 2   | F     | 257 | ASP  |
| 2   | F     | 259 | GLU  |
| 2   | F     | 260 | ASP  |
| 2   | F     | 266 | VAL  |
| 2   | F     | 271 | GLU  |
| 2   | F     | 272 | HIS  |
| 2   | F     | 281 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28)

such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1098 | ASN  |
| 2   | B     | 46   | GLN  |
| 2   | B     | 48   | GLN  |
| 2   | B     | 50   | GLN  |
| 2   | B     | 135  | ASN  |
| 2   | B     | 176  | ASN  |
| 2   | B     | 183  | ASN  |
| 2   | B     | 246  | ASN  |
| 1   | C     | 1093 | HIS  |
| 1   | C     | 1098 | ASN  |
| 1   | C     | 1101 | GLN  |
| 2   | D     | 46   | GLN  |
| 2   | D     | 48   | GLN  |
| 2   | D     | 50   | GLN  |
| 2   | D     | 176  | ASN  |
| 2   | D     | 183  | ASN  |
| 2   | D     | 246  | ASN  |
| 1   | E     | 1098 | ASN  |
| 2   | F     | 9    | ASN  |
| 2   | F     | 14   | ASN  |
| 2   | F     | 17   | GLN  |
| 2   | F     | 46   | GLN  |
| 2   | F     | 48   | GLN  |
| 2   | F     | 50   | GLN  |
| 2   | F     | 115  | ASN  |
| 2   | F     | 135  | ASN  |
| 2   | F     | 176  | ASN  |
| 2   | F     | 183  | 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

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 296/325 (91%)   | -0.25  | 0       | 100 | 100 | 47, 89, 147, 193      | 0     |
| 1   | C     | 296/325 (91%)   | -0.26  | 0       | 100 | 100 | 56, 111, 179, 201     | 0     |
| 1   | E     | 296/325 (91%)   | 0.11   | 5 (1%)  | 69  | 50  | 113, 171, 201, 201    | 0     |
| 2   | B     | 290/310 (93%)   | -0.27  | 0       | 100 | 100 | 44, 96, 169, 188      | 0     |
| 2   | D     | 290/310 (93%)   | -0.17  | 1 (0%)  | 90  | 82  | 59, 110, 173, 201     | 0     |
| 2   | F     | 290/310 (93%)   | 0.05   | 0       | 100 | 100 | 92, 177, 201, 201     | 0     |
| All | All   | 1758/1905 (92%) | -0.13  | 6 (0%)  | 90  | 82  | 44, 127, 196, 201     | 0     |

All (6) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | E     | 1141 | PHE  | 3.2  |
| 1   | E     | 1129 | ALA  | 2.6  |
| 1   | E     | 1044 | TYR  | 2.4  |
| 2   | D     | 50   | GLN  | 2.4  |
| 1   | E     | 927  | LEU  | 2.2  |
| 1   | E     | 1114 | SER  | 2.1  |

### 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 [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.