



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:43 AM UTC

PDB ID : 3I9V / pdb\_00003i9v  
Title : Crystal structure of the hydrophilic domain of respiratory complex I from  
Thermus thermophilus, oxidized, 2 mol/ASU  
Authors : Sazanov, L.A.; Berrisford, J.M.  
Deposited on : 2009-07-13  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

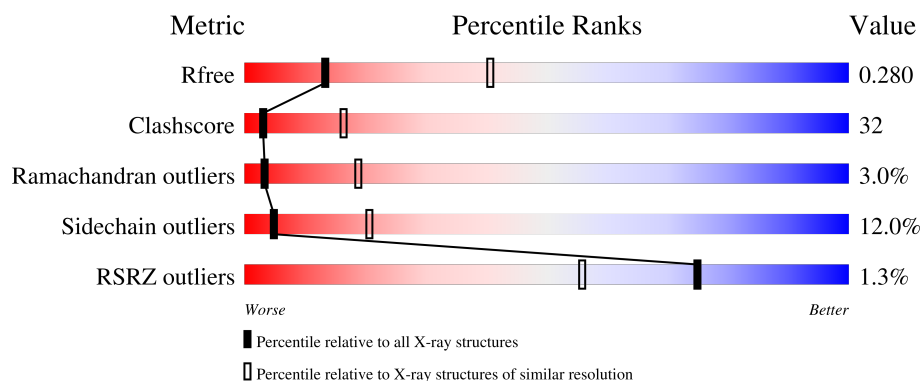
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

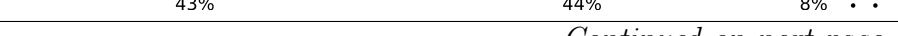
The reported resolution of this entry is 3.10 Å.

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                      | 1456 (3.10-3.10)                                      |
| Clashscore            | 190562                      | 1539 (3.10-3.10)                                      |
| Ramachandran outliers | 187476                      | 1467 (3.10-3.10)                                      |
| Sidechain outliers    | 187428                      | 1467 (3.10-3.10)                                      |
| RSRZ outliers         | 180081                      | 1456 (3.10-3.10)                                      |

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   | 1     | 438    |  |
| 1   | A     | 438    |  |
| 2   | 2     | 181    |  |
| 2   | B     | 181    |  |
| 3   | 3     | 783    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | C     | 783    |                  |
| 4   | 4     | 409    |                  |
| 4   | D     | 409    |                  |
| 5   | 5     | 207    |                  |
| 5   | E     | 207    |                  |
| 6   | 6     | 181    |                  |
| 6   | F     | 181    |                  |
| 7   | 9     | 182    |                  |
| 7   | G     | 182    |                  |
| 8   | 7     | 129    |                  |
| 8   | H     | 129    |                  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 9   | SF4  | 1     | 439 | -         | -        | X       | -                |
| 9   | SF4  | 3     | 784 | -         | -        | X       | -                |
| 9   | SF4  | 3     | 786 | -         | -        | X       | -                |
| 9   | SF4  | 6     | 182 | -         | -        | X       | -                |
| 9   | SF4  | C     | 784 | -         | -        | X       | -                |
| 9   | SF4  | C     | 786 | -         | -        | X       | -                |
| 9   | SF4  | F     | 182 | -         | -        | X       | -                |

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 37520 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 NADH-quinone oxidoreductase subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | 1     | 437      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3417  | 2180 | 595 | 624 | 18 |         |         |       |
| 1   | A     | 437      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3417  | 2180 | 595 | 624 | 18 |         |         |       |

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | 2     | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1406  | 895 | 238 | 265 | 8 |         |         |       |
| 2   | B     | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1406  | 895 | 238 | 265 | 8 |         |         |       |

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit 3.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3   | 3     | 754      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 5880  | 3743 | 1055 | 1051 | 31 |         |         |       |
| 3   | C     | 754      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 5880  | 3743 | 1055 | 1051 | 31 |         |         |       |

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | 4     | 377      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3011  | 1941 | 510 | 549 | 11 |         |         |       |
| 4   | D     | 377      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3011  | 1941 | 510 | 549 | 11 |         |         |       |

- Molecule 5 is a protein called NADH-quinone oxidoreductase subunit 5.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | 5     | 196      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1607  | 1043 | 273 | 288 | 3 |         |         |       |
| 5   | E     | 196      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1607  | 1043 | 273 | 288 | 3 |         |         |       |

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit 6.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 6   | 6     | 145      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1113  | 706 | 196 | 198 | 13 |         |         |       |
| 6   | F     | 145      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1113  | 706 | 196 | 198 | 13 |         |         |       |

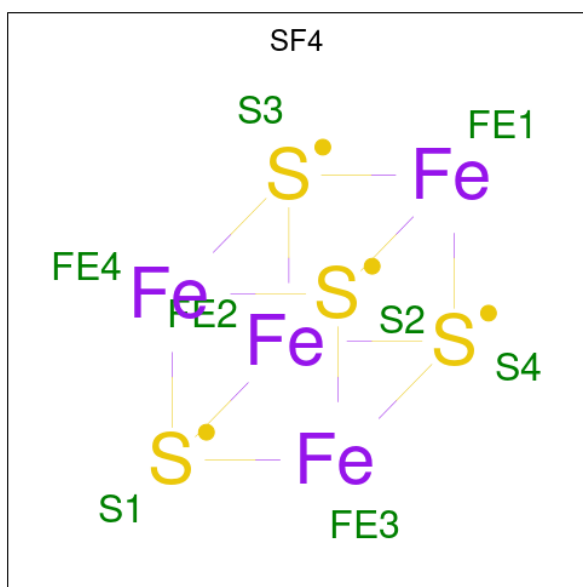
- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit 9.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 7   | 9     | 154      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1193  | 759 | 201 | 222 | 11 |         |         |       |
| 7   | G     | 154      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1193  | 759 | 201 | 222 | 11 |         |         |       |

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit 15.

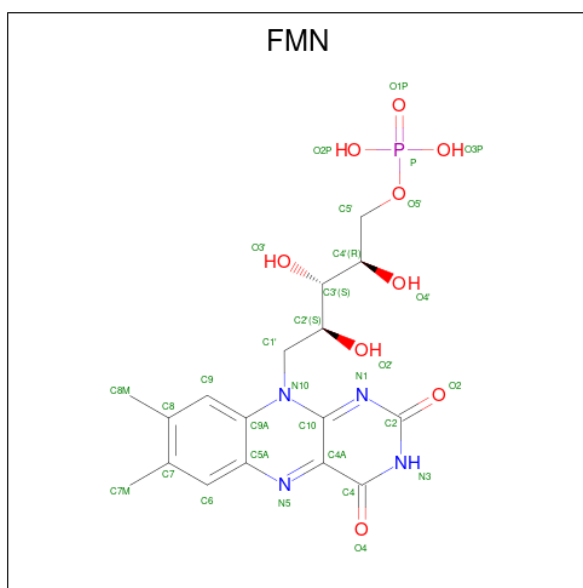
| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | 7     | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1031  | 664 | 183 | 181 | 3 |         |         |       |
| 8   | H     | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1031  | 664 | 183 | 181 | 3 |         |         |       |

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



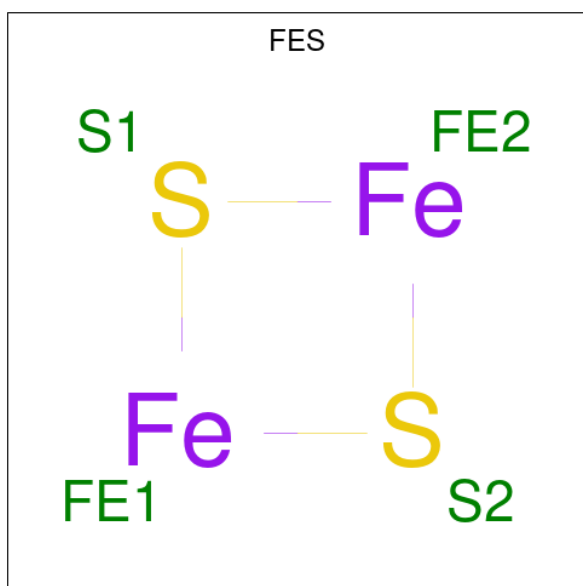
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 9   | 1     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | 3     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | 3     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | 3     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | 6     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | 9     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | 9     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | A     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | C     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | C     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | C     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | F     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | G     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | G     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

- Molecule 10 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 10  | 1     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |         |
| 10  | A     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |         |

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $Fe_2S_2$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 11  | 2     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |

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| Mol | Chain | Residues | Atoms      |         |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|--------|---------|---------|
| 11  | 3     | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       | 0       |
| 11  | B     | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       | 0       |
| 11  | C     | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       | 0       |

- Molecule 12 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 12  | 2     | 1        | Total<br>1 | Mn<br>1 | 0       | 0       |
| 12  | 3     | 2        | Total<br>2 | Mn<br>2 | 0       | 0       |
| 12  | 4     | 2        | Total<br>2 | Mn<br>2 | 0       | 0       |
| 12  | 5     | 1        | Total<br>1 | Mn<br>1 | 0       | 0       |
| 12  | 7     | 1        | Total<br>1 | Mn<br>1 | 0       | 0       |
| 12  | C     | 2        | Total<br>2 | Mn<br>2 | 0       | 0       |
| 12  | D     | 1        | Total<br>1 | Mn<br>1 | 0       | 0       |
| 12  | E     | 1        | Total<br>1 | Mn<br>1 | 0       | 0       |
| 12  | H     | 1        | Total<br>1 | Mn<br>1 | 0       | 0       |

- Molecule 13 is CALCIUM ION (CCD ID: CA) (formula: Ca).

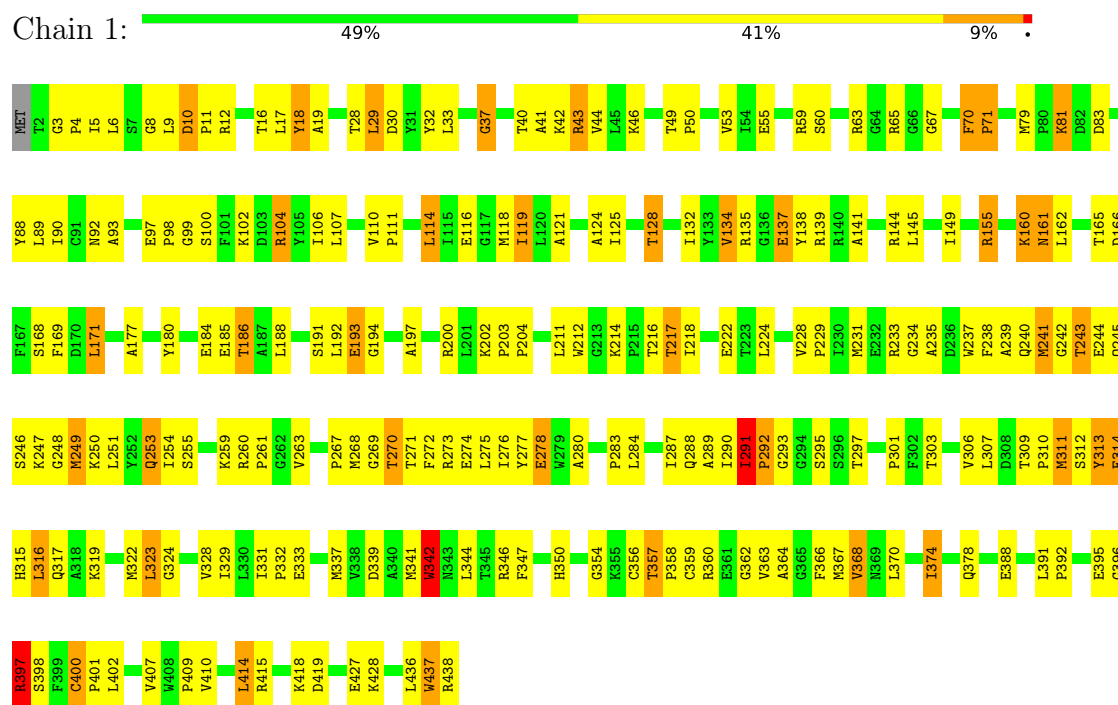
| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 13  | 3     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 13  | C     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |



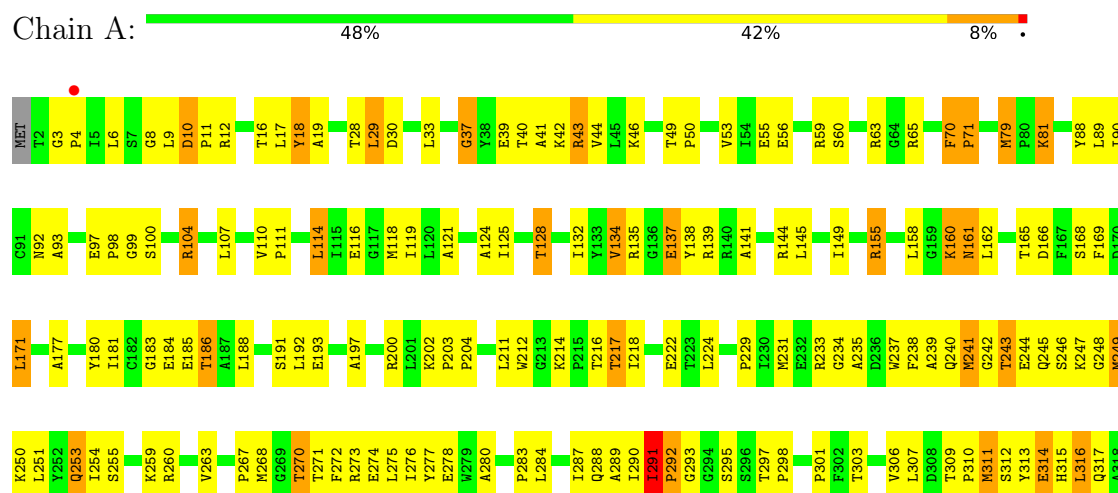
### 3 Residue-property plots [i](#)

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.

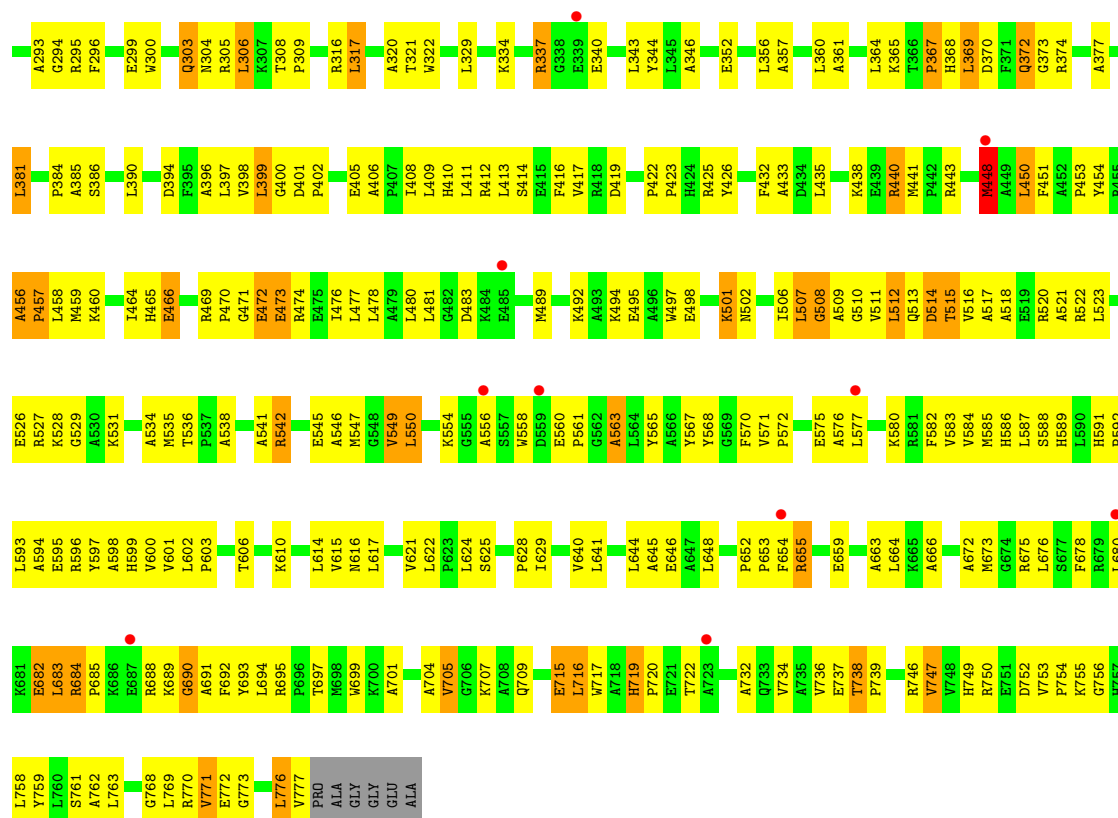
#### • Molecule 1: NADH-quinone oxidoreductase subunit 1



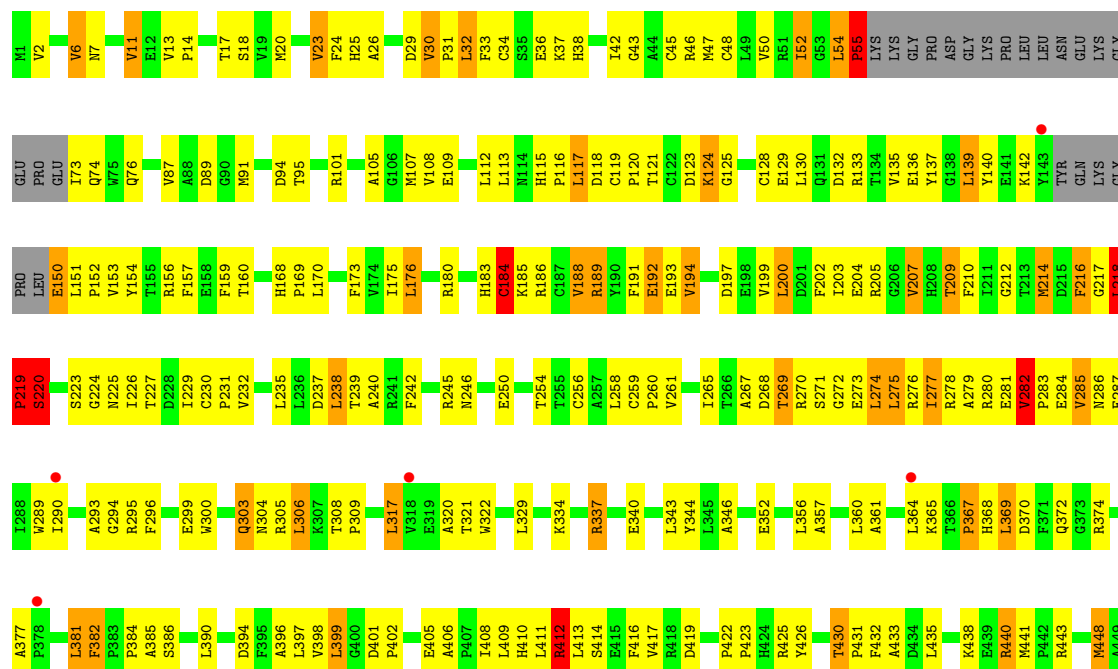
#### • Molecule 1: NADH-quinone oxidoreductase subunit 1

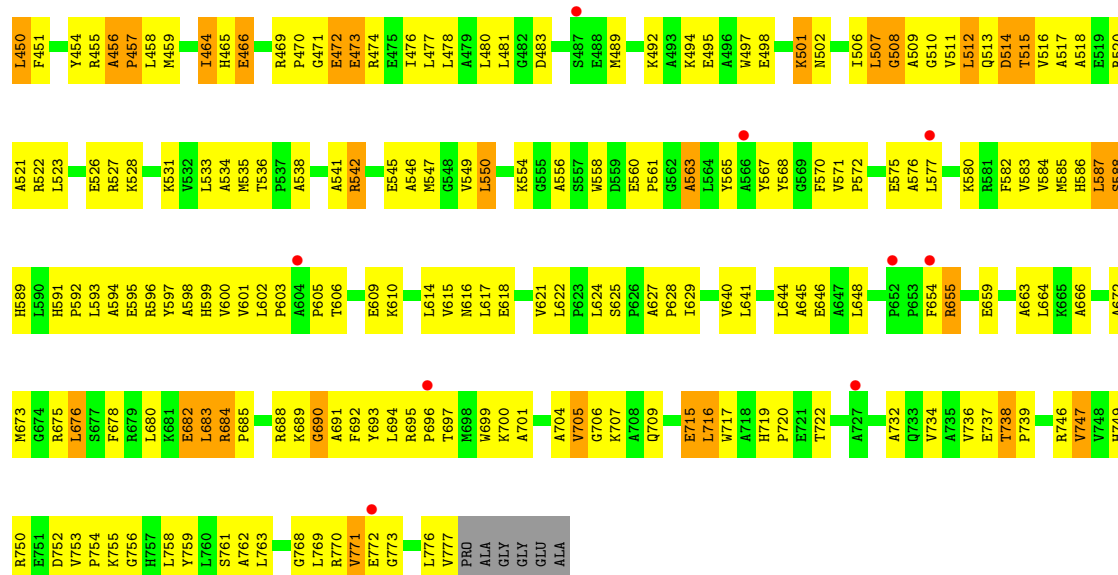




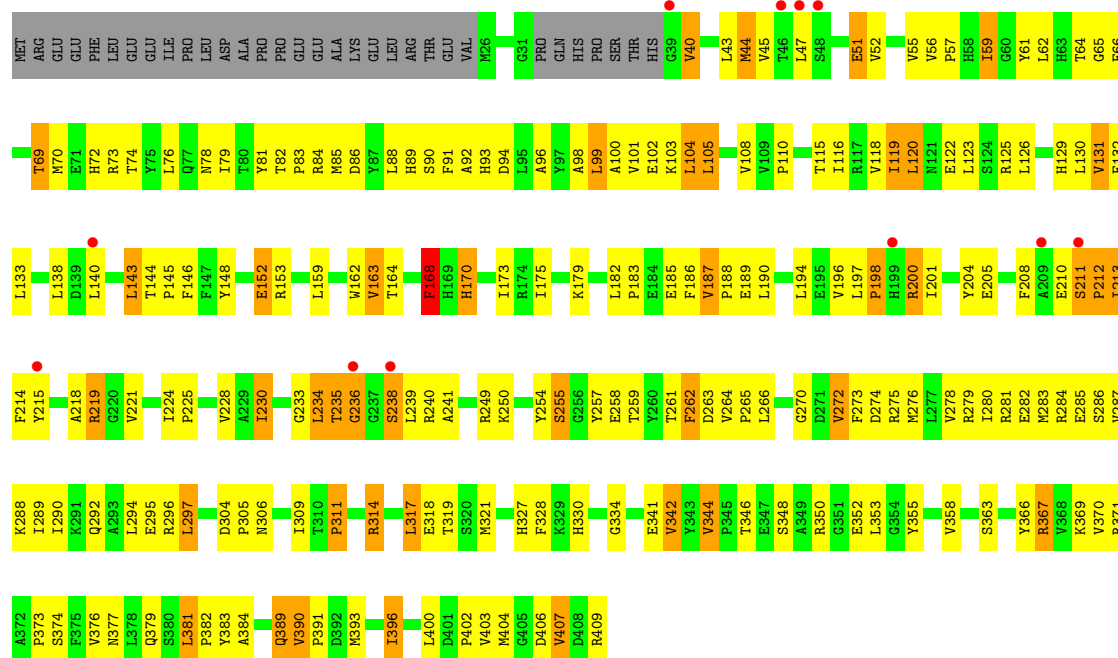


• Molecule 3: NADH-quinone oxidoreductase subunit 3

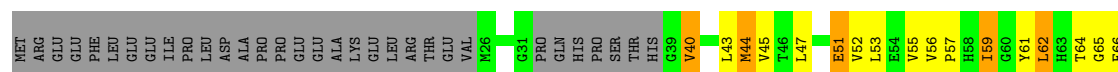
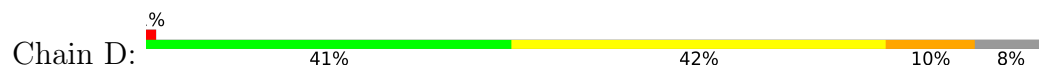


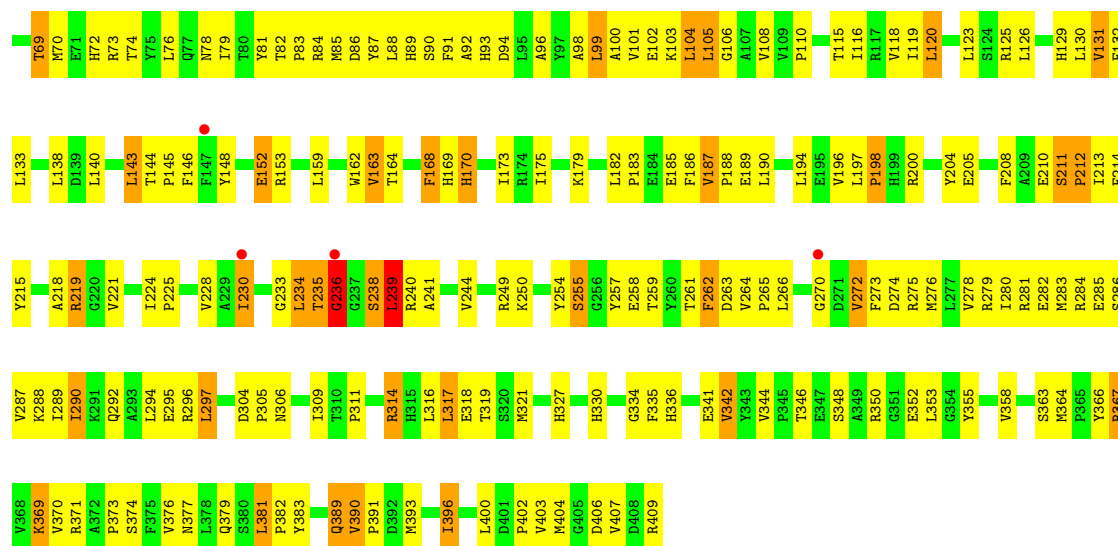


• Molecule 4: NADH-quinone oxidoreductase subunit 4

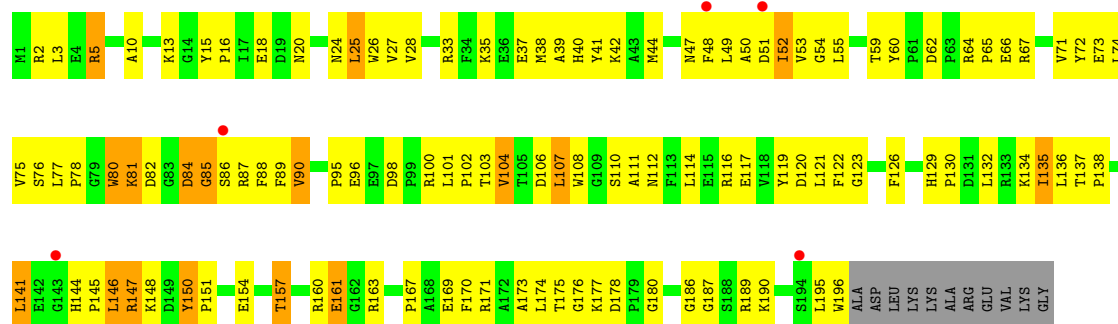


• Molecule 4: NADH-quinone oxidoreductase subunit 4

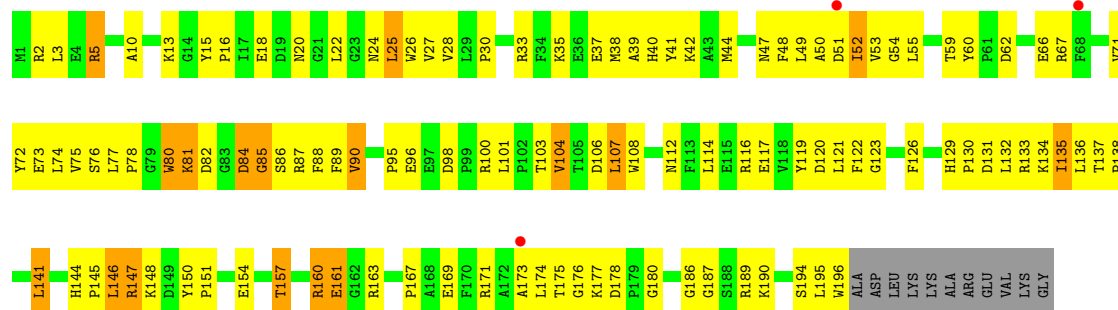




• Molecule 5: NADH-quinone oxidoreductase subunit 5

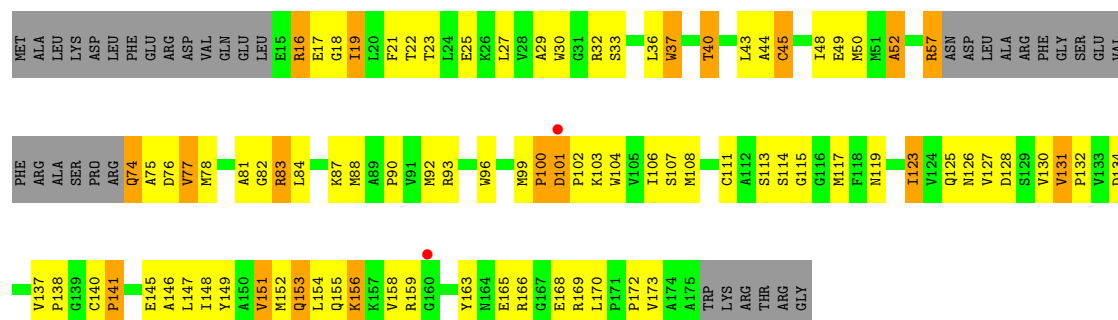


• Molecule 5: NADH-quinone oxidoreductase subunit 5

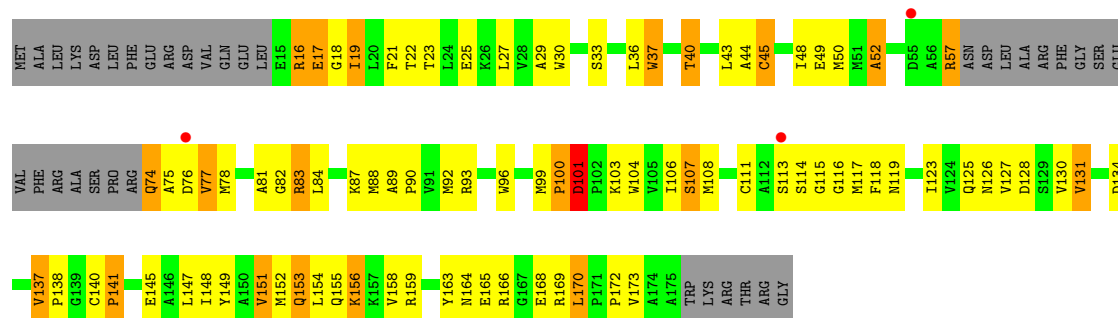


• Molecule 6: NADH-quinone oxidoreductase subunit 6

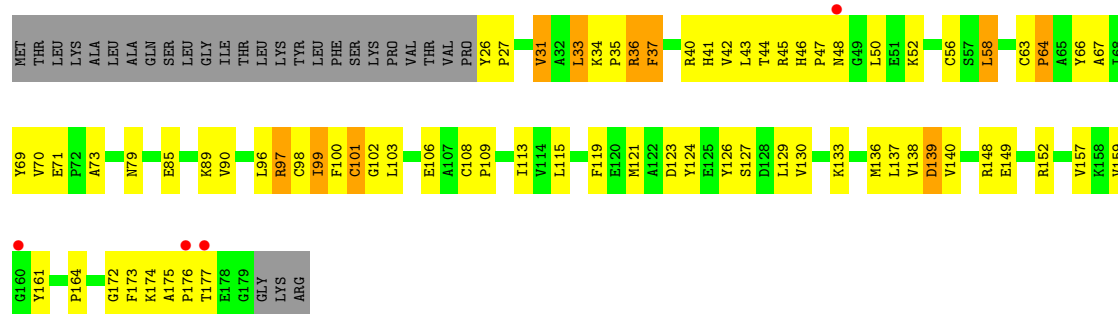
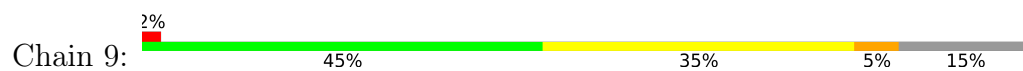




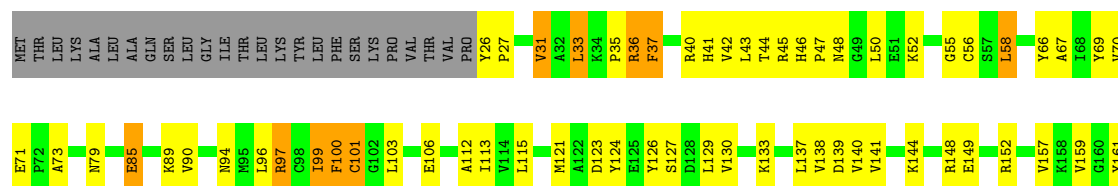
• Molecule 6: NADH-quinone oxidoreductase subunit 6

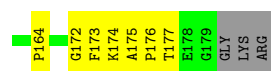


• Molecule 7: NADH-quinone oxidoreductase subunit 9

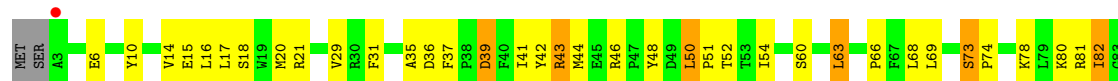


• Molecule 7: NADH-quinone oxidoreductase subunit 9





• Molecule 8: NADH-quinone oxidoreductase subunit 15



• Molecule 8: NADH-quinone oxidoreductase subunit 15



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 108.96Å 150.51Å 216.73Å<br>90.00° 92.19° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 29.93 – 3.10<br>29.93 – 3.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 81.0 (29.93-3.10)<br>80.9 (29.93-3.10)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.14                                                        | Depositor        |
| $R_{sym}$                                                               | 0.14                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.00 (at 3.06Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.235 , 0.283<br>0.233 , 0.280                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2215 reflections (1.84%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 62.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.388                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 57.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$ | Xtriage          |
| Estimated twinning fraction                                             | 0.048 for h,-k,-l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 37520                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 64.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, FES, CA, SF4, FMN

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   | 1     | 0.62         | 0/3506  | 1.05        | 15/4745 (0.3%)   |
| 1   | A     | 0.60         | 0/3506  | 1.04        | 16/4745 (0.3%)   |
| 2   | 2     | 0.62         | 0/1439  | 1.05        | 6/1953 (0.3%)    |
| 2   | B     | 0.56         | 0/1439  | 1.03        | 6/1953 (0.3%)    |
| 3   | 3     | 0.59         | 0/6019  | 1.04        | 30/8163 (0.4%)   |
| 3   | C     | 0.56         | 0/6019  | 1.04        | 35/8163 (0.4%)   |
| 4   | 4     | 0.57         | 0/3089  | 0.99        | 11/4197 (0.3%)   |
| 4   | D     | 0.52         | 0/3089  | 0.99        | 5/4197 (0.1%)    |
| 5   | 5     | 0.53         | 0/1656  | 1.05        | 14/2246 (0.6%)   |
| 5   | E     | 0.48         | 0/1656  | 1.05        | 12/2246 (0.5%)   |
| 6   | 6     | 0.63         | 0/1137  | 1.09        | 6/1542 (0.4%)    |
| 6   | F     | 0.64         | 0/1137  | 1.10        | 6/1542 (0.4%)    |
| 7   | 9     | 0.64         | 0/1224  | 1.04        | 5/1663 (0.3%)    |
| 7   | G     | 0.60         | 0/1224  | 1.01        | 3/1663 (0.2%)    |
| 8   | 7     | 0.57         | 0/1059  | 0.99        | 7/1429 (0.5%)    |
| 8   | H     | 0.57         | 0/1059  | 1.00        | 5/1429 (0.3%)    |
| All | All   | 0.58         | 0/38258 | 1.03        | 182/51876 (0.4%) |

There are no bond length outliers.

All (182) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | 4     | 238 | SER  | N-CA-C | -8.96 | 101.66      | 112.59   |
| 1   | 1     | 291 | ILE  | CA-C-N | 8.72  | 130.74      | 119.84   |
| 1   | 1     | 291 | ILE  | C-N-CA | 8.72  | 130.74      | 119.84   |
| 1   | A     | 291 | ILE  | CA-C-N | 8.66  | 130.66      | 119.84   |
| 1   | A     | 291 | ILE  | C-N-CA | 8.66  | 130.66      | 119.84   |
| 3   | 3     | 625 | SER  | CA-C-N | 8.58  | 130.56      | 119.84   |
| 3   | 3     | 625 | SER  | C-N-CA | 8.58  | 130.56      | 119.84   |
| 3   | C     | 625 | SER  | CA-C-N | 8.29  | 130.20      | 119.84   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | C     | 625 | SER  | C-N-CA  | 8.29  | 130.20      | 119.84   |
| 2   | B     | 19  | PRO  | CA-C-N  | 8.16  | 127.72      | 119.24   |
| 2   | B     | 19  | PRO  | C-N-CA  | 8.16  | 127.72      | 119.24   |
| 5   | E     | 160 | ARG  | N-CA-C  | 8.12  | 119.83      | 110.97   |
| 4   | D     | 238 | SER  | N-CA-C  | -8.10 | 102.70      | 112.59   |
| 1   | A     | 342 | TRP  | N-CA-C  | -7.96 | 101.55      | 111.11   |
| 3   | C     | 194 | VAL  | CA-C-N  | -7.83 | 110.06      | 119.84   |
| 3   | C     | 194 | VAL  | C-N-CA  | -7.83 | 110.06      | 119.84   |
| 6   | F     | 137 | VAL  | N-CA-C  | 7.77  | 115.84      | 108.15   |
| 5   | 5     | 160 | ARG  | N-CA-C  | 7.73  | 119.39      | 110.97   |
| 2   | 2     | 19  | PRO  | CA-C-N  | 7.70  | 127.25      | 119.24   |
| 2   | 2     | 19  | PRO  | C-N-CA  | 7.70  | 127.25      | 119.24   |
| 6   | 6     | 170 | LEU  | CA-C-N  | 7.66  | 128.26      | 120.38   |
| 6   | 6     | 170 | LEU  | C-N-CA  | 7.66  | 128.26      | 120.38   |
| 2   | 2     | 139 | GLU  | CA-C-N  | 7.62  | 129.36      | 119.84   |
| 2   | 2     | 139 | GLU  | C-N-CA  | 7.62  | 129.36      | 119.84   |
| 6   | F     | 170 | LEU  | CA-C-N  | 7.58  | 128.19      | 120.38   |
| 6   | F     | 170 | LEU  | C-N-CA  | 7.58  | 128.19      | 120.38   |
| 5   | 5     | 135 | ILE  | CB-CA-C | -7.52 | 105.31      | 111.71   |
| 1   | 1     | 400 | CYS  | CA-C-N  | 7.48  | 127.50      | 119.28   |
| 1   | 1     | 400 | CYS  | C-N-CA  | 7.48  | 127.50      | 119.28   |
| 5   | 5     | 85  | GLY  | N-CA-C  | -7.38 | 103.91      | 116.01   |
| 2   | B     | 139 | GLU  | CA-C-N  | 7.35  | 129.03      | 119.84   |
| 2   | B     | 139 | GLU  | C-N-CA  | 7.35  | 129.03      | 119.84   |
| 3   | C     | 14  | PRO  | CA-C-N  | 7.30  | 126.83      | 119.24   |
| 3   | C     | 14  | PRO  | C-N-CA  | 7.30  | 126.83      | 119.24   |
| 5   | E     | 85  | GLY  | N-CA-C  | -7.24 | 104.14      | 116.01   |
| 7   | 9     | 79  | ASN  | CA-C-N  | 7.20  | 127.12      | 119.85   |
| 7   | 9     | 79  | ASN  | C-N-CA  | 7.20  | 127.12      | 119.85   |
| 3   | C     | 406 | ALA  | CA-C-N  | 7.15  | 126.68      | 119.24   |
| 3   | C     | 406 | ALA  | C-N-CA  | 7.15  | 126.68      | 119.24   |
| 3   | 3     | 14  | PRO  | CA-C-N  | 7.02  | 126.54      | 119.24   |
| 3   | 3     | 14  | PRO  | C-N-CA  | 7.02  | 126.54      | 119.24   |
| 3   | 3     | 194 | VAL  | CA-C-N  | -7.00 | 111.09      | 119.84   |
| 3   | 3     | 194 | VAL  | C-N-CA  | -7.00 | 111.09      | 119.84   |
| 3   | C     | 218 | LEU  | CA-C-N  | 6.96  | 128.54      | 119.84   |
| 3   | C     | 218 | LEU  | C-N-CA  | 6.96  | 128.54      | 119.84   |
| 5   | E     | 135 | ILE  | CB-CA-C | -6.93 | 105.82      | 111.71   |
| 3   | C     | 55  | PRO  | CB-CA-C | -6.85 | 97.08       | 110.10   |
| 7   | G     | 79  | ASN  | CA-C-N  | 6.76  | 126.68      | 119.85   |
| 7   | G     | 79  | ASN  | C-N-CA  | 6.76  | 126.68      | 119.85   |
| 1   | 1     | 378 | GLN  | N-CA-C  | -6.70 | 104.24      | 112.88   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | 3     | 55  | PRO  | CB-CA-C | -6.61 | 97.54       | 110.10   |
| 3   | 3     | 218 | LEU  | CA-C-N  | 6.59  | 128.08      | 119.84   |
| 3   | 3     | 218 | LEU  | C-N-CA  | 6.59  | 128.08      | 119.84   |
| 5   | 5     | 60  | TYR  | CA-C-N  | 6.49  | 125.99      | 119.24   |
| 5   | 5     | 60  | TYR  | C-N-CA  | 6.49  | 125.99      | 119.24   |
| 4   | D     | 306 | ASN  | CA-C-N  | 6.45  | 126.38      | 119.28   |
| 4   | D     | 306 | ASN  | C-N-CA  | 6.45  | 126.38      | 119.28   |
| 1   | A     | 378 | GLN  | N-CA-C  | -6.45 | 104.56      | 112.88   |
| 3   | C     | 456 | ALA  | CA-C-N  | 6.42  | 127.86      | 119.84   |
| 3   | C     | 456 | ALA  | C-N-CA  | 6.42  | 127.86      | 119.84   |
| 6   | 6     | 101 | ASP  | CA-C-N  | -6.32 | 111.94      | 119.84   |
| 6   | 6     | 101 | ASP  | C-N-CA  | -6.32 | 111.94      | 119.84   |
| 5   | E     | 60  | TYR  | CA-C-N  | 6.29  | 125.78      | 119.24   |
| 5   | E     | 60  | TYR  | C-N-CA  | 6.29  | 125.78      | 119.24   |
| 1   | A     | 400 | CYS  | CA-C-N  | 6.22  | 126.12      | 119.28   |
| 1   | A     | 400 | CYS  | C-N-CA  | 6.22  | 126.12      | 119.28   |
| 6   | F     | 101 | ASP  | CA-C-N  | -6.19 | 112.10      | 119.84   |
| 6   | F     | 101 | ASP  | C-N-CA  | -6.19 | 112.10      | 119.84   |
| 3   | 3     | 282 | VAL  | CA-C-N  | 6.19  | 126.65      | 119.47   |
| 3   | 3     | 282 | VAL  | C-N-CA  | 6.19  | 126.65      | 119.47   |
| 1   | A     | 137 | GLU  | N-CA-C  | -6.18 | 106.37      | 114.04   |
| 3   | 3     | 456 | ALA  | CA-C-N  | 6.17  | 127.56      | 119.84   |
| 3   | 3     | 456 | ALA  | C-N-CA  | 6.17  | 127.56      | 119.84   |
| 5   | 5     | 160 | ARG  | CA-C-N  | -6.16 | 114.77      | 123.03   |
| 5   | 5     | 160 | ARG  | C-N-CA  | -6.16 | 114.77      | 123.03   |
| 1   | A     | 70  | PHE  | CA-C-N  | 6.14  | 127.52      | 119.84   |
| 1   | A     | 70  | PHE  | C-N-CA  | 6.14  | 127.52      | 119.84   |
| 1   | 1     | 137 | GLU  | N-CA-C  | -6.14 | 106.43      | 114.04   |
| 4   | 4     | 306 | ASN  | CA-C-N  | 6.05  | 125.94      | 119.28   |
| 4   | 4     | 306 | ASN  | C-N-CA  | 6.05  | 125.94      | 119.28   |
| 1   | 1     | 70  | PHE  | CA-C-N  | 6.02  | 127.36      | 119.84   |
| 1   | 1     | 70  | PHE  | C-N-CA  | 6.02  | 127.36      | 119.84   |
| 8   | H     | 37  | PHE  | CA-C-N  | -5.97 | 113.53      | 119.56   |
| 8   | H     | 37  | PHE  | C-N-CA  | -5.97 | 113.53      | 119.56   |
| 3   | 3     | 216 | PHE  | N-CA-C  | 5.97  | 121.22      | 111.37   |
| 1   | 1     | 356 | CYS  | CB-CA-C | -5.87 | 99.84       | 109.53   |
| 3   | C     | 282 | VAL  | CA-C-N  | 5.87  | 126.28      | 119.47   |
| 3   | C     | 282 | VAL  | C-N-CA  | 5.87  | 126.28      | 119.47   |
| 3   | 3     | 719 | HIS  | CA-C-N  | 5.77  | 127.05      | 119.84   |
| 3   | 3     | 719 | HIS  | C-N-CA  | 5.77  | 127.05      | 119.84   |
| 3   | C     | 377 | ALA  | CA-C-N  | 5.75  | 126.04      | 119.83   |
| 3   | C     | 377 | ALA  | C-N-CA  | 5.75  | 126.04      | 119.83   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | C     | 216 | PHE  | N-CA-C | 5.74  | 120.85      | 111.37   |
| 1   | A     | 397 | ARG  | N-CA-C | 5.73  | 116.77      | 107.32   |
| 8   | 7     | 35  | ALA  | N-CA-C | 5.71  | 117.08      | 108.46   |
| 8   | H     | 35  | ALA  | N-CA-C | 5.67  | 117.02      | 108.46   |
| 1   | 1     | 342 | TRP  | N-CA-C | -5.59 | 102.14      | 111.37   |
| 3   | C     | 430 | THR  | CA-C-N | 5.58  | 125.59      | 119.89   |
| 3   | C     | 430 | THR  | C-N-CA | 5.58  | 125.59      | 119.89   |
| 7   | 9     | 102 | GLY  | N-CA-C | -5.57 | 107.58      | 115.43   |
| 5   | E     | 104 | VAL  | N-CA-C | -5.57 | 106.88      | 112.17   |
| 2   | 2     | 7   | LYS  | N-CA-C | 5.56  | 116.38      | 108.54   |
| 3   | C     | 52  | ILE  | N-CA-C | 5.55  | 115.89      | 108.11   |
| 3   | C     | 472 | GLU  | N-CA-C | -5.54 | 106.35      | 114.39   |
| 2   | B     | 7   | LYS  | N-CA-C | 5.54  | 116.35      | 108.54   |
| 5   | 5     | 104 | VAL  | N-CA-C | -5.51 | 106.94      | 112.17   |
| 3   | 3     | 377 | ALA  | CA-C-N | 5.50  | 125.77      | 119.83   |
| 3   | 3     | 377 | ALA  | C-N-CA | 5.50  | 125.77      | 119.83   |
| 5   | E     | 62  | ASP  | CA-C-N | 5.50  | 125.25      | 119.76   |
| 5   | E     | 62  | ASP  | C-N-CA | 5.50  | 125.25      | 119.76   |
| 3   | C     | 719 | HIS  | CA-C-N | 5.48  | 126.69      | 119.84   |
| 3   | C     | 719 | HIS  | C-N-CA | 5.48  | 126.69      | 119.84   |
| 3   | C     | 691 | ALA  | N-CA-C | -5.46 | 105.73      | 112.72   |
| 5   | 5     | 62  | ASP  | CA-C-N | 5.46  | 125.22      | 119.76   |
| 5   | 5     | 62  | ASP  | C-N-CA | 5.46  | 125.22      | 119.76   |
| 3   | 3     | 691 | ALA  | N-CA-C | -5.45 | 105.74      | 112.72   |
| 7   | G     | 70  | VAL  | N-CA-C | 5.45  | 115.84      | 107.77   |
| 2   | 2     | 172 | CYS  | N-CA-C | 5.44  | 117.29      | 108.26   |
| 1   | A     | 429 | ARG  | CA-C-N | 5.43  | 125.34      | 119.85   |
| 1   | A     | 429 | ARG  | C-N-CA | 5.43  | 125.34      | 119.85   |
| 4   | 4     | 56  | VAL  | CA-C-N | 5.43  | 125.33      | 119.85   |
| 4   | 4     | 56  | VAL  | C-N-CA | 5.43  | 125.33      | 119.85   |
| 5   | E     | 178 | ASP  | CA-C-N | 5.41  | 125.03      | 119.56   |
| 5   | E     | 178 | ASP  | C-N-CA | 5.41  | 125.03      | 119.56   |
| 4   | 4     | 344 | VAL  | CA-C-N | 5.41  | 126.24      | 120.13   |
| 4   | 4     | 344 | VAL  | C-N-CA | 5.41  | 126.24      | 120.13   |
| 3   | 3     | 52  | ILE  | N-CA-C | 5.41  | 115.68      | 108.11   |
| 3   | C     | 588 | SER  | N-CA-C | -5.40 | 106.63      | 113.43   |
| 3   | 3     | 448 | MET  | N-CA-C | 5.39  | 117.38      | 109.24   |
| 3   | C     | 412 | ARG  | N-CA-C | -5.38 | 106.56      | 113.23   |
| 3   | 3     | 171 | SER  | N-CA-C | -5.36 | 103.30      | 108.07   |
| 5   | E     | 160 | ARG  | CA-C-N | -5.33 | 115.85      | 123.20   |
| 5   | E     | 160 | ARG  | C-N-CA | -5.33 | 115.85      | 123.20   |
| 1   | 1     | 67  | GLY  | N-CA-C | -5.32 | 108.15      | 114.48   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | 4     | 119 | ILE  | CB-CA-C | -5.32 | 105.17      | 111.97   |
| 2   | B     | 172 | CYS  | N-CA-C  | 5.31  | 117.07      | 108.26   |
| 6   | F     | 52  | ALA  | N-CA-C  | -5.30 | 106.70      | 114.39   |
| 4   | D     | 239 | LEU  | N-CA-C  | -5.29 | 104.43      | 112.04   |
| 7   | 9     | 70  | VAL  | N-CA-C  | 5.28  | 115.72      | 108.12   |
| 3   | 3     | 406 | ALA  | CA-C-N  | 5.26  | 126.42      | 119.84   |
| 3   | 3     | 406 | ALA  | C-N-CA  | 5.26  | 126.42      | 119.84   |
| 8   | 7     | 37  | PHE  | CA-C-N  | -5.24 | 114.27      | 119.56   |
| 8   | 7     | 37  | PHE  | C-N-CA  | -5.24 | 114.27      | 119.56   |
| 3   | C     | 382 | PHE  | CA-C-N  | 5.24  | 125.78      | 120.38   |
| 3   | C     | 382 | PHE  | C-N-CA  | 5.24  | 125.78      | 120.38   |
| 8   | 7     | 46  | ARG  | CA-C-N  | 5.20  | 125.11      | 119.85   |
| 8   | 7     | 46  | ARG  | C-N-CA  | 5.20  | 125.11      | 119.85   |
| 1   | A     | 79  | MET  | CA-C-N  | 5.20  | 125.49      | 119.93   |
| 1   | A     | 79  | MET  | C-N-CA  | 5.20  | 125.49      | 119.93   |
| 3   | 3     | 30  | VAL  | CA-C-N  | 5.18  | 125.17      | 119.89   |
| 3   | 3     | 30  | VAL  | C-N-CA  | 5.18  | 125.17      | 119.89   |
| 4   | 4     | 168 | PHE  | N-CA-C  | 5.17  | 116.15      | 108.86   |
| 1   | A     | 331 | ILE  | CA-C-N  | 5.14  | 124.91      | 119.76   |
| 1   | A     | 331 | ILE  | C-N-CA  | 5.14  | 124.91      | 119.76   |
| 3   | C     | 466 | GLU  | N-CA-C  | 5.14  | 117.73      | 108.48   |
| 3   | C     | 30  | VAL  | CA-C-N  | 5.13  | 125.12      | 119.89   |
| 3   | C     | 30  | VAL  | C-N-CA  | 5.13  | 125.12      | 119.89   |
| 8   | H     | 46  | ARG  | CA-C-N  | 5.12  | 125.02      | 119.85   |
| 8   | H     | 46  | ARG  | C-N-CA  | 5.12  | 125.02      | 119.85   |
| 4   | 4     | 311 | PRO  | CA-C-N  | 5.11  | 125.65      | 120.38   |
| 4   | 4     | 311 | PRO  | C-N-CA  | 5.11  | 125.65      | 120.38   |
| 6   | 6     | 52  | ALA  | N-CA-C  | -5.11 | 106.97      | 114.39   |
| 6   | 6     | 123 | ILE  | N-CA-C  | 5.11  | 115.47      | 108.12   |
| 3   | C     | 184 | CYS  | CA-C-N  | -5.10 | 113.98      | 122.08   |
| 3   | C     | 184 | CYS  | C-N-CA  | -5.10 | 113.98      | 122.08   |
| 5   | 5     | 178 | ASP  | CA-C-N  | 5.09  | 124.70      | 119.56   |
| 5   | 5     | 178 | ASP  | C-N-CA  | 5.09  | 124.70      | 119.56   |
| 8   | 7     | 73  | SER  | CA-C-N  | 5.09  | 126.20      | 119.84   |
| 8   | 7     | 73  | SER  | C-N-CA  | 5.09  | 126.20      | 119.84   |
| 3   | C     | 176 | LEU  | N-CA-C  | 5.08  | 116.98      | 107.99   |
| 7   | 9     | 64  | PRO  | N-CA-C  | -5.07 | 107.79      | 114.03   |
| 5   | 5     | 150 | TYR  | CA-C-N  | 5.04  | 124.95      | 119.76   |
| 5   | 5     | 150 | TYR  | C-N-CA  | 5.04  | 124.95      | 119.76   |
| 3   | 3     | 289 | TRP  | N-CA-C  | 5.04  | 117.70      | 109.59   |
| 1   | 1     | 119 | ILE  | CB-CA-C | -5.03 | 105.45      | 111.88   |
| 1   | 1     | 397 | ARG  | N-CA-C  | 5.02  | 115.62      | 107.23   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | 3     | 400 | GLY  | N-CA-C | -5.01 | 106.53      | 111.85   |
| 3   | 3     | 466 | GLU  | N-CA-C | 5.01  | 117.50      | 108.48   |
| 1   | 1     | 260 | ARG  | CA-C-N | 5.01  | 125.28      | 119.92   |
| 1   | 1     | 260 | ARG  | C-N-CA | 5.01  | 125.28      | 119.92   |
| 3   | 3     | 472 | GLU  | N-CA-C | -5.01 | 107.13      | 114.39   |
| 4   | D     | 236 | GLY  | N-CA-C | 5.00  | 125.04      | 113.18   |

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   | 1     | 3417  | 0        | 3388     | 215     | 1            |
| 1   | A     | 3417  | 0        | 3388     | 218     | 0            |
| 2   | 2     | 1406  | 0        | 1373     | 78      | 0            |
| 2   | B     | 1406  | 0        | 1373     | 76      | 0            |
| 3   | 3     | 5880  | 0        | 5911     | 412     | 1            |
| 3   | C     | 5880  | 0        | 5911     | 423     | 0            |
| 4   | 4     | 3011  | 0        | 3000     | 225     | 0            |
| 4   | D     | 3011  | 0        | 3000     | 236     | 0            |
| 5   | 5     | 1607  | 0        | 1574     | 107     | 0            |
| 5   | E     | 1607  | 0        | 1574     | 113     | 0            |
| 6   | 6     | 1113  | 0        | 1121     | 105     | 0            |
| 6   | F     | 1113  | 0        | 1121     | 109     | 0            |
| 7   | 9     | 1193  | 0        | 1160     | 70      | 0            |
| 7   | G     | 1193  | 0        | 1160     | 68      | 0            |
| 8   | 7     | 1031  | 0        | 1029     | 44      | 0            |
| 8   | H     | 1031  | 0        | 1029     | 47      | 0            |
| 9   | 1     | 8     | 0        | 0        | 2       | 0            |
| 9   | 3     | 24    | 0        | 0        | 7       | 0            |
| 9   | 6     | 8     | 0        | 0        | 4       | 0            |
| 9   | 9     | 16    | 0        | 0        | 0       | 0            |
| 9   | A     | 8     | 0        | 0        | 1       | 0            |
| 9   | C     | 24    | 0        | 0        | 5       | 0            |
| 9   | F     | 8     | 0        | 0        | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | G     | 16    | 0        | 0        | 2       | 0            |
| 10  | 1     | 31    | 0        | 19       | 8       | 0            |
| 10  | A     | 31    | 0        | 19       | 4       | 0            |
| 11  | 2     | 4     | 0        | 0        | 0       | 0            |
| 11  | 3     | 4     | 0        | 0        | 1       | 0            |
| 11  | B     | 4     | 0        | 0        | 1       | 0            |
| 11  | C     | 4     | 0        | 0        | 1       | 0            |
| 12  | 2     | 1     | 0        | 0        | 0       | 0            |
| 12  | 3     | 2     | 0        | 0        | 0       | 0            |
| 12  | 4     | 2     | 0        | 0        | 0       | 0            |
| 12  | 5     | 1     | 0        | 0        | 0       | 0            |
| 12  | 7     | 1     | 0        | 0        | 0       | 0            |
| 12  | C     | 2     | 0        | 0        | 0       | 0            |
| 12  | D     | 1     | 0        | 0        | 0       | 0            |
| 12  | E     | 1     | 0        | 0        | 0       | 0            |
| 12  | H     | 1     | 0        | 0        | 0       | 0            |
| 13  | 3     | 1     | 0        | 0        | 0       | 0            |
| 13  | C     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 37520 | 0        | 37150    | 2354    | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (2354) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:561:PRO:HB3  | 3:C:576:ALA:HA   | 1.28                     | 1.15              |
| 3:3:474:ARG:NH2  | 3:3:516:VAL:HG21 | 1.60                     | 1.15              |
| 3:3:117:LEU:N    | 4:4:321:MET:HE1  | 1.62                     | 1.13              |
| 7:G:40:ARG:HB2   | 7:G:121:MET:HE1  | 1.32                     | 1.12              |
| 3:C:117:LEU:N    | 4:D:321:MET:HE1  | 1.66                     | 1.10              |
| 3:C:474:ARG:NH2  | 3:C:516:VAL:HG21 | 1.65                     | 1.10              |
| 3:3:561:PRO:HB3  | 3:3:576:ALA:HA   | 1.30                     | 1.10              |
| 1:1:437:TRP:HB3  | 2:2:92:GLY:HA3   | 1.10                     | 1.09              |
| 5:E:66:GLU:HG2   | 5:E:95:PRO:HA    | 1.13                     | 1.09              |
| 7:9:40:ARG:HB2   | 7:9:121:MET:HE1  | 1.33                     | 1.08              |
| 5:5:66:GLU:HG2   | 5:5:95:PRO:HA    | 1.16                     | 1.08              |
| 6:6:117:MET:HE2  | 7:9:99:ILE:HG12  | 1.27                     | 1.07              |
| 3:C:738:THR:HG22 | 3:C:739:PRO:HD2  | 1.36                     | 1.07              |
| 1:A:437:TRP:HB3  | 2:B:92:GLY:HA3   | 1.07                     | 1.06              |
| 3:3:474:ARG:HH21 | 3:3:516:VAL:HG21 | 1.12                     | 1.04              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:115:HIS:CD2  | 3:3:116:PRO:HD2  | 1.91                     | 1.04              |
| 6:F:117:MET:HE2  | 7:G:99:ILE:HG12  | 1.39                     | 1.03              |
| 3:C:115:HIS:CD2  | 3:C:116:PRO:HD2  | 1.92                     | 1.02              |
| 3:3:738:THR:HG22 | 3:3:739:PRO:HD2  | 1.37                     | 1.02              |
| 3:C:440:ARG:HG2  | 3:C:440:ARG:HH11 | 1.24                     | 1.02              |
| 7:G:41:HIS:HB3   | 7:G:113:ILE:HD11 | 1.43                     | 1.01              |
| 1:A:16:THR:HG21  | 1:A:229:PRO:HB3  | 1.40                     | 1.00              |
| 3:C:655:ARG:HB2  | 3:C:655:ARG:HH11 | 1.27                     | 1.00              |
| 4:4:367:ARG:HH11 | 4:4:367:ARG:HG3  | 1.22                     | 1.00              |
| 6:6:145:GLU:HG2  | 7:9:31:VAL:HG21  | 1.43                     | 0.99              |
| 3:3:440:ARG:HG2  | 3:3:440:ARG:HH11 | 1.20                     | 0.99              |
| 1:1:186:THR:HG23 | 1:1:200:ARG:H    | 1.27                     | 0.99              |
| 3:3:501:LYS:H    | 3:3:501:LYS:HD2  | 1.27                     | 0.99              |
| 1:1:16:THR:HG21  | 1:1:229:PRO:HB3  | 1.44                     | 0.99              |
| 3:3:655:ARG:HB2  | 3:3:655:ARG:HH11 | 1.26                     | 0.98              |
| 4:D:367:ARG:HH11 | 4:D:367:ARG:HG3  | 1.26                     | 0.98              |
| 7:9:41:HIS:HB3   | 7:9:113:ILE:HD11 | 1.42                     | 0.97              |
| 3:C:501:LYS:H    | 3:C:501:LYS:HD2  | 1.28                     | 0.97              |
| 3:C:474:ARG:HH21 | 3:C:516:VAL:HG21 | 1.15                     | 0.96              |
| 1:1:104:ARG:HH21 | 2:2:127:SER:HB3  | 1.31                     | 0.95              |
| 1:A:186:THR:HG23 | 1:A:200:ARG:H    | 1.29                     | 0.95              |
| 1:A:395:GLU:HB2  | 1:A:407:VAL:HG21 | 1.49                     | 0.95              |
| 3:C:722:THR:HG21 | 3:C:756:GLY:H    | 1.31                     | 0.95              |
| 1:A:246:SER:HB3  | 1:A:268:MET:HG2  | 1.47                     | 0.94              |
| 6:F:145:GLU:HG2  | 7:G:31:VAL:HG21  | 1.46                     | 0.94              |
| 1:1:358:PRO:O    | 1:1:362:GLY:HA3  | 1.66                     | 0.94              |
| 3:C:279:ALA:HB2  | 3:C:290:ILE:HG12 | 1.48                     | 0.94              |
| 4:4:254:TYR:HD1  | 4:4:255:SER:H    | 1.15                     | 0.94              |
| 1:A:358:PRO:O    | 1:A:362:GLY:HA3  | 1.68                     | 0.94              |
| 1:1:395:GLU:HB2  | 1:1:407:VAL:HG21 | 1.50                     | 0.93              |
| 3:3:440:ARG:HH11 | 3:3:440:ARG:CG   | 1.80                     | 0.93              |
| 4:4:238:SER:HB3  | 4:4:279:ARG:NH2  | 1.83                     | 0.93              |
| 1:A:90:ILE:HD11  | 1:A:211:LEU:HD22 | 1.50                     | 0.93              |
| 1:A:104:ARG:HH21 | 2:B:127:SER:HB3  | 1.32                     | 0.93              |
| 1:1:331:ILE:HD12 | 1:1:337:MET:HE1  | 1.51                     | 0.93              |
| 3:C:343:LEU:HD12 | 3:C:361:ALA:HB2  | 1.50                     | 0.92              |
| 1:1:246:SER:HB3  | 1:1:268:MET:HG2  | 1.49                     | 0.92              |
| 1:1:90:ILE:HD11  | 1:1:211:LEU:HD22 | 1.48                     | 0.92              |
| 3:3:20:MET:HE2   | 3:3:433:ALA:HB2  | 1.49                     | 0.91              |
| 4:D:238:SER:HB3  | 4:D:279:ARG:NH2  | 1.86                     | 0.91              |
| 3:3:722:THR:HG21 | 3:3:756:GLY:H    | 1.34                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:254:TYR:HD1  | 4:D:255:SER:H    | 1.12                     | 0.91              |
| 3:3:343:LEU:HD12 | 3:3:361:ALA:HB2  | 1.50                     | 0.91              |
| 3:C:20:MET:HE2   | 3:C:433:ALA:HB2  | 1.53                     | 0.91              |
| 3:C:440:ARG:HH11 | 3:C:440:ARG:CG   | 1.84                     | 0.90              |
| 3:C:509:ALA:HB1  | 3:C:768:GLY:HA3  | 1.53                     | 0.90              |
| 1:A:242:GLY:HA2  | 1:A:268:MET:O    | 1.71                     | 0.90              |
| 1:A:331:ILE:HD12 | 1:A:337:MET:HE1  | 1.52                     | 0.89              |
| 1:1:40:THR:O     | 1:1:44:VAL:HG23  | 1.70                     | 0.89              |
| 3:3:509:ALA:HB1  | 3:3:768:GLY:HA3  | 1.50                     | 0.89              |
| 5:E:161:GLU:HG3  | 5:E:163:ARG:NH2  | 1.88                     | 0.89              |
| 3:3:136:GLU:HG2  | 5:5:189:ARG:HG2  | 1.55                     | 0.88              |
| 1:A:186:THR:CG2  | 1:A:200:ARG:H    | 1.86                     | 0.88              |
| 3:3:374:ARG:NH2  | 3:3:684:ARG:HG3  | 1.87                     | 0.88              |
| 3:C:226:ILE:HD12 | 3:C:235:LEU:HD13 | 1.54                     | 0.88              |
| 3:C:396:ALA:HB3  | 3:C:448:MET:HB2  | 1.55                     | 0.88              |
| 3:3:279:ALA:HB2  | 3:3:290:ILE:HG12 | 1.56                     | 0.88              |
| 3:3:115:HIS:CG   | 3:3:116:PRO:HD2  | 2.09                     | 0.88              |
| 8:H:87:PRO:O     | 8:H:88:ARG:HB2   | 1.73                     | 0.88              |
| 3:C:87:VAL:HA    | 3:C:91:MET:HE1   | 1.55                     | 0.87              |
| 5:E:18:GLU:HB2   | 5:E:26:TRP:HB2   | 1.57                     | 0.87              |
| 3:C:115:HIS:CG   | 3:C:116:PRO:HD2  | 2.09                     | 0.87              |
| 1:1:186:THR:CG2  | 1:1:200:ARG:H    | 1.87                     | 0.87              |
| 1:1:242:GLY:HA2  | 1:1:268:MET:O    | 1.75                     | 0.87              |
| 5:5:18:GLU:HB2   | 5:5:26:TRP:HB2   | 1.55                     | 0.87              |
| 1:A:437:TRP:CB   | 2:B:92:GLY:HA3   | 2.00                     | 0.87              |
| 1:A:297:THR:HG22 | 1:A:322:MET:HG3  | 1.57                     | 0.86              |
| 3:3:689:LYS:HE3  | 3:3:771:VAL:HG13 | 1.55                     | 0.86              |
| 1:A:270:THR:O    | 1:A:311:MET:HG3  | 1.75                     | 0.86              |
| 3:3:396:ALA:HB3  | 3:3:448:MET:HB2  | 1.57                     | 0.86              |
| 4:D:230:ILE:HD13 | 5:E:77:LEU:HD12  | 1.57                     | 0.86              |
| 1:A:40:THR:O     | 1:A:44:VAL:HG23  | 1.76                     | 0.86              |
| 1:1:245:GLN:HB2  | 1:1:314:GLU:OE1  | 1.75                     | 0.86              |
| 1:A:437:TRP:HB3  | 2:B:92:GLY:CA    | 2.01                     | 0.86              |
| 3:3:226:ILE:HD12 | 3:3:235:LEU:HD13 | 1.58                     | 0.85              |
| 1:A:360:ARG:O    | 1:A:364:ALA:HB3  | 1.75                     | 0.85              |
| 1:1:162:LEU:O    | 1:1:165:THR:HG22 | 1.76                     | 0.85              |
| 3:C:689:LYS:HG3  | 3:C:771:VAL:HA   | 1.58                     | 0.85              |
| 3:C:374:ARG:NH2  | 3:C:684:ARG:HG3  | 1.92                     | 0.85              |
| 3:3:402:PRO:HG3  | 3:3:535:MET:HE1  | 1.58                     | 0.85              |
| 1:A:162:LEU:O    | 1:A:165:THR:HG22 | 1.76                     | 0.85              |
| 3:3:87:VAL:HA    | 3:3:91:MET:HE1   | 1.58                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:88:TYR:HB2   | 1:A:216:THR:HG22 | 1.58                     | 0.84              |
| 3:C:689:LYS:HE3  | 3:C:771:VAL:HG13 | 1.58                     | 0.84              |
| 4:D:115:THR:HG21 | 4:D:297:LEU:HD13 | 1.58                     | 0.84              |
| 1:A:253:GLN:N    | 1:A:253:GLN:HE21 | 1.73                     | 0.84              |
| 3:3:689:LYS:HG3  | 3:3:771:VAL:HA   | 1.59                     | 0.84              |
| 4:4:115:THR:HG21 | 4:4:297:LEU:HD13 | 1.60                     | 0.84              |
| 1:1:297:THR:HG22 | 1:1:322:MET:HG3  | 1.58                     | 0.84              |
| 3:C:117:LEU:H    | 4:D:321:MET:HE1  | 1.37                     | 0.84              |
| 5:E:121:LEU:HB3  | 5:E:146:LEU:HB2  | 1.57                     | 0.84              |
| 3:C:186:ARG:HD2  | 3:C:231:PRO:HD3  | 1.60                     | 0.84              |
| 8:7:87:PRO:O     | 8:7:88:ARG:HB2   | 1.74                     | 0.83              |
| 5:E:52:ILE:CG2   | 5:E:114:LEU:HB3  | 2.06                     | 0.83              |
| 5:5:52:ILE:CG2   | 5:5:114:LEU:HB3  | 2.07                     | 0.83              |
| 1:1:253:GLN:N    | 1:1:253:GLN:HE21 | 1.75                     | 0.83              |
| 4:4:230:ILE:HD13 | 5:5:77:LEU:HD12  | 1.61                     | 0.83              |
| 5:5:121:LEU:HB3  | 5:5:146:LEU:HB2  | 1.60                     | 0.83              |
| 1:A:245:GLN:HB2  | 1:A:314:GLU:OE1  | 1.79                     | 0.82              |
| 3:3:186:ARG:HD2  | 3:3:231:PRO:HD3  | 1.61                     | 0.82              |
| 1:1:88:TYR:HB2   | 1:1:216:THR:HG22 | 1.60                     | 0.82              |
| 1:A:104:ARG:HH21 | 2:B:127:SER:CB   | 1.93                     | 0.82              |
| 3:C:739:PRO:HG2  | 3:C:771:VAL:CG1  | 2.10                     | 0.82              |
| 3:3:120:PRO:HG2  | 8:7:42:TYR:OH    | 1.80                     | 0.82              |
| 3:C:561:PRO:CB   | 3:C:576:ALA:HA   | 2.10                     | 0.82              |
| 10:1:440:FMN:N1  | 10:1:440:FMN:O3' | 2.13                     | 0.81              |
| 1:A:104:ARG:NH2  | 2:B:127:SER:HB3  | 1.94                     | 0.81              |
| 3:C:722:THR:HG21 | 3:C:756:GLY:N    | 1.94                     | 0.81              |
| 6:6:96:TRP:HA    | 6:6:99:MET:HE3   | 1.61                     | 0.81              |
| 3:C:386:SER:HB2  | 3:C:675:ARG:NH1  | 1.95                     | 0.81              |
| 3:C:413:LEU:HD13 | 3:C:448:MET:HE1  | 1.62                     | 0.81              |
| 3:3:11:VAL:HG11  | 3:3:25:HIS:CD2   | 2.16                     | 0.81              |
| 3:3:117:LEU:H    | 4:4:321:MET:HE1  | 1.44                     | 0.81              |
| 1:A:293:GLY:HA3  | 1:A:324:GLY:H    | 1.45                     | 0.81              |
| 4:4:311:PRO:HD3  | 4:4:330:HIS:CE1  | 2.15                     | 0.81              |
| 3:C:237:ASP:OD1  | 3:C:239:THR:HG22 | 1.81                     | 0.81              |
| 3:C:2:VAL:HG13   | 3:C:89:ASP:HA    | 1.62                     | 0.80              |
| 1:1:437:TRP:CB   | 2:2:92:GLY:HA3   | 2.04                     | 0.80              |
| 5:5:161:GLU:HG3  | 5:5:163:ARG:NH2  | 1.95                     | 0.80              |
| 4:D:212:PRO:HG2  | 4:D:213:ILE:HD12 | 1.64                     | 0.80              |
| 4:D:238:SER:HB3  | 4:D:279:ARG:HH22 | 1.46                     | 0.80              |
| 3:3:237:ASP:OD1  | 3:3:239:THR:HG22 | 1.81                     | 0.80              |
| 3:3:722:THR:HG21 | 3:3:756:GLY:N    | 1.97                     | 0.80              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:3:739:PRO:HG2  | 3:3:771:VAL:CG1   | 2.11                     | 0.80              |
| 3:C:538:ALA:HB3  | 3:C:541:ALA:HB2   | 1.64                     | 0.80              |
| 3:3:2:VAL:HG13   | 3:3:89:ASP:HA     | 1.63                     | 0.79              |
| 4:4:212:PRO:HG2  | 4:4:213:ILE:HD12  | 1.64                     | 0.79              |
| 3:C:11:VAL:HG11  | 3:C:25:HIS:CD2    | 2.18                     | 0.79              |
| 1:1:160:LYS:HG3  | 1:1:161:ASN:H     | 1.46                     | 0.79              |
| 3:3:250:GLU:HG3  | 5:5:169:GLU:CD    | 2.05                     | 0.79              |
| 1:1:104:ARG:HH21 | 2:2:127:SER:CB    | 1.94                     | 0.79              |
| 6:F:96:TRP:HA    | 6:F:99:MET:HE3    | 1.65                     | 0.79              |
| 1:1:293:GLY:HA3  | 1:1:324:GLY:H     | 1.47                     | 0.79              |
| 1:A:401:PRO:HB2  | 10:A:440:FMN:HM82 | 1.65                     | 0.79              |
| 3:C:584:VAL:HG12 | 3:C:600:VAL:HB    | 1.64                     | 0.79              |
| 4:D:250:LYS:HE2  | 4:D:262:PHE:HB3   | 1.65                     | 0.79              |
| 3:3:584:VAL:HG12 | 3:3:600:VAL:HB    | 1.64                     | 0.78              |
| 3:C:511:VAL:O    | 3:C:518:ALA:HB2   | 1.84                     | 0.78              |
| 1:1:104:ARG:NH2  | 2:2:127:SER:HB3   | 1.97                     | 0.78              |
| 3:3:694:LEU:HB3  | 3:3:762:ALA:HB2   | 1.64                     | 0.78              |
| 1:A:341:MET:HE1  | 1:A:409:PRO:HB2   | 1.65                     | 0.78              |
| 3:C:55:PRO:HD3   | 3:C:74:GLN:H      | 1.49                     | 0.78              |
| 3:3:655:ARG:HB2  | 3:3:655:ARG:NH1   | 1.98                     | 0.78              |
| 6:F:148:ILE:HG21 | 7:G:27:PRO:HG3    | 1.66                     | 0.78              |
| 1:1:415:ARG:O    | 1:1:415:ARG:HG2   | 1.82                     | 0.78              |
| 1:A:415:ARG:O    | 1:A:415:ARG:HG2   | 1.84                     | 0.78              |
| 4:4:238:SER:HB3  | 4:4:279:ARG:HH22  | 1.45                     | 0.78              |
| 5:5:37:GLU:O     | 5:5:41:TYR:HD1    | 1.67                     | 0.78              |
| 3:C:300:TRP:HB3  | 3:C:705:VAL:HG21  | 1.66                     | 0.77              |
| 3:C:694:LEU:HB3  | 3:C:762:ALA:HB2   | 1.66                     | 0.77              |
| 2:2:61:MET:HE2   | 3:3:214:MET:HG2   | 1.67                     | 0.77              |
| 5:E:106:ASP:HB2  | 5:E:107:LEU:HD12  | 1.66                     | 0.77              |
| 3:C:136:GLU:HG2  | 5:E:189:ARG:HG2   | 1.65                     | 0.77              |
| 5:E:174:LEU:HD21 | 5:E:180:GLY:HA2   | 1.66                     | 0.77              |
| 3:C:116:PRO:O    | 3:C:117:LEU:HB2   | 1.84                     | 0.77              |
| 3:C:402:PRO:HG3  | 3:C:535:MET:HE1   | 1.67                     | 0.77              |
| 3:C:337:ARG:H    | 3:C:337:ARG:CD    | 1.97                     | 0.77              |
| 4:D:371:ARG:NH2  | 4:D:376:VAL:HG21  | 2.00                     | 0.77              |
| 7:G:33:LEU:HD11  | 7:G:161:TYR:HB2   | 1.67                     | 0.77              |
| 4:D:389:GLN:HG3  | 4:D:390:VAL:H     | 1.49                     | 0.77              |
| 1:A:160:LYS:HG3  | 1:A:161:ASN:H     | 1.48                     | 0.77              |
| 3:C:337:ARG:H    | 3:C:337:ARG:HD2   | 1.50                     | 0.76              |
| 7:G:44:THR:HA    | 7:G:138:VAL:CG1   | 2.14                     | 0.76              |
| 4:D:40:VAL:HG13  | 4:D:404:MET:HG3   | 1.67                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:368:HIS:CB   | 3:3:556:ALA:HB3  | 2.15                     | 0.76              |
| 3:3:511:VAL:O    | 3:3:518:ALA:HB2  | 1.86                     | 0.76              |
| 4:4:249:ARG:HB3  | 4:4:257:TYR:HD1  | 1.49                     | 0.76              |
| 3:3:160:THR:OG1  | 8:7:73:SER:HB3   | 1.86                     | 0.76              |
| 3:3:337:ARG:H    | 3:3:337:ARG:HD2  | 1.50                     | 0.76              |
| 3:C:655:ARG:HB2  | 3:C:655:ARG:NH1  | 1.99                     | 0.76              |
| 4:D:249:ARG:HB3  | 4:D:257:TYR:HD1  | 1.49                     | 0.76              |
| 3:3:368:HIS:HB3  | 3:3:556:ALA:HB3  | 1.67                     | 0.76              |
| 7:9:33:LEU:HD11  | 7:9:161:TYR:HB2  | 1.67                     | 0.76              |
| 4:D:311:PRO:HD3  | 4:D:330:HIS:CE1  | 2.21                     | 0.76              |
| 3:3:413:LEU:HD13 | 3:3:448:MET:HE1  | 1.68                     | 0.75              |
| 3:3:738:THR:CG2  | 3:3:739:PRO:HD2  | 2.17                     | 0.75              |
| 4:4:389:GLN:HG3  | 4:4:390:VAL:H    | 1.51                     | 0.75              |
| 2:B:136:VAL:HG21 | 2:B:163:LEU:HD13 | 1.67                     | 0.75              |
| 3:C:368:HIS:CB   | 3:C:556:ALA:HB3  | 2.17                     | 0.75              |
| 1:1:98:PRO:HA    | 2:2:124:CYS:SG   | 2.26                     | 0.75              |
| 7:9:44:THR:HA    | 7:9:138:VAL:CG1  | 2.16                     | 0.75              |
| 5:E:5:ARG:HH11   | 5:E:5:ARG:HG3    | 1.52                     | 0.75              |
| 3:3:337:ARG:H    | 3:3:337:ARG:CD   | 1.98                     | 0.75              |
| 8:H:121:ARG:HH11 | 8:H:121:ARG:HG3  | 1.52                     | 0.75              |
| 3:C:205:ARG:HA   | 3:C:209:THR:HG22 | 1.66                     | 0.75              |
| 3:C:506:ILE:HG21 | 3:C:535:MET:HE3  | 1.69                     | 0.75              |
| 6:F:163:TYR:HD1  | 7:G:152:ARG:NH1  | 1.83                     | 0.75              |
| 1:1:243:THR:HG22 | 1:1:244:GLU:H    | 1.51                     | 0.75              |
| 4:4:283:MET:O    | 4:4:287:VAL:HG23 | 1.87                     | 0.75              |
| 5:5:174:LEU:HD21 | 5:5:180:GLY:HA2  | 1.67                     | 0.75              |
| 3:3:561:PRO:CB   | 3:3:576:ALA:HA   | 2.12                     | 0.75              |
| 3:C:160:THR:OG1  | 8:H:73:SER:HB3   | 1.87                     | 0.75              |
| 4:4:85:MET:HE3   | 4:4:409:ARG:HG3  | 1.69                     | 0.74              |
| 5:E:103:THR:HG22 | 5:E:126:PHE:HB3  | 1.68                     | 0.74              |
| 7:G:44:THR:HA    | 7:G:138:VAL:HG13 | 1.67                     | 0.74              |
| 4:D:85:MET:HE3   | 4:D:409:ARG:HG3  | 1.70                     | 0.74              |
| 4:D:285:GLU:O    | 4:D:289:ILE:HG12 | 1.87                     | 0.74              |
| 1:1:360:ARG:O    | 1:1:364:ALA:HB3  | 1.88                     | 0.74              |
| 1:1:437:TRP:HB3  | 2:2:92:GLY:CA    | 2.05                     | 0.74              |
| 4:4:390:VAL:HB   | 4:4:391:PRO:HD3  | 1.69                     | 0.74              |
| 3:3:615:VAL:HG22 | 3:3:621:VAL:HG12 | 1.70                     | 0.74              |
| 5:5:5:ARG:HH11   | 5:5:5:ARG:HG3    | 1.51                     | 0.74              |
| 3:C:186:ARG:HD3  | 3:C:229:ILE:HG22 | 1.69                     | 0.74              |
| 5:E:37:GLU:O     | 5:E:41:TYR:HD1   | 1.70                     | 0.74              |
| 3:3:186:ARG:HD3  | 3:3:229:ILE:HG22 | 1.69                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:368:HIS:HB3  | 3:C:556:ALA:HB3  | 1.70                     | 0.74              |
| 3:C:494:LYS:O    | 3:C:498:GLU:HG2  | 1.87                     | 0.74              |
| 6:F:81:ALA:HA    | 6:F:108:MET:HB3  | 1.69                     | 0.74              |
| 6:F:99:MET:HG2   | 6:F:100:PRO:HD2  | 1.70                     | 0.74              |
| 4:4:250:LYS:HE2  | 4:4:262:PHE:HB3  | 1.69                     | 0.74              |
| 6:6:99:MET:HG2   | 6:6:100:PRO:HD2  | 1.69                     | 0.74              |
| 3:C:501:LYS:HD2  | 3:C:501:LYS:N    | 2.03                     | 0.74              |
| 4:D:314:ARG:HH11 | 4:D:314:ARG:HG2  | 1.53                     | 0.74              |
| 6:6:81:ALA:HA    | 6:6:108:MET:HB3  | 1.69                     | 0.73              |
| 1:A:303:THR:OG1  | 1:A:306:VAL:HG23 | 1.86                     | 0.73              |
| 1:1:270:THR:O    | 1:1:311:MET:HG3  | 1.88                     | 0.73              |
| 3:C:300:TRP:HB3  | 3:C:705:VAL:CG2  | 2.17                     | 0.73              |
| 1:A:341:MET:CE   | 1:A:409:PRO:HB2  | 2.19                     | 0.73              |
| 3:3:31:PRO:HG3   | 3:3:137:TYR:CD1  | 2.24                     | 0.73              |
| 3:3:300:TRP:HB3  | 3:3:705:VAL:HG21 | 1.71                     | 0.73              |
| 6:6:165:GLU:HG2  | 7:9:148:ARG:HH11 | 1.53                     | 0.73              |
| 3:C:43:GLY:HA2   | 11:C:787:FES:S1  | 2.29                     | 0.73              |
| 3:3:690:GLY:HA3  | 3:3:770:ARG:NH2  | 2.02                     | 0.73              |
| 1:1:341:MET:HE1  | 1:1:409:PRO:HB2  | 1.70                     | 0.73              |
| 3:3:55:PRO:HD3   | 3:3:74:GLN:H     | 1.53                     | 0.73              |
| 3:3:386:SER:HB2  | 3:3:675:ARG:NH1  | 2.04                     | 0.73              |
| 4:4:371:ARG:NH2  | 4:4:376:VAL:HG21 | 2.02                     | 0.73              |
| 5:5:103:THR:HG22 | 5:5:126:PHE:HB3  | 1.71                     | 0.73              |
| 3:C:591:HIS:ND1  | 3:C:592:PRO:HD2  | 2.03                     | 0.73              |
| 3:3:494:LYS:O    | 3:3:498:GLU:HG2  | 1.88                     | 0.73              |
| 3:C:615:VAL:HG22 | 3:C:621:VAL:HG12 | 1.70                     | 0.73              |
| 3:3:438:LYS:O    | 3:3:441:MET:HG3  | 1.88                     | 0.72              |
| 5:5:106:ASP:HB2  | 5:5:107:LEU:HD12 | 1.71                     | 0.72              |
| 3:3:101:ARG:HB3  | 3:3:101:ARG:NH1  | 2.03                     | 0.72              |
| 3:C:279:ALA:CB   | 3:C:290:ILE:HG12 | 2.19                     | 0.72              |
| 3:3:398:VAL:HB   | 3:3:450:LEU:HD22 | 1.71                     | 0.72              |
| 3:3:501:LYS:HD2  | 3:3:501:LYS:N    | 2.02                     | 0.72              |
| 2:2:24:ARG:O     | 2:2:27:ILE:HG13  | 1.89                     | 0.72              |
| 3:C:739:PRO:HG2  | 3:C:771:VAL:HG12 | 1.70                     | 0.72              |
| 3:3:538:ALA:HB3  | 3:3:541:ALA:HB2  | 1.72                     | 0.72              |
| 4:4:105:LEU:HD13 | 4:4:309:ILE:HD13 | 1.72                     | 0.72              |
| 7:9:73:ALA:HB2   | 7:9:89:LYS:HB2   | 1.71                     | 0.72              |
| 3:C:506:ILE:CG2  | 3:C:535:MET:HE3  | 2.19                     | 0.72              |
| 4:D:371:ARG:HG3  | 5:E:51:ASP:OD1   | 1.89                     | 0.72              |
| 2:2:109:GLY:HA2  | 8:7:91:ILE:HD13  | 1.72                     | 0.72              |
| 1:A:16:THR:HG21  | 1:A:229:PRO:CB   | 2.16                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:116:PRO:O    | 3:3:117:LEU:HB2  | 1.88                     | 0.72              |
| 1:A:288:GLN:HB3  | 1:A:333:GLU:HG2  | 1.72                     | 0.72              |
| 3:C:738:THR:CG2  | 3:C:739:PRO:HD2  | 2.15                     | 0.72              |
| 4:D:261:THR:H    | 4:D:292:GLN:HE22 | 1.37                     | 0.72              |
| 1:1:16:THR:HG21  | 1:1:229:PRO:CB   | 2.18                     | 0.72              |
| 3:3:217:GLY:O    | 3:3:218:LEU:HB2  | 1.90                     | 0.72              |
| 4:4:314:ARG:HG2  | 4:4:314:ARG:HH11 | 1.53                     | 0.72              |
| 2:B:24:ARG:O     | 2:B:27:ILE:HG13  | 1.90                     | 0.72              |
| 3:C:232:VAL:HB   | 9:C:784:SF4:S2   | 2.30                     | 0.72              |
| 4:D:105:LEU:HD13 | 4:D:309:ILE:HD13 | 1.71                     | 0.72              |
| 5:5:3:LEU:HB2    | 5:5:86:SER:HB2   | 1.71                     | 0.71              |
| 4:4:47:LEU:HD13  | 4:4:52:VAL:HA    | 1.72                     | 0.71              |
| 1:A:53:VAL:HG23  | 1:A:231:MET:HE2  | 1.72                     | 0.71              |
| 3:C:238:LEU:HD12 | 3:C:238:LEU:O    | 1.91                     | 0.71              |
| 4:D:236:GLY:C    | 4:D:238:SER:H    | 1.99                     | 0.71              |
| 4:4:261:THR:H    | 4:4:292:GLN:HE22 | 1.39                     | 0.71              |
| 6:6:148:ILE:HG21 | 7:9:27:PRO:HG3   | 1.70                     | 0.71              |
| 6:6:151:VAL:O    | 6:6:155:GLN:HB2  | 1.91                     | 0.71              |
| 3:C:690:GLY:HA3  | 3:C:770:ARG:NH2  | 2.05                     | 0.71              |
| 5:E:50:ALA:HB3   | 5:E:73:GLU:HB3   | 1.71                     | 0.71              |
| 4:D:390:VAL:HB   | 4:D:391:PRO:HD3  | 1.71                     | 0.71              |
| 4:4:371:ARG:HG3  | 5:5:51:ASP:OD1   | 1.91                     | 0.71              |
| 3:3:205:ARG:HA   | 3:3:209:THR:HG22 | 1.71                     | 0.71              |
| 3:3:300:TRP:HB3  | 3:3:705:VAL:CG2  | 2.20                     | 0.71              |
| 4:D:235:THR:HG21 | 4:D:352:GLU:HB2  | 1.71                     | 0.71              |
| 3:C:217:GLY:O    | 3:C:218:LEU:HB2  | 1.90                     | 0.71              |
| 5:E:3:LEU:HB2    | 5:E:86:SER:HB2   | 1.73                     | 0.71              |
| 4:4:168:PHE:HE1  | 6:6:141:PRO:HG3  | 1.54                     | 0.71              |
| 1:1:267:PRO:O    | 1:1:270:THR:HG23 | 1.91                     | 0.70              |
| 3:3:367:PRO:HB2  | 3:3:554:LYS:HB2  | 1.73                     | 0.70              |
| 5:5:80:TRP:HA    | 5:5:80:TRP:CE3   | 2.25                     | 0.70              |
| 1:A:243:THR:HG22 | 1:A:244:GLU:H    | 1.54                     | 0.70              |
| 3:C:367:PRO:HB2  | 3:C:554:LYS:HB2  | 1.72                     | 0.70              |
| 4:D:371:ARG:HH22 | 4:D:376:VAL:HG21 | 1.56                     | 0.70              |
| 1:1:222:GLU:HG3  | 1:1:251:LEU:HD22 | 1.72                     | 0.70              |
| 3:3:185:LYS:HG2  | 3:3:188:VAL:HG22 | 1.73                     | 0.70              |
| 4:4:285:GLU:O    | 4:4:289:ILE:HG12 | 1.91                     | 0.70              |
| 4:4:367:ARG:HH11 | 4:4:367:ARG:CG   | 1.99                     | 0.70              |
| 1:A:203:PRO:HB2  | 1:A:204:PRO:HD3  | 1.72                     | 0.70              |
| 1:A:267:PRO:O    | 1:A:270:THR:HG23 | 1.91                     | 0.70              |
| 4:4:263:ASP:HB2  | 4:4:285:GLU:CD   | 2.17                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:259:LYS:HA   | 1:A:284:LEU:HD21 | 1.72                     | 0.70              |
| 1:1:370:LEU:O    | 1:1:374:ILE:HG22 | 1.92                     | 0.70              |
| 7:9:44:THR:HA    | 7:9:138:VAL:HG13 | 1.73                     | 0.70              |
| 1:A:149:ILE:HD13 | 1:A:171:LEU:HB3  | 1.74                     | 0.70              |
| 3:C:185:LYS:HG2  | 3:C:188:VAL:HG22 | 1.72                     | 0.70              |
| 3:C:586:HIS:NE2  | 3:C:640:VAL:HG21 | 2.05                     | 0.70              |
| 3:C:701:ALA:HB2  | 3:C:763:LEU:HB2  | 1.74                     | 0.70              |
| 4:D:168:PHE:HE1  | 6:F:141:PRO:HG3  | 1.57                     | 0.70              |
| 5:5:186:GLY:HA2  | 5:5:190:LYS:HD3  | 1.74                     | 0.70              |
| 6:F:151:VAL:O    | 6:F:155:GLN:HB2  | 1.91                     | 0.70              |
| 2:2:136:VAL:HG21 | 2:2:163:LEU:HD13 | 1.72                     | 0.70              |
| 1:1:149:ILE:HD13 | 1:1:171:LEU:HB3  | 1.74                     | 0.70              |
| 4:4:235:THR:HG21 | 4:4:352:GLU:HB2  | 1.73                     | 0.70              |
| 3:3:739:PRO:HG2  | 3:3:771:VAL:HG12 | 1.72                     | 0.70              |
| 3:C:120:PRO:HG2  | 8:H:42:TYR:OH    | 1.92                     | 0.70              |
| 4:D:116:ILE:O    | 4:D:120:LEU:HB2  | 1.92                     | 0.70              |
| 3:C:306:LEU:HD11 | 3:C:308:THR:O    | 1.92                     | 0.69              |
| 4:D:218:ALA:HB1  | 4:D:272:VAL:HG22 | 1.73                     | 0.69              |
| 1:1:259:LYS:HA   | 1:1:284:LEU:HD21 | 1.72                     | 0.69              |
| 3:3:101:ARG:NH1  | 3:3:140:TYR:CD1  | 2.59                     | 0.69              |
| 3:3:591:HIS:ND1  | 3:3:592:PRO:HD2  | 2.07                     | 0.69              |
| 4:4:371:ARG:HH22 | 4:4:376:VAL:HG21 | 1.57                     | 0.69              |
| 3:C:101:ARG:HB3  | 3:C:101:ARG:NH1  | 2.07                     | 0.69              |
| 3:C:438:LYS:O    | 3:C:441:MET:HG3  | 1.92                     | 0.69              |
| 1:1:303:THR:OG1  | 1:1:306:VAL:HG23 | 1.91                     | 0.69              |
| 1:A:222:GLU:HG3  | 1:A:251:LEU:HD22 | 1.74                     | 0.69              |
| 7:G:40:ARG:HB2   | 7:G:121:MET:CE   | 2.17                     | 0.69              |
| 1:1:203:PRO:HB2  | 1:1:204:PRO:HD3  | 1.75                     | 0.69              |
| 3:3:309:PRO:HG2  | 3:3:320:ALA:O    | 1.92                     | 0.69              |
| 5:5:5:ARG:HG3    | 5:5:5:ARG:NH1    | 2.07                     | 0.69              |
| 2:B:61:MET:HE2   | 3:C:214:MET:HG2  | 1.74                     | 0.69              |
| 3:C:294:GLY:HA3  | 9:C:786:SF4:S4   | 2.33                     | 0.69              |
| 4:D:44:MET:HE2   | 4:D:44:MET:HA    | 1.74                     | 0.69              |
| 5:E:5:ARG:HG3    | 5:E:5:ARG:NH1    | 2.07                     | 0.69              |
| 5:E:80:TRP:HA    | 5:E:80:TRP:CE3   | 2.27                     | 0.69              |
| 1:1:312:SER:N    | 1:1:316:LEU:HD12 | 2.07                     | 0.69              |
| 5:5:33:ARG:O     | 5:5:37:GLU:HB2   | 1.92                     | 0.69              |
| 1:1:402:LEU:HD13 | 9:1:439:SF4:S1   | 2.33                     | 0.69              |
| 4:4:40:VAL:HG13  | 4:4:404:MET:HG3  | 1.73                     | 0.69              |
| 1:A:297:THR:HG22 | 1:A:322:MET:CG   | 2.20                     | 0.69              |
| 3:C:309:PRO:HG2  | 3:C:320:ALA:O    | 1.92                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:236:GLY:C    | 4:4:238:SER:H    | 2.00                     | 0.68              |
| 3:C:398:VAL:HB   | 3:C:450:LEU:HD22 | 1.74                     | 0.68              |
| 5:E:33:ARG:O     | 5:E:37:GLU:HB2   | 1.92                     | 0.68              |
| 1:1:341:MET:CE   | 1:1:409:PRO:HB2  | 2.23                     | 0.68              |
| 4:D:47:LEU:HD13  | 4:D:52:VAL:HA    | 1.74                     | 0.68              |
| 2:2:77:LYS:H     | 2:2:116:LEU:HA   | 1.58                     | 0.68              |
| 3:3:459:MET:HG2  | 3:3:465:HIS:HB2  | 1.75                     | 0.68              |
| 4:4:96:ALA:HB2   | 4:4:346:THR:HG21 | 1.76                     | 0.68              |
| 4:4:224:ILE:HD11 | 4:4:275:ARG:NH1  | 2.09                     | 0.68              |
| 5:E:2:ARG:HG3    | 5:E:84:ASP:OD2   | 1.93                     | 0.68              |
| 1:1:29:LEU:HD22  | 1:1:33:LEU:HG    | 1.75                     | 0.68              |
| 3:3:693:TYR:HB3  | 3:3:759:TYR:HD2  | 1.57                     | 0.68              |
| 4:4:218:ALA:HB1  | 4:4:272:VAL:HG22 | 1.74                     | 0.68              |
| 6:6:163:TYR:HD1  | 7:9:152:ARG:NH1  | 1.91                     | 0.68              |
| 3:C:250:GLU:HG3  | 5:E:169:GLU:CD   | 2.18                     | 0.68              |
| 3:3:374:ARG:HH21 | 3:3:684:ARG:HG3  | 1.57                     | 0.68              |
| 1:A:289:ALA:HB3  | 1:A:337:MET:HE3  | 1.75                     | 0.68              |
| 3:C:285:VAL:HG22 | 3:C:286:ASN:H    | 1.57                     | 0.68              |
| 4:D:283:MET:O    | 4:D:287:VAL:HG23 | 1.93                     | 0.68              |
| 5:5:2:ARG:HG3    | 5:5:84:ASP:OD2   | 1.94                     | 0.68              |
| 6:F:153:GLN:HG3  | 7:G:124:TYR:OH   | 1.94                     | 0.68              |
| 7:G:73:ALA:HB2   | 7:G:89:LYS:HB2   | 1.75                     | 0.68              |
| 1:A:29:LEU:HD22  | 1:A:33:LEU:HG    | 1.74                     | 0.68              |
| 1:1:312:SER:H    | 1:1:316:LEU:HD12 | 1.59                     | 0.68              |
| 3:3:279:ALA:CB   | 3:3:290:ILE:HG12 | 2.24                     | 0.68              |
| 3:3:506:ILE:HG21 | 3:3:535:MET:HE3  | 1.74                     | 0.68              |
| 2:B:86:LEU:O     | 2:B:90:LEU:HD12  | 1.94                     | 0.68              |
| 3:C:374:ARG:HH21 | 3:C:684:ARG:HG3  | 1.60                     | 0.68              |
| 5:5:163:ARG:HD2  | 7:9:69:TYR:CD1   | 2.29                     | 0.67              |
| 3:C:175:ILE:HB   | 3:C:238:LEU:HD22 | 1.76                     | 0.67              |
| 3:C:216:PHE:CZ   | 8:H:128:PHE:HD2  | 2.12                     | 0.67              |
| 3:3:175:ILE:HB   | 3:3:238:LEU:HD22 | 1.75                     | 0.67              |
| 4:4:311:PRO:HD3  | 4:4:330:HIS:NE2  | 2.09                     | 0.67              |
| 4:D:93:HIS:CE1   | 4:D:353:LEU:HD11 | 2.30                     | 0.67              |
| 1:1:253:GLN:HE21 | 1:1:253:GLN:H    | 1.42                     | 0.67              |
| 4:4:98:ALA:O     | 4:4:102:GLU:HG3  | 1.94                     | 0.67              |
| 8:7:121:ARG:HH11 | 8:7:121:ARG:HG3  | 1.58                     | 0.67              |
| 3:C:693:TYR:HB3  | 3:C:759:TYR:HD2  | 1.58                     | 0.67              |
| 3:3:542:ARG:HB2  | 3:3:542:ARG:HH11 | 1.58                     | 0.67              |
| 1:A:370:LEU:O    | 1:A:374:ILE:HG22 | 1.94                     | 0.67              |
| 3:C:205:ARG:CA   | 3:C:209:THR:HG22 | 2.24                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:40:VAL:O     | 4:4:40:VAL:HG22  | 1.94                     | 0.67              |
| 2:B:40:TRP:CD1   | 2:B:74:PRO:HA    | 2.30                     | 0.67              |
| 4:D:96:ALA:HB2   | 4:D:346:THR:HG21 | 1.76                     | 0.67              |
| 3:3:567:TYR:HA   | 3:3:584:VAL:HG23 | 1.75                     | 0.67              |
| 3:C:101:ARG:NH1  | 3:C:140:TYR:CD1  | 2.63                     | 0.67              |
| 3:C:459:MET:HG2  | 3:C:465:HIS:HB2  | 1.76                     | 0.67              |
| 4:D:40:VAL:O     | 4:D:40:VAL:HG22  | 1.94                     | 0.67              |
| 4:D:263:ASP:O    | 4:D:265:PRO:HD3  | 1.94                     | 0.67              |
| 1:1:288:GLN:HB3  | 1:1:333:GLU:HG2  | 1.77                     | 0.67              |
| 1:1:272:PHE:HZ   | 1:1:316:LEU:HD21 | 1.60                     | 0.66              |
| 3:3:715:GLU:HB3  | 3:3:746:ARG:CZ   | 2.25                     | 0.66              |
| 1:A:272:PHE:HZ   | 1:A:316:LEU:HD21 | 1.61                     | 0.66              |
| 4:D:215:TYR:CE2  | 4:D:219:ARG:HG3  | 2.30                     | 0.66              |
| 3:3:586:HIS:NE2  | 3:3:640:VAL:HG21 | 2.10                     | 0.66              |
| 4:D:224:ILE:HD11 | 4:D:275:ARG:NH1  | 2.10                     | 0.66              |
| 4:4:254:TYR:CE2  | 4:4:346:THR:HA   | 2.31                     | 0.66              |
| 3:C:367:PRO:CB   | 3:C:554:LYS:HB2  | 2.25                     | 0.66              |
| 3:C:567:TYR:HA   | 3:C:584:VAL:HG23 | 1.77                     | 0.66              |
| 6:F:16:ARG:HA    | 6:F:21:PHE:CD2   | 2.30                     | 0.66              |
| 1:1:93:ALA:HB1   | 1:1:107:LEU:HD11 | 1.75                     | 0.66              |
| 3:3:117:LEU:CD2  | 4:4:321:MET:HA   | 2.26                     | 0.66              |
| 4:4:99:LEU:HB3   | 4:4:344:VAL:HG21 | 1.77                     | 0.66              |
| 3:C:716:LEU:HD21 | 3:C:758:LEU:HB3  | 1.77                     | 0.66              |
| 4:D:274:ASP:O    | 4:D:278:VAL:HG23 | 1.95                     | 0.66              |
| 3:3:132:ASP:O    | 3:3:136:GLU:HG3  | 1.95                     | 0.66              |
| 3:3:402:PRO:CG   | 3:3:535:MET:HE1  | 2.26                     | 0.66              |
| 3:3:440:ARG:CG   | 3:3:440:ARG:NH1  | 2.46                     | 0.66              |
| 6:6:113:SER:HB3  | 7:9:96:LEU:HD13  | 1.75                     | 0.66              |
| 1:A:253:GLN:HE21 | 1:A:253:GLN:H    | 1.42                     | 0.66              |
| 4:D:99:LEU:HB3   | 4:D:344:VAL:HG21 | 1.78                     | 0.66              |
| 4:D:254:TYR:CE2  | 4:D:346:THR:HA   | 2.30                     | 0.66              |
| 5:E:126:PHE:H    | 5:E:132:LEU:HD11 | 1.61                     | 0.66              |
| 6:F:163:TYR:HD1  | 7:G:152:ARG:HH11 | 1.43                     | 0.66              |
| 1:A:16:THR:CG2   | 1:A:229:PRO:HB3  | 2.23                     | 0.66              |
| 1:A:402:LEU:HD13 | 9:A:439:SF4:S1   | 2.35                     | 0.66              |
| 3:C:224:GLY:O    | 3:C:227:THR:HB   | 1.96                     | 0.66              |
| 5:E:66:GLU:CG    | 5:E:95:PRO:HA    | 2.08                     | 0.66              |
| 2:2:86:LEU:O     | 2:2:90:LEU:HD12  | 1.96                     | 0.66              |
| 4:4:44:MET:HE2   | 4:4:44:MET:HA    | 1.78                     | 0.66              |
| 6:6:119:ASN:HA   | 6:6:125:GLN:HE22 | 1.61                     | 0.66              |
| 3:C:117:LEU:HD23 | 4:D:321:MET:HA   | 1.78                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:93:ALA:HB1   | 1:A:107:LEU:HD11 | 1.78                     | 0.66              |
| 3:C:715:GLU:HB3  | 3:C:746:ARG:CZ   | 2.26                     | 0.66              |
| 4:D:263:ASP:HB2  | 4:D:285:GLU:CD   | 2.21                     | 0.66              |
| 1:A:92:ASN:ND2   | 10:A:440:FMN:O3' | 2.29                     | 0.66              |
| 5:E:10:ALA:HB1   | 5:E:15:TYR:HB2   | 1.78                     | 0.66              |
| 3:3:583:VAL:CG2  | 3:3:598:ALA:HA   | 2.27                     | 0.65              |
| 1:A:274:GLU:HG3  | 1:A:278:GLU:HG3  | 1.77                     | 0.65              |
| 4:D:225:PRO:HG2  | 4:D:228:VAL:HB   | 1.78                     | 0.65              |
| 4:4:116:ILE:O    | 4:4:120:LEU:HB2  | 1.96                     | 0.65              |
| 4:4:274:ASP:O    | 4:4:278:VAL:HG23 | 1.96                     | 0.65              |
| 4:4:404:MET:HA   | 4:4:407:VAL:CG1  | 2.27                     | 0.65              |
| 3:C:546:ALA:O    | 3:C:547:MET:HE2  | 1.97                     | 0.65              |
| 3:C:583:VAL:CG2  | 3:C:598:ALA:HA   | 2.27                     | 0.65              |
| 3:3:367:PRO:CB   | 3:3:554:LYS:HB2  | 2.26                     | 0.65              |
| 5:E:39:ALA:HA    | 5:E:107:LEU:HD23 | 1.79                     | 0.65              |
| 1:1:437:TRP:CZ3  | 2:2:96:LEU:HB2   | 2.31                     | 0.65              |
| 3:3:117:LEU:HD23 | 4:4:321:MET:HA   | 1.77                     | 0.65              |
| 4:4:341:GLU:HG2  | 4:4:358:VAL:HG22 | 1.77                     | 0.65              |
| 4:D:404:MET:HA   | 4:D:407:VAL:CG1  | 2.27                     | 0.65              |
| 1:1:53:VAL:HG23  | 1:1:231:MET:HE2  | 1.77                     | 0.65              |
| 1:1:289:ALA:HB3  | 1:1:337:MET:HE3  | 1.79                     | 0.65              |
| 3:3:689:LYS:HE3  | 3:3:771:VAL:CG1  | 2.27                     | 0.65              |
| 3:C:738:THR:HG22 | 3:C:739:PRO:CD   | 2.21                     | 0.65              |
| 7:G:175:ALA:HB1  | 7:G:176:PRO:HD2  | 1.79                     | 0.65              |
| 3:3:506:ILE:CG2  | 3:3:535:MET:HE3  | 2.27                     | 0.65              |
| 7:9:40:ARG:HB2   | 7:9:121:MET:CE   | 2.18                     | 0.65              |
| 2:B:109:GLY:HA2  | 8:H:91:ILE:HD13  | 1.78                     | 0.65              |
| 5:E:20:ASN:HD21  | 5:E:24:ASN:HB2   | 1.62                     | 0.65              |
| 1:A:312:SER:N    | 1:A:316:LEU:HD12 | 2.10                     | 0.65              |
| 3:C:360:LEU:O    | 3:C:364:LEU:HB3  | 1.96                     | 0.65              |
| 1:1:297:THR:HG22 | 1:1:322:MET:CG   | 2.26                     | 0.64              |
| 5:5:50:ALA:HB3   | 5:5:73:GLU:HB3   | 1.77                     | 0.64              |
| 5:5:144:HIS:HB2  | 5:5:147:ARG:HD3  | 1.79                     | 0.64              |
| 1:1:274:GLU:HG3  | 1:1:278:GLU:HG3  | 1.80                     | 0.64              |
| 3:3:739:PRO:HG2  | 3:3:771:VAL:HG11 | 1.79                     | 0.64              |
| 6:6:16:ARG:HA    | 6:6:21:PHE:CD2   | 2.32                     | 0.64              |
| 3:C:600:VAL:HG12 | 3:C:602:LEU:HD11 | 1.79                     | 0.64              |
| 3:C:750:ARG:HB2  | 3:C:753:VAL:HG23 | 1.79                     | 0.64              |
| 1:1:99:GLY:HA3   | 1:1:329:ILE:HD11 | 1.79                     | 0.64              |
| 3:3:205:ARG:CA   | 3:3:209:THR:HG22 | 2.28                     | 0.64              |
| 3:3:285:VAL:HG22 | 3:3:286:ASN:H    | 1.61                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:72:HIS:O     | 4:D:73:ARG:HD2   | 1.98                     | 0.64              |
| 4:4:65:GLY:O     | 4:4:69:THR:HG22  | 1.98                     | 0.64              |
| 3:C:285:VAL:HG22 | 3:C:286:ASN:N    | 2.13                     | 0.64              |
| 7:G:101:CYS:HB2  | 7:G:103:LEU:H    | 1.62                     | 0.64              |
| 7:9:56:CYS:SG    | 7:9:58:LEU:HB2   | 2.37                     | 0.64              |
| 2:B:77:LYS:H     | 2:B:116:LEU:HA   | 1.62                     | 0.64              |
| 3:C:692:PHE:HE1  | 3:C:773:GLY:O    | 1.80                     | 0.64              |
| 1:A:312:SER:H    | 1:A:316:LEU:HD12 | 1.62                     | 0.64              |
| 5:5:120:ASP:CG   | 5:5:134:LYS:HG3  | 2.22                     | 0.64              |
| 7:9:101:CYS:HB2  | 7:9:103:LEU:H    | 1.63                     | 0.64              |
| 3:C:31:PRO:HG3   | 3:C:137:TYR:CD1  | 2.32                     | 0.64              |
| 3:3:11:VAL:HG11  | 3:3:25:HIS:HD2   | 1.60                     | 0.64              |
| 3:3:489:MET:HE2  | 3:3:492:LYS:HD2  | 1.79                     | 0.64              |
| 6:6:117:MET:CE   | 7:9:99:ILE:HG12  | 2.17                     | 0.64              |
| 4:D:65:GLY:O     | 4:D:69:THR:HG22  | 1.98                     | 0.64              |
| 2:2:40:TRP:CH2   | 2:2:42:ARG:HG2   | 2.33                     | 0.64              |
| 1:A:185:GLU:HB2  | 1:A:218:ILE:HD12 | 1.80                     | 0.64              |
| 6:F:119:ASN:HA   | 6:F:125:GLN:HE22 | 1.63                     | 0.64              |
| 3:C:739:PRO:HG2  | 3:C:771:VAL:HG11 | 1.80                     | 0.64              |
| 4:4:93:HIS:CE1   | 4:4:353:LEU:HD11 | 2.33                     | 0.63              |
| 7:G:67:ALA:HB2   | 7:G:97:ARG:HB3   | 1.80                     | 0.63              |
| 5:E:186:GLY:HA2  | 5:E:190:LYS:HD3  | 1.79                     | 0.63              |
| 1:1:116:GLU:HA   | 1:1:119:ILE:HD12 | 1.80                     | 0.63              |
| 2:B:40:TRP:CH2   | 2:B:42:ARG:HG2   | 2.33                     | 0.63              |
| 6:F:107:SER:O    | 6:F:137:VAL:HG12 | 1.99                     | 0.63              |
| 3:3:306:LEU:HD11 | 3:3:308:THR:O    | 1.97                     | 0.63              |
| 7:9:46:HIS:HB3   | 7:9:47:PRO:HD2   | 1.79                     | 0.63              |
| 1:1:50:PRO:O     | 1:1:53:VAL:HG12  | 1.99                     | 0.63              |
| 3:3:205:ARG:C    | 3:3:209:THR:HG22 | 2.23                     | 0.63              |
| 1:A:139:ARG:HG2  | 2:B:139:GLU:HA   | 1.81                     | 0.63              |
| 3:C:300:TRP:CB   | 3:C:705:VAL:HG21 | 2.28                     | 0.63              |
| 6:F:141:PRO:HB3  | 9:F:182:SF4:S1   | 2.38                     | 0.63              |
| 3:3:216:PHE:CZ   | 8:7:128:PHE:HD2  | 2.15                     | 0.63              |
| 3:3:546:ALA:O    | 3:3:547:MET:HE2  | 1.98                     | 0.63              |
| 4:4:225:PRO:HG2  | 4:4:228:VAL:HB   | 1.81                     | 0.63              |
| 1:A:99:GLY:HA3   | 1:A:329:ILE:HD11 | 1.81                     | 0.63              |
| 4:D:130:LEU:HD11 | 4:D:152:GLU:HB3  | 1.79                     | 0.63              |
| 3:3:304:ASN:O    | 3:3:589:HIS:CD2  | 2.52                     | 0.63              |
| 4:4:263:ASP:O    | 4:4:265:PRO:HD3  | 1.98                     | 0.63              |
| 3:C:115:HIS:HB3  | 4:D:321:MET:HE3  | 1.81                     | 0.63              |
| 3:C:205:ARG:C    | 3:C:209:THR:HG22 | 2.24                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:3:394:ASP:OD2  | 3:3:501:LYS:HB2   | 1.98                     | 0.62              |
| 7:G:56:CYS:SG    | 7:G:58:LEU:HB2    | 2.39                     | 0.62              |
| 3:3:701:ALA:HB2  | 3:3:763:LEU:HB2   | 1.80                     | 0.62              |
| 3:C:216:PHE:HZ   | 8:H:128:PHE:HD2   | 1.47                     | 0.62              |
| 3:C:368:HIS:CE1  | 3:C:563:ALA:HB2   | 2.34                     | 0.62              |
| 6:6:153:GLN:HG3  | 7:9:124:TYR:OH    | 1.99                     | 0.62              |
| 3:C:117:LEU:CD2  | 4:D:321:MET:HA    | 2.29                     | 0.62              |
| 4:4:70:MET:HG2   | 4:4:78:ASN:OD1    | 2.00                     | 0.62              |
| 4:4:72:HIS:O     | 4:4:73:ARG:HD2    | 2.00                     | 0.62              |
| 3:C:132:ASP:O    | 3:C:136:GLU:HG3   | 1.99                     | 0.62              |
| 4:D:98:ALA:O     | 4:D:102:GLU:HG3   | 1.98                     | 0.62              |
| 1:1:401:PRO:HB2  | 10:1:440:FMN:HM82 | 1.81                     | 0.62              |
| 4:4:88:LEU:HD21  | 6:6:48:ILE:HD13   | 1.82                     | 0.62              |
| 5:5:10:ALA:HB1   | 5:5:15:TYR:HB2    | 1.81                     | 0.62              |
| 6:6:83:ARG:HH11  | 6:6:83:ARG:HG3    | 1.64                     | 0.62              |
| 1:A:50:PRO:O     | 1:A:53:VAL:HG12   | 1.99                     | 0.62              |
| 4:D:70:MET:HG2   | 4:D:78:ASN:OD1    | 1.99                     | 0.62              |
| 4:D:367:ARG:HH11 | 4:D:367:ARG:CG    | 2.04                     | 0.62              |
| 5:E:167:PRO:C    | 5:E:171:ARG:HH12  | 2.07                     | 0.62              |
| 3:3:224:GLY:O    | 3:3:227:THR:HB    | 1.99                     | 0.62              |
| 1:A:98:PRO:HA    | 2:B:124:CYS:SG    | 2.40                     | 0.62              |
| 5:E:52:ILE:HG23  | 5:E:114:LEU:HB3   | 1.81                     | 0.62              |
| 5:5:20:ASN:HD21  | 5:5:24:ASN:HB2    | 1.65                     | 0.62              |
| 1:1:92:ASN:ND2   | 10:1:440:FMN:O3'  | 2.33                     | 0.62              |
| 5:5:52:ILE:HG23  | 5:5:114:LEU:HB3   | 1.82                     | 0.62              |
| 3:C:489:MET:HE2  | 3:C:492:LYS:HD2   | 1.81                     | 0.62              |
| 4:4:70:MET:HE3   | 4:4:81:TYR:CB     | 2.29                     | 0.62              |
| 1:A:17:LEU:HD12  | 1:A:251:LEU:HD11  | 1.81                     | 0.62              |
| 3:C:290:ILE:HG21 | 3:C:295:ARG:HB2   | 1.81                     | 0.62              |
| 4:D:314:ARG:HG2  | 4:D:314:ARG:NH1   | 2.13                     | 0.62              |
| 4:4:215:TYR:CE2  | 4:4:219:ARG:HG3   | 2.35                     | 0.62              |
| 4:4:314:ARG:HG2  | 4:4:314:ARG:NH1   | 2.13                     | 0.62              |
| 5:5:107:LEU:HD12 | 5:5:107:LEU:N     | 2.14                     | 0.62              |
| 1:A:116:GLU:HA   | 1:A:119:ILE:HD12  | 1.81                     | 0.62              |
| 5:5:72:TYR:HB2   | 5:5:90:VAL:HG13   | 1.82                     | 0.61              |
| 6:6:140:CYS:SG   | 7:9:99:ILE:HG13   | 2.39                     | 0.61              |
| 1:1:186:THR:HG23 | 1:1:200:ARG:N     | 2.09                     | 0.61              |
| 3:3:360:LEU:O    | 3:3:364:LEU:HB3   | 2.00                     | 0.61              |
| 5:5:39:ALA:HA    | 5:5:107:LEU:HD23  | 1.82                     | 0.61              |
| 6:6:165:GLU:HG2  | 7:9:148:ARG:NH1   | 2.15                     | 0.61              |
| 3:C:11:VAL:HG11  | 3:C:25:HIS:HD2    | 1.64                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:341:GLU:HG2  | 4:D:358:VAL:HG22 | 1.82                     | 0.61              |
| 3:3:285:VAL:HG22 | 3:3:286:ASN:N    | 2.15                     | 0.61              |
| 5:E:144:HIS:HB2  | 5:E:147:ARG:HD3  | 1.80                     | 0.61              |
| 5:5:174:LEU:CD2  | 5:5:180:GLY:HA2  | 2.30                     | 0.61              |
| 3:C:732:ALA:O    | 3:C:747:VAL:HG12 | 2.00                     | 0.61              |
| 3:3:738:THR:HG22 | 3:3:739:PRO:CD   | 2.22                     | 0.61              |
| 6:6:163:TYR:HB3  | 6:6:168:GLU:O    | 2.01                     | 0.61              |
| 4:4:130:LEU:HD11 | 4:4:152:GLU:HB3  | 1.83                     | 0.61              |
| 5:5:5:ARG:HH11   | 5:5:5:ARG:CG     | 2.12                     | 0.61              |
| 5:E:5:ARG:HH11   | 5:E:5:ARG:CG     | 2.13                     | 0.61              |
| 2:2:40:TRP:CD1   | 2:2:74:PRO:HA    | 2.36                     | 0.61              |
| 4:4:263:ASP:HB2  | 4:4:285:GLU:OE1  | 2.01                     | 0.61              |
| 1:1:401:PRO:HB2  | 10:1:440:FMN:C8M | 2.29                     | 0.61              |
| 3:3:282:VAL:HG22 | 3:3:285:VAL:HG12 | 1.82                     | 0.61              |
| 3:3:512:LEU:HD21 | 3:3:534:ALA:HB1  | 1.83                     | 0.61              |
| 3:C:282:VAL:HG22 | 3:C:285:VAL:HG12 | 1.83                     | 0.61              |
| 3:3:716:LEU:HD21 | 3:3:758:LEU:HB3  | 1.81                     | 0.61              |
| 3:3:750:ARG:HB2  | 3:3:753:VAL:HG23 | 1.82                     | 0.61              |
| 1:A:139:ARG:CG   | 2:B:140:PRO:HD3  | 2.30                     | 0.61              |
| 1:A:437:TRP:CZ3  | 2:B:96:LEU:HB2   | 2.36                     | 0.61              |
| 4:D:76:LEU:HD12  | 4:D:79:ILE:HD12  | 1.81                     | 0.61              |
| 6:6:107:SER:O    | 6:6:137:VAL:HG12 | 2.01                     | 0.61              |
| 8:7:6:GLU:CD     | 8:7:80:LYS:HE3   | 2.26                     | 0.61              |
| 4:D:311:PRO:HD3  | 4:D:330:HIS:NE2  | 2.15                     | 0.61              |
| 5:E:39:ALA:HA    | 5:E:107:LEU:CD2  | 2.30                     | 0.61              |
| 8:H:60:SER:HA    | 8:H:66:PRO:HA    | 1.82                     | 0.61              |
| 3:3:368:HIS:CE1  | 3:3:563:ALA:HB2  | 2.36                     | 0.60              |
| 1:A:184:GLU:OE1  | 1:A:186:THR:HG22 | 2.01                     | 0.60              |
| 7:G:44:THR:OG1   | 7:G:52:LYS:HD2   | 2.00                     | 0.60              |
| 5:5:126:PHE:H    | 5:5:132:LEU:HD11 | 1.65                     | 0.60              |
| 3:3:692:PHE:HE1  | 3:3:773:GLY:O    | 1.82                     | 0.60              |
| 7:9:175:ALA:HB1  | 7:9:176:PRO:HD2  | 1.83                     | 0.60              |
| 1:A:88:TYR:HB2   | 1:A:216:THR:CG2  | 2.31                     | 0.60              |
| 4:D:241:ALA:CB   | 4:D:278:VAL:HG21 | 2.31                     | 0.60              |
| 3:3:732:ALA:O    | 3:3:747:VAL:HG12 | 2.00                     | 0.60              |
| 4:D:393:MET:HA   | 4:D:396:ILE:CG2  | 2.32                     | 0.60              |
| 5:E:72:TYR:HB2   | 5:E:90:VAL:HG13  | 1.84                     | 0.60              |
| 5:E:80:TRP:HA    | 5:E:80:TRP:HE3   | 1.66                     | 0.60              |
| 5:E:107:LEU:HD12 | 5:E:107:LEU:N    | 2.16                     | 0.60              |
| 5:E:134:LYS:HD3  | 5:E:137:THR:OG1  | 2.01                     | 0.60              |
| 1:1:6:LEU:HD21   | 1:1:12:ARG:HG3   | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:92:ASN:HD21  | 10:1:440:FMN:C2  | 2.14                     | 0.60              |
| 3:C:542:ARG:HB2  | 3:C:542:ARG:HH11 | 1.65                     | 0.60              |
| 4:D:40:VAL:CG1   | 4:D:404:MET:HG3  | 2.31                     | 0.60              |
| 5:E:167:PRO:C    | 5:E:171:ARG:NH1  | 2.60                     | 0.60              |
| 5:E:174:LEU:CD2  | 5:E:180:GLY:HA2  | 2.30                     | 0.60              |
| 1:1:29:LEU:O     | 1:1:33:LEU:HG    | 2.01                     | 0.60              |
| 5:5:80:TRP:HA    | 5:5:80:TRP:HE3   | 1.65                     | 0.60              |
| 3:C:242:PHE:HE2  | 7:G:85:GLU:O     | 1.85                     | 0.60              |
| 3:C:583:VAL:HG21 | 3:C:598:ALA:HA   | 1.84                     | 0.60              |
| 4:D:250:LYS:CE   | 4:D:262:PHE:HB3  | 2.32                     | 0.60              |
| 4:4:393:MET:HA   | 4:4:396:ILE:CG2  | 2.32                     | 0.60              |
| 3:C:655:ARG:NH1  | 3:C:659:GLU:HG3  | 2.17                     | 0.60              |
| 6:F:83:ARG:HH11  | 6:F:83:ARG:HG3   | 1.66                     | 0.60              |
| 1:1:110:VAL:N    | 1:1:111:PRO:HD3  | 2.17                     | 0.60              |
| 7:9:45:ARG:NH2   | 7:9:137:LEU:HD23 | 2.17                     | 0.60              |
| 3:C:717:TRP:HB2  | 3:C:759:TYR:HB2  | 1.84                     | 0.60              |
| 6:F:93:ARG:NH1   | 6:F:96:TRP:CE3   | 2.70                     | 0.60              |
| 8:H:6:GLU:CD     | 8:H:80:LYS:HE3   | 2.27                     | 0.60              |
| 1:A:104:ARG:NH2  | 2:B:127:SER:CB   | 2.60                     | 0.59              |
| 1:A:313:TYR:CE1  | 1:A:323:LEU:HD13 | 2.37                     | 0.59              |
| 3:C:394:ASP:OD2  | 3:C:501:LYS:HB2  | 2.02                     | 0.59              |
| 4:D:404:MET:HA   | 4:D:407:VAL:HG12 | 1.84                     | 0.59              |
| 7:G:41:HIS:CD2   | 7:G:115:LEU:CD2  | 2.85                     | 0.59              |
| 7:G:46:HIS:HB3   | 7:G:47:PRO:HD2   | 1.82                     | 0.59              |
| 5:5:39:ALA:HA    | 5:5:107:LEU:CD2  | 2.32                     | 0.59              |
| 6:6:156:LYS:HG2  | 6:6:156:LYS:O    | 2.01                     | 0.59              |
| 3:C:304:ASN:O    | 3:C:589:HIS:CD2  | 2.55                     | 0.59              |
| 3:C:337:ARG:HD2  | 3:C:337:ARG:N    | 2.17                     | 0.59              |
| 7:G:133:LYS:O    | 7:G:137:LEU:HD13 | 2.03                     | 0.59              |
| 3:3:356:LEU:HD13 | 3:3:654:PHE:HD1  | 1.67                     | 0.59              |
| 3:3:399:LEU:N    | 3:3:399:LEU:HD12 | 2.18                     | 0.59              |
| 7:9:43:LEU:O     | 7:9:138:VAL:HG13 | 2.03                     | 0.59              |
| 8:H:82:ILE:HG23  | 8:H:95:ALA:HB3   | 1.84                     | 0.59              |
| 1:1:185:GLU:HB2  | 1:1:218:ILE:HD12 | 1.84                     | 0.59              |
| 1:1:214:LYS:O    | 1:1:216:THR:HG23 | 2.03                     | 0.59              |
| 3:3:693:TYR:HB3  | 3:3:759:TYR:CD2  | 2.37                     | 0.59              |
| 4:4:76:LEU:HD12  | 4:4:79:ILE:HD12  | 1.84                     | 0.59              |
| 5:5:134:LYS:HD3  | 5:5:137:THR:OG1  | 2.03                     | 0.59              |
| 8:7:6:GLU:OE1    | 8:7:80:LYS:HE3   | 2.01                     | 0.59              |
| 1:A:29:LEU:CD1   | 1:A:155:ARG:HG3  | 2.32                     | 0.59              |
| 4:D:70:MET:HE3   | 4:D:81:TYR:CB    | 2.33                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:583:VAL:HG21 | 3:3:598:ALA:HA   | 1.83                     | 0.59              |
| 3:C:385:ALA:HB2  | 3:C:531:LYS:HB2  | 1.84                     | 0.59              |
| 3:C:216:PHE:HZ   | 8:H:128:PHE:CD2  | 2.21                     | 0.59              |
| 3:C:583:VAL:HG21 | 3:C:597:TYR:O    | 2.03                     | 0.59              |
| 1:1:313:TYR:CE1  | 1:1:323:LEU:HD13 | 2.38                     | 0.59              |
| 1:1:344:LEU:O    | 1:1:347:PHE:HB3  | 2.03                     | 0.59              |
| 3:3:300:TRP:CB   | 3:3:705:VAL:HG21 | 2.32                     | 0.59              |
| 4:4:404:MET:HA   | 4:4:407:VAL:HG12 | 1.84                     | 0.59              |
| 5:E:120:ASP:CG   | 5:E:134:LYS:HG3  | 2.27                     | 0.59              |
| 4:4:393:MET:O    | 4:4:396:ILE:HG22 | 2.03                     | 0.58              |
| 3:C:398:VAL:C    | 3:C:399:LEU:HD12 | 2.28                     | 0.58              |
| 3:C:509:ALA:HB1  | 3:C:768:GLY:CA   | 2.32                     | 0.58              |
| 4:D:219:ARG:NH1  | 4:D:273:PHE:CD2  | 2.71                     | 0.58              |
| 7:G:45:ARG:NH2   | 7:G:137:LEU:HD23 | 2.18                     | 0.58              |
| 1:1:184:GLU:OE1  | 1:1:186:THR:HG22 | 2.03                     | 0.58              |
| 3:3:290:ILE:HG21 | 3:3:295:ARG:HB2  | 1.85                     | 0.58              |
| 4:4:40:VAL:HG23  | 6:6:88:MET:HE2   | 1.85                     | 0.58              |
| 7:9:67:ALA:HB2   | 7:9:97:ARG:HB3   | 1.85                     | 0.58              |
| 3:3:655:ARG:NH1  | 3:3:659:GLU:HG3  | 2.18                     | 0.58              |
| 1:A:246:SER:HB3  | 1:A:268:MET:CG   | 2.29                     | 0.58              |
| 7:G:43:LEU:O     | 7:G:138:VAL:HG13 | 2.03                     | 0.58              |
| 3:3:546:ALA:HA   | 3:3:678:PHE:CE2  | 2.39                     | 0.58              |
| 4:4:89:HIS:CE1   | 4:4:92:ALA:HB2   | 2.39                     | 0.58              |
| 4:4:225:PRO:HG3  | 4:4:383:TYR:OH   | 2.04                     | 0.58              |
| 4:4:355:TYR:CE2  | 4:4:370:VAL:HG22 | 2.38                     | 0.58              |
| 5:5:37:GLU:O     | 5:5:41:TYR:CD1   | 2.52                     | 0.58              |
| 1:A:310:PRO:HG2  | 1:A:315:HIS:CD2  | 2.38                     | 0.58              |
| 4:D:64:THR:HG21  | 6:F:118:PHE:CD1  | 2.38                     | 0.58              |
| 1:1:65:ARG:HD2   | 1:1:250:LYS:HD3  | 1.86                     | 0.58              |
| 2:B:175:HIS:CE1  | 2:B:176:VAL:HG22 | 2.39                     | 0.58              |
| 6:F:163:TYR:HB3  | 6:F:168:GLU:O    | 2.04                     | 0.58              |
| 3:3:246:ASN:H    | 3:3:246:ASN:HD22 | 1.52                     | 0.58              |
| 3:3:474:ARG:NH2  | 3:3:516:VAL:CG2  | 2.53                     | 0.58              |
| 7:9:26:TYR:N     | 7:9:27:PRO:HD3   | 2.19                     | 0.58              |
| 1:A:289:ALA:HB3  | 1:A:337:MET:CE   | 2.34                     | 0.58              |
| 3:C:512:LEU:HD21 | 3:C:534:ALA:HB1  | 1.86                     | 0.58              |
| 4:D:280:ILE:HG23 | 4:D:283:MET:HE2  | 1.86                     | 0.58              |
| 5:5:167:PRO:C    | 5:5:171:ARG:HH12 | 2.11                     | 0.58              |
| 6:6:43:LEU:HB2   | 6:6:82:GLY:HA3   | 1.86                     | 0.58              |
| 3:C:402:PRO:CG   | 3:C:535:MET:HE1  | 2.32                     | 0.58              |
| 4:D:85:MET:HE3   | 4:D:409:ARG:HB2  | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:167:PRO:CB   | 5:E:171:ARG:HH12 | 2.16                     | 0.58              |
| 6:F:128:ASP:HA   | 6:F:131:VAL:O    | 2.04                     | 0.58              |
| 1:1:17:LEU:HD12  | 1:1:251:LEU:HD11 | 1.86                     | 0.58              |
| 1:1:53:VAL:HG23  | 1:1:231:MET:CE   | 2.34                     | 0.58              |
| 3:3:337:ARG:HD2  | 3:3:337:ARG:N    | 2.16                     | 0.58              |
| 3:3:337:ARG:HG2  | 3:3:340:GLU:HG2  | 1.86                     | 0.58              |
| 3:3:495:GLU:O    | 3:3:498:GLU:HB2  | 2.04                     | 0.58              |
| 4:4:367:ARG:HG3  | 4:4:367:ARG:NH1  | 2.03                     | 0.58              |
| 7:9:33:LEU:H     | 7:9:33:LEU:HD12  | 1.69                     | 0.58              |
| 1:A:301:PRO:HB2  | 1:A:303:THR:HG23 | 1.86                     | 0.58              |
| 3:C:55:PRO:CD    | 3:C:74:GLN:H     | 2.17                     | 0.58              |
| 3:C:689:LYS:HE3  | 3:C:771:VAL:CG1  | 2.30                     | 0.58              |
| 1:1:247:LYS:O    | 1:1:268:MET:HE2  | 2.03                     | 0.58              |
| 3:3:238:LEU:HD12 | 3:3:238:LEU:O    | 2.02                     | 0.58              |
| 3:3:583:VAL:HG21 | 3:3:597:TYR:O    | 2.04                     | 0.58              |
| 4:4:241:ALA:CB   | 4:4:278:VAL:HG21 | 2.34                     | 0.58              |
| 7:9:46:HIS:HB3   | 7:9:47:PRO:CD    | 2.34                     | 0.58              |
| 8:7:60:SER:HA    | 8:7:66:PRO:HA    | 1.84                     | 0.58              |
| 3:C:655:ARG:HH12 | 3:C:659:GLU:HG3  | 1.69                     | 0.58              |
| 3:C:684:ARG:HG2  | 3:C:684:ARG:HH11 | 1.69                     | 0.58              |
| 5:E:123:GLY:HA2  | 5:E:144:HIS:CE1  | 2.39                     | 0.58              |
| 8:H:50:LEU:HD12  | 8:H:51:PRO:HD3   | 1.86                     | 0.58              |
| 1:1:241:MET:HG2  | 1:1:267:PRO:HB3  | 1.86                     | 0.57              |
| 3:3:309:PRO:HA   | 3:3:603:PRO:HD2  | 1.86                     | 0.57              |
| 7:9:44:THR:OG1   | 7:9:52:LYS:HD2   | 2.04                     | 0.57              |
| 1:A:29:LEU:O     | 1:A:33:LEU:HG    | 2.04                     | 0.57              |
| 1:A:354:GLY:O    | 1:A:360:ARG:NH1  | 2.37                     | 0.57              |
| 3:C:469:ARG:HB3  | 3:C:754:PRO:CB   | 2.34                     | 0.57              |
| 1:1:88:TYR:HB2   | 1:1:216:THR:CG2  | 2.32                     | 0.57              |
| 6:6:16:ARG:HD3   | 6:6:17:GLU:OE1   | 2.04                     | 0.57              |
| 1:1:315:HIS:O    | 1:1:319:LYS:HB2  | 2.05                     | 0.57              |
| 2:2:58:THR:HG21  | 3:3:200:LEU:N    | 2.20                     | 0.57              |
| 2:2:175:HIS:CE1  | 2:2:176:VAL:HG22 | 2.38                     | 0.57              |
| 3:3:202:PHE:O    | 3:3:203:ILE:HD13 | 2.04                     | 0.57              |
| 3:3:655:ARG:HH12 | 3:3:659:GLU:HG3  | 1.70                     | 0.57              |
| 4:4:278:VAL:O    | 4:4:282:GLU:HG3  | 2.04                     | 0.57              |
| 5:5:175:THR:O    | 5:5:177:LYS:N    | 2.36                     | 0.57              |
| 1:A:191:SER:HB2  | 1:A:197:ALA:HB2  | 1.84                     | 0.57              |
| 3:C:405:GLU:OE1  | 3:C:508:GLY:HA3  | 2.03                     | 0.57              |
| 3:C:440:ARG:CG   | 3:C:440:ARG:NH1  | 2.49                     | 0.57              |
| 3:C:546:ALA:HA   | 3:C:678:PHE:CE2  | 2.39                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:2:146:THR:HG23 | 2:2:149:ARG:HB2  | 1.87                     | 0.57              |
| 4:4:85:MET:HE3   | 4:4:409:ARG:HB2  | 1.86                     | 0.57              |
| 1:A:6:LEU:HD21   | 1:A:12:ARG:HG3   | 1.87                     | 0.57              |
| 3:C:693:TYR:HB3  | 3:C:759:TYR:CD2  | 2.39                     | 0.57              |
| 1:A:65:ARG:HD2   | 1:A:250:LYS:HD3  | 1.87                     | 0.57              |
| 2:B:86:LEU:CD1   | 2:B:90:LEU:HD11  | 2.35                     | 0.57              |
| 6:F:77:VAL:HA    | 6:F:104:TRP:O    | 2.03                     | 0.57              |
| 6:F:156:LYS:HG2  | 6:F:156:LYS:O    | 2.02                     | 0.57              |
| 3:3:682:GLU:OE1  | 3:3:684:ARG:NH2  | 2.38                     | 0.57              |
| 6:6:93:ARG:NH1   | 6:6:96:TRP:CE3   | 2.73                     | 0.57              |
| 3:C:279:ALA:HB2  | 3:C:290:ILE:CG1  | 2.30                     | 0.57              |
| 4:D:254:TYR:HE2  | 4:D:346:THR:HA   | 1.69                     | 0.57              |
| 6:F:77:VAL:O     | 6:F:77:VAL:HG12  | 2.04                     | 0.57              |
| 6:F:153:GLN:HG3  | 7:G:124:TYR:CZ   | 2.40                     | 0.57              |
| 3:3:183:HIS:C    | 3:3:184:CYS:O    | 2.48                     | 0.57              |
| 2:B:27:ILE:HG22  | 2:B:31:LEU:CD2   | 2.33                     | 0.57              |
| 6:F:29:ALA:HB1   | 6:F:158:VAL:O    | 2.05                     | 0.57              |
| 3:3:197:ASP:O    | 3:3:199:VAL:HG22 | 2.05                     | 0.57              |
| 8:7:82:ILE:HG23  | 8:7:95:ALA:HB3   | 1.87                     | 0.57              |
| 1:A:63:ARG:HD3   | 1:A:313:TYR:HD2  | 1.69                     | 0.57              |
| 3:C:701:ALA:HB2  | 3:C:763:LEU:CB   | 2.35                     | 0.57              |
| 4:D:61:TYR:CZ    | 6:F:87:LYS:HE2   | 2.40                     | 0.57              |
| 6:F:16:ARG:NH1   | 6:F:17:GLU:OE2   | 2.38                     | 0.57              |
| 6:F:50:MET:HE2   | 6:F:108:MET:HE2  | 1.87                     | 0.57              |
| 1:1:16:THR:CG2   | 1:1:229:PRO:HB3  | 2.28                     | 0.57              |
| 1:1:202:LYS:O    | 1:1:203:PRO:C    | 2.48                     | 0.57              |
| 2:B:27:ILE:HG22  | 2:B:31:LEU:HD22  | 1.87                     | 0.57              |
| 3:C:459:MET:CG   | 3:C:465:HIS:HB2  | 2.35                     | 0.57              |
| 4:D:278:VAL:O    | 4:D:282:GLU:HG3  | 2.04                     | 0.57              |
| 4:D:89:HIS:CE1   | 4:D:92:ALA:HB2   | 2.39                     | 0.57              |
| 4:D:261:THR:N    | 4:D:292:GLN:HE22 | 2.03                     | 0.57              |
| 5:E:66:GLU:HG2   | 5:E:95:PRO:CA    | 2.08                     | 0.57              |
| 8:H:6:GLU:OE1    | 8:H:80:LYS:HE3   | 2.04                     | 0.57              |
| 3:3:385:ALA:HB2  | 3:3:531:LYS:HB2  | 1.87                     | 0.56              |
| 3:3:753:VAL:HG13 | 3:3:759:TYR:CE1  | 2.40                     | 0.56              |
| 4:4:352:GLU:HB3  | 4:4:371:ARG:NE   | 2.20                     | 0.56              |
| 1:A:247:LYS:O    | 1:A:268:MET:HE2  | 2.05                     | 0.56              |
| 1:A:291:ILE:O    | 1:A:328:VAL:HA   | 2.04                     | 0.56              |
| 3:C:52:ILE:O     | 3:C:76:GLN:HG2   | 2.05                     | 0.56              |
| 6:F:43:LEU:HB2   | 6:F:82:GLY:HA3   | 1.87                     | 0.56              |
| 6:F:113:SER:HB3  | 7:G:96:LEU:HD13  | 1.86                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:6:83:ARG:HD3   | 9:6:182:SF4:S4   | 2.44                     | 0.56              |
| 2:B:143:GLU:C    | 2:B:144:CYS:SG   | 2.88                     | 0.56              |
| 3:C:337:ARG:HG2  | 3:C:340:GLU:HG2  | 1.87                     | 0.56              |
| 3:C:507:LEU:HD22 | 3:C:511:VAL:HG11 | 1.87                     | 0.56              |
| 3:C:565:TYR:HD1  | 3:C:582:PHE:CB   | 2.18                     | 0.56              |
| 5:E:75:VAL:HG12  | 5:E:76:SER:N     | 2.20                     | 0.56              |
| 6:F:165:GLU:HG2  | 7:G:148:ARG:HH11 | 1.70                     | 0.56              |
| 1:1:139:ARG:HG2  | 2:2:139:GLU:HA   | 1.85                     | 0.56              |
| 2:2:74:PRO:HB2   | 8:7:121:ARG:HH21 | 1.70                     | 0.56              |
| 3:3:459:MET:CG   | 3:3:465:HIS:HB2  | 2.35                     | 0.56              |
| 3:3:469:ARG:HB3  | 3:3:754:PRO:HB3  | 1.86                     | 0.56              |
| 3:3:717:TRP:HB2  | 3:3:759:TYR:HB2  | 1.88                     | 0.56              |
| 4:4:85:MET:HE3   | 4:4:409:ARG:CG   | 2.35                     | 0.56              |
| 4:4:219:ARG:NH1  | 4:4:273:PHE:CD2  | 2.73                     | 0.56              |
| 1:A:53:VAL:HG23  | 1:A:231:MET:CE   | 2.34                     | 0.56              |
| 1:A:314:GLU:HA   | 1:A:317:GLN:HB3  | 1.87                     | 0.56              |
| 1:A:344:LEU:O    | 1:A:347:PHE:HB3  | 2.06                     | 0.56              |
| 4:D:85:MET:HE3   | 4:D:409:ARG:CG   | 2.36                     | 0.56              |
| 1:1:314:GLU:HA   | 1:1:317:GLN:HB3  | 1.87                     | 0.56              |
| 2:B:135:GLN:HB2  | 2:B:141:TYR:HD1  | 1.71                     | 0.56              |
| 3:C:591:HIS:ND1  | 3:C:592:PRO:CD   | 2.69                     | 0.56              |
| 4:D:197:LEU:N    | 4:D:198:PRO:HD2  | 2.20                     | 0.56              |
| 5:E:37:GLU:O     | 5:E:41:TYR:CD1   | 2.55                     | 0.56              |
| 6:F:83:ARG:HD3   | 9:F:182:SF4:S4   | 2.45                     | 0.56              |
| 1:1:177:ALA:HB3  | 2:2:67:TYR:CG    | 2.41                     | 0.56              |
| 2:2:86:LEU:CD1   | 2:2:90:LEU:HD11  | 2.35                     | 0.56              |
| 3:3:405:GLU:OE1  | 3:3:508:GLY:HA3  | 2.06                     | 0.56              |
| 6:6:163:TYR:HD1  | 7:9:152:ARG:HH11 | 1.54                     | 0.56              |
| 2:B:10:PHE:CZ    | 2:B:33:ARG:HG3   | 2.41                     | 0.56              |
| 3:3:101:ARG:HH12 | 3:3:140:TYR:HD1  | 1.47                     | 0.56              |
| 3:3:295:ARG:HD2  | 3:3:296:PHE:CE2  | 2.41                     | 0.56              |
| 4:4:40:VAL:CG1   | 4:4:404:MET:HG3  | 2.36                     | 0.56              |
| 1:A:89:LEU:HD12  | 1:A:217:THR:HG22 | 1.87                     | 0.56              |
| 1:A:107:LEU:O    | 1:A:111:PRO:HG3  | 2.05                     | 0.56              |
| 1:A:315:HIS:O    | 1:A:319:LYS:HB2  | 2.06                     | 0.56              |
| 3:C:410:HIS:HA   | 3:C:458:LEU:HD21 | 1.87                     | 0.56              |
| 4:D:59:ILE:H     | 4:D:59:ILE:HD13  | 1.71                     | 0.56              |
| 4:D:115:THR:CG2  | 4:D:297:LEU:HD13 | 2.32                     | 0.56              |
| 4:D:225:PRO:HG3  | 4:D:383:TYR:OH   | 2.06                     | 0.56              |
| 4:D:355:TYR:CE2  | 4:D:370:VAL:HG22 | 2.40                     | 0.56              |
| 3:3:117:LEU:CA   | 4:4:321:MET:HE1  | 2.34                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:398:VAL:C    | 3:3:399:LEU:HD12 | 2.30                     | 0.56              |
| 3:3:568:TYR:CD1  | 3:3:572:PRO:HG3  | 2.40                     | 0.56              |
| 3:3:600:VAL:HG12 | 3:3:602:LEU:HD11 | 1.88                     | 0.56              |
| 3:C:55:PRO:HG3   | 3:C:74:GLN:HB2   | 1.87                     | 0.56              |
| 3:C:309:PRO:HA   | 3:C:603:PRO:HD2  | 1.87                     | 0.56              |
| 3:C:469:ARG:HB3  | 3:C:754:PRO:HB3  | 1.87                     | 0.56              |
| 3:C:568:TYR:CD1  | 3:C:572:PRO:HG3  | 2.41                     | 0.56              |
| 4:D:45:VAL:HG13  | 4:D:55:VAL:HG22  | 1.88                     | 0.56              |
| 7:G:26:TYR:N     | 7:G:27:PRO:HD3   | 2.20                     | 0.56              |
| 8:H:121:ARG:HG3  | 8:H:121:ARG:NH1  | 2.20                     | 0.56              |
| 1:1:312:SER:O    | 1:1:316:LEU:HB2  | 2.06                     | 0.56              |
| 2:2:27:ILE:HG22  | 2:2:31:LEU:CD2   | 2.36                     | 0.56              |
| 4:4:261:THR:H    | 4:4:292:GLN:NE2  | 2.04                     | 0.56              |
| 5:5:163:ARG:HD2  | 7:9:69:TYR:CE1   | 2.41                     | 0.56              |
| 1:A:42:LYS:HG3   | 1:A:46:LYS:HE3   | 1.88                     | 0.56              |
| 3:C:295:ARG:HD2  | 3:C:296:PHE:CE2  | 2.41                     | 0.56              |
| 4:4:374:SER:HB2  | 4:4:406:ASP:HB3  | 1.88                     | 0.56              |
| 7:9:33:LEU:HD22  | 7:9:37:PHE:CD2   | 2.41                     | 0.56              |
| 7:9:123:ASP:CG   | 7:9:148:ARG:HH22 | 2.14                     | 0.56              |
| 5:E:53:VAL:HG13  | 5:E:71:VAL:HB    | 1.88                     | 0.56              |
| 7:G:101:CYS:SG   | 7:G:103:LEU:HD12 | 2.46                     | 0.56              |
| 2:2:10:PHE:CZ    | 2:2:33:ARG:HG3   | 2.42                     | 0.55              |
| 4:4:115:THR:CG2  | 4:4:297:LEU:HD13 | 2.32                     | 0.55              |
| 3:C:20:MET:HE3   | 3:C:432:PHE:HB3  | 1.87                     | 0.55              |
| 3:C:495:GLU:O    | 3:C:498:GLU:HB2  | 2.05                     | 0.55              |
| 3:C:715:GLU:H    | 3:C:761:SER:HB2  | 1.72                     | 0.55              |
| 5:E:175:THR:O    | 5:E:177:LYS:N    | 2.39                     | 0.55              |
| 1:1:211:LEU:H    | 1:1:216:THR:HG21 | 1.71                     | 0.55              |
| 3:3:470:PRO:HG3  | 3:3:759:TYR:HE2  | 1.71                     | 0.55              |
| 4:4:183:PRO:HD3  | 7:9:36:ARG:NH2   | 2.20                     | 0.55              |
| 4:4:409:ARG:NH2  | 5:5:117:GLU:OE2  | 2.39                     | 0.55              |
| 1:A:313:TYR:HE1  | 1:A:323:LEU:HD13 | 1.70                     | 0.55              |
| 4:D:105:LEU:CD1  | 4:D:309:ILE:HD13 | 2.36                     | 0.55              |
| 2:2:135:GLN:HB2  | 2:2:141:TYR:HD1  | 1.70                     | 0.55              |
| 4:4:280:ILE:HG23 | 4:4:283:MET:HE2  | 1.87                     | 0.55              |
| 3:C:401:ASP:OD2  | 3:C:457:PRO:HD2  | 2.07                     | 0.55              |
| 4:D:197:LEU:HA   | 4:D:200:ARG:HB3  | 1.88                     | 0.55              |
| 5:E:42:LYS:HB2   | 5:E:108:TRP:CZ2  | 2.41                     | 0.55              |
| 1:1:29:LEU:CD1   | 1:1:155:ARG:HG3  | 2.36                     | 0.55              |
| 3:3:293:ALA:HA   | 3:3:699:TRP:CZ3  | 2.42                     | 0.55              |
| 4:4:94:ASP:HB3   | 4:4:173:ILE:HG21 | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:6:50:MET:HE2   | 6:6:108:MET:HE2  | 1.86                     | 0.55              |
| 7:9:175:ALA:O    | 7:9:177:THR:HG23 | 2.06                     | 0.55              |
| 3:C:218:LEU:N    | 3:C:219:PRO:CD   | 2.70                     | 0.55              |
| 3:C:399:LEU:HD12 | 3:C:399:LEU:N    | 2.21                     | 0.55              |
| 3:C:472:GLU:O    | 3:C:476:ILE:HD12 | 2.07                     | 0.55              |
| 6:F:83:ARG:HA    | 6:F:111:CYS:HB3  | 1.89                     | 0.55              |
| 7:G:33:LEU:H     | 7:G:33:LEU:HD12  | 1.71                     | 0.55              |
| 3:3:20:MET:CE    | 3:3:433:ALA:HB2  | 2.30                     | 0.55              |
| 6:6:29:ALA:HB1   | 6:6:158:VAL:O    | 2.07                     | 0.55              |
| 1:A:110:VAL:N    | 1:A:111:PRO:HD3  | 2.20                     | 0.55              |
| 3:C:356:LEU:HD13 | 3:C:654:PHE:HD1  | 1.71                     | 0.55              |
| 1:1:301:PRO:HB2  | 1:1:303:THR:HG23 | 1.89                     | 0.55              |
| 1:1:354:GLY:O    | 1:1:360:ARG:NH1  | 2.38                     | 0.55              |
| 1:1:366:PHE:CD1  | 1:1:370:LEU:HD21 | 2.42                     | 0.55              |
| 2:2:86:LEU:O     | 2:2:89:LYS:HB3   | 2.07                     | 0.55              |
| 4:4:212:PRO:HG2  | 4:4:213:ILE:H    | 1.71                     | 0.55              |
| 6:6:40:THR:HB    | 6:6:50:MET:SD    | 2.47                     | 0.55              |
| 1:1:63:ARG:HD3   | 1:1:313:TYR:HD2  | 1.71                     | 0.55              |
| 2:2:101:THR:HG23 | 2:2:106:ILE:O    | 2.07                     | 0.55              |
| 3:3:216:PHE:CZ   | 8:7:128:PHE:CD2  | 2.94                     | 0.55              |
| 4:4:105:LEU:HD13 | 4:4:309:ILE:CD1  | 2.36                     | 0.55              |
| 4:4:208:PHE:O    | 4:4:211:SER:HB3  | 2.06                     | 0.55              |
| 6:6:76:ASP:O     | 6:6:77:VAL:HB    | 2.07                     | 0.55              |
| 7:9:45:ARG:HH21  | 7:9:137:LEU:HD23 | 1.71                     | 0.55              |
| 1:A:29:LEU:HD22  | 1:A:29:LEU:O     | 2.06                     | 0.55              |
| 3:C:361:ALA:HB3  | 3:C:369:LEU:HD13 | 1.89                     | 0.55              |
| 4:D:261:THR:H    | 4:D:292:GLN:NE2  | 2.03                     | 0.55              |
| 4:D:367:ARG:HG3  | 4:D:367:ARG:NH1  | 2.06                     | 0.55              |
| 3:3:715:GLU:H    | 3:3:761:SER:HB2  | 1.71                     | 0.55              |
| 6:6:130:VAL:HG23 | 6:6:131:VAL:HG13 | 1.89                     | 0.55              |
| 1:A:186:THR:HG23 | 1:A:200:ARG:N    | 2.10                     | 0.55              |
| 2:B:116:LEU:HD23 | 2:B:116:LEU:N    | 2.22                     | 0.55              |
| 3:C:510:GLY:O    | 3:C:514:ASP:HB3  | 2.07                     | 0.55              |
| 4:D:381:LEU:HD13 | 4:D:400:LEU:HD12 | 1.89                     | 0.55              |
| 1:1:107:LEU:O    | 1:1:111:PRO:HG3  | 2.06                     | 0.55              |
| 3:3:136:GLU:CG   | 5:5:189:ARG:HG2  | 2.32                     | 0.55              |
| 3:3:218:LEU:N    | 3:3:219:PRO:CD   | 2.69                     | 0.55              |
| 3:3:507:LEU:HD22 | 3:3:511:VAL:HG11 | 1.88                     | 0.55              |
| 3:3:707:LYS:C    | 3:3:709:GLN:H    | 2.14                     | 0.55              |
| 4:4:45:VAL:HG13  | 4:4:55:VAL:HG22  | 1.87                     | 0.55              |
| 4:4:133:LEU:HD21 | 4:4:204:TYR:CD2  | 2.42                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:5:25:LEU:HD23  | 5:5:25:LEU:H     | 1.72                     | 0.55              |
| 6:6:77:VAL:HA    | 6:6:104:TRP:O    | 2.06                     | 0.55              |
| 2:B:106:ILE:CG2  | 2:B:110:GLU:HB2  | 2.37                     | 0.55              |
| 3:C:720:PRO:HG3  | 3:C:749:HIS:HB3  | 1.89                     | 0.55              |
| 4:D:86:ASP:O     | 4:D:90:SER:HA    | 2.07                     | 0.55              |
| 5:E:25:LEU:N     | 5:E:25:LEU:HD23  | 2.22                     | 0.55              |
| 7:G:40:ARG:NH1   | 7:G:41:HIS:O     | 2.40                     | 0.55              |
| 6:6:141:PRO:HB3  | 9:6:182:SF4:S1   | 2.46                     | 0.55              |
| 7:9:41:HIS:CD2   | 7:9:115:LEU:CD2  | 2.89                     | 0.55              |
| 3:C:246:ASN:H    | 3:C:246:ASN:HD22 | 1.55                     | 0.55              |
| 4:D:85:MET:HE1   | 4:D:370:VAL:HG21 | 1.89                     | 0.55              |
| 3:3:565:TYR:HD1  | 3:3:582:PHE:CB   | 2.20                     | 0.54              |
| 4:4:105:LEU:CD1  | 4:4:309:ILE:HD13 | 2.37                     | 0.54              |
| 1:A:283:PRO:HB3  | 1:A:287:ILE:HD13 | 1.89                     | 0.54              |
| 1:A:312:SER:HG   | 1:A:315:HIS:HD1  | 1.54                     | 0.54              |
| 4:D:263:ASP:HB2  | 4:D:285:GLU:OE1  | 2.06                     | 0.54              |
| 5:E:163:ARG:HD2  | 7:G:69:TYR:CD1   | 2.42                     | 0.54              |
| 6:F:156:LYS:HA   | 6:F:159:ARG:HD2  | 1.88                     | 0.54              |
| 1:1:310:PRO:HG2  | 1:1:315:HIS:CD2  | 2.41                     | 0.54              |
| 3:3:52:ILE:O     | 3:3:76:GLN:HG2   | 2.07                     | 0.54              |
| 3:3:550:LEU:HD12 | 3:3:550:LEU:N    | 2.22                     | 0.54              |
| 4:4:70:MET:HE3   | 4:4:81:TYR:HB3   | 1.89                     | 0.54              |
| 4:D:241:ALA:HB2  | 4:D:278:VAL:HG21 | 1.89                     | 0.54              |
| 5:E:25:LEU:HD23  | 5:E:25:LEU:H     | 1.73                     | 0.54              |
| 1:1:191:SER:HB2  | 1:1:197:ALA:HB2  | 1.88                     | 0.54              |
| 3:3:87:VAL:CA    | 3:3:91:MET:HE1   | 2.35                     | 0.54              |
| 4:4:197:LEU:HA   | 4:4:200:ARG:HB3  | 1.89                     | 0.54              |
| 4:4:262:PHE:CD1  | 4:4:289:ILE:HD11 | 2.43                     | 0.54              |
| 5:5:16:PRO:HB2   | 5:5:28:VAL:HG12  | 1.90                     | 0.54              |
| 5:5:167:PRO:C    | 5:5:171:ARG:NH1  | 2.65                     | 0.54              |
| 1:A:8:GLY:C      | 1:A:10:ASP:H     | 2.15                     | 0.54              |
| 3:C:753:VAL:HG13 | 3:C:759:TYR:CE1  | 2.43                     | 0.54              |
| 4:4:205:GLU:OE2  | 4:4:281:ARG:NE   | 2.27                     | 0.54              |
| 1:A:401:PRO:HB2  | 10:A:440:FMN:C8M | 2.36                     | 0.54              |
| 3:C:202:PHE:O    | 3:C:203:ILE:HD13 | 2.08                     | 0.54              |
| 3:C:409:LEU:HD12 | 3:C:535:MET:HE2  | 1.90                     | 0.54              |
| 4:D:346:THR:HG22 | 4:D:353:LEU:O    | 2.08                     | 0.54              |
| 6:F:22:THR:HA    | 6:F:25:GLU:HG2   | 1.90                     | 0.54              |
| 5:5:25:LEU:HD23  | 5:5:25:LEU:N     | 2.22                     | 0.54              |
| 4:D:208:PHE:O    | 4:D:211:SER:HB3  | 2.08                     | 0.54              |
| 4:D:374:SER:HB2  | 4:D:406:ASP:HB3  | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:393:MET:HA   | 4:D:396:ILE:HG22 | 1.89                     | 0.54              |
| 3:3:54:LEU:H     | 3:3:55:PRO:HD3   | 1.73                     | 0.54              |
| 3:3:410:HIS:HA   | 3:3:458:LEU:HD21 | 1.90                     | 0.54              |
| 3:3:473:GLU:O    | 3:3:477:LEU:CD1  | 2.56                     | 0.54              |
| 1:A:60:SER:HA    | 1:A:235:ALA:HB1  | 1.90                     | 0.54              |
| 3:C:20:MET:CE    | 3:C:433:ALA:HB2  | 2.34                     | 0.54              |
| 3:C:46:ARG:HG2   | 3:C:46:ARG:HH11  | 1.72                     | 0.54              |
| 1:1:104:ARG:NH2  | 2:2:127:SER:CB   | 2.64                     | 0.54              |
| 1:1:332:PRO:HD2  | 2:2:90:LEU:CD2   | 2.38                     | 0.54              |
| 3:3:401:ASP:OD2  | 3:3:457:PRO:HD2  | 2.08                     | 0.54              |
| 1:A:312:SER:O    | 1:A:316:LEU:HB2  | 2.07                     | 0.54              |
| 3:C:456:ALA:O    | 3:C:459:MET:HB2  | 2.08                     | 0.54              |
| 4:D:212:PRO:HG2  | 4:D:213:ILE:H    | 1.72                     | 0.54              |
| 5:E:54:GLY:C     | 5:E:55:LEU:HD12  | 2.33                     | 0.54              |
| 7:G:175:ALA:O    | 7:G:177:THR:HG23 | 2.08                     | 0.54              |
| 3:3:43:GLY:HA2   | 11:3:787:FES:S1  | 2.48                     | 0.54              |
| 1:A:366:PHE:CD1  | 1:A:370:LEU:HD21 | 2.42                     | 0.54              |
| 4:D:183:PRO:HD3  | 7:G:36:ARG:NH2   | 2.22                     | 0.54              |
| 7:G:33:LEU:HD22  | 7:G:37:PHE:CD2   | 2.42                     | 0.54              |
| 1:1:283:PRO:HB3  | 1:1:287:ILE:HD13 | 1.90                     | 0.54              |
| 3:3:684:ARG:HG2  | 3:3:684:ARG:HH11 | 1.73                     | 0.54              |
| 4:4:70:MET:HE3   | 4:4:81:TYR:HB2   | 1.89                     | 0.54              |
| 4:4:140:LEU:HD11 | 4:4:214:PHE:HB2  | 1.90                     | 0.54              |
| 6:6:57:ARG:C     | 6:6:57:ARG:NE    | 2.66                     | 0.54              |
| 3:C:55:PRO:HD3   | 3:C:74:GLN:N     | 2.20                     | 0.54              |
| 7:G:123:ASP:CG   | 7:G:148:ARG:HH22 | 2.16                     | 0.54              |
| 1:1:9:LEU:O      | 1:1:9:LEU:HG     | 2.08                     | 0.54              |
| 1:1:272:PHE:CD2  | 1:1:311:MET:HE3  | 2.43                     | 0.54              |
| 3:3:510:GLY:O    | 3:3:514:ASP:HB3  | 2.08                     | 0.54              |
| 4:4:250:LYS:CE   | 4:4:262:PHE:HB3  | 2.36                     | 0.54              |
| 4:4:254:TYR:HE2  | 4:4:346:THR:HA   | 1.72                     | 0.54              |
| 8:7:50:LEU:HD12  | 8:7:51:PRO:HD3   | 1.90                     | 0.54              |
| 3:C:54:LEU:H     | 3:C:55:PRO:HD3   | 1.72                     | 0.54              |
| 4:D:352:GLU:HB3  | 4:D:371:ARG:NE   | 2.22                     | 0.54              |
| 4:D:381:LEU:O    | 4:D:381:LEU:HG   | 2.08                     | 0.54              |
| 6:F:50:MET:HB2   | 6:F:108:MET:CE   | 2.37                     | 0.54              |
| 6:F:96:TRP:HA    | 6:F:99:MET:CE    | 2.36                     | 0.54              |
| 7:G:45:ARG:HH21  | 7:G:137:LEU:HD23 | 1.73                     | 0.54              |
| 3:3:305:ARG:HG2  | 3:3:588:SER:O    | 2.08                     | 0.53              |
| 4:4:86:ASP:O     | 4:4:90:SER:HA    | 2.08                     | 0.53              |
| 6:6:83:ARG:HA    | 6:6:111:CYS:HB3  | 1.89                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:192:LEU:HD22 | 1:A:211:LEU:HD11 | 1.90                     | 0.53              |
| 1:A:202:LYS:O    | 1:A:203:PRO:C    | 2.50                     | 0.53              |
| 3:C:33:PHE:HB2   | 3:C:45:CYS:SG    | 2.48                     | 0.53              |
| 3:C:229:ILE:HD11 | 3:C:289:TRP:CZ3  | 2.42                     | 0.53              |
| 4:D:94:ASP:HB3   | 4:D:173:ILE:HG21 | 1.89                     | 0.53              |
| 4:D:350:ARG:O    | 4:D:373:PRO:HB2  | 2.08                     | 0.53              |
| 1:1:138:TYR:HB3  | 1:1:141:ALA:HB3  | 1.88                     | 0.53              |
| 1:1:332:PRO:HD2  | 2:2:90:LEU:HD23  | 1.89                     | 0.53              |
| 3:3:720:PRO:HG3  | 3:3:749:HIS:HB3  | 1.91                     | 0.53              |
| 4:4:381:LEU:HD13 | 4:4:400:LEU:HD12 | 1.90                     | 0.53              |
| 7:9:133:LYS:O    | 7:9:137:LEU:HD13 | 2.07                     | 0.53              |
| 3:C:229:ILE:HD11 | 3:C:289:TRP:HZ3  | 1.72                     | 0.53              |
| 5:E:135:ILE:HG22 | 5:E:136:LEU:HG   | 1.90                     | 0.53              |
| 6:F:104:TRP:CE2  | 6:F:173:VAL:HG22 | 2.44                     | 0.53              |
| 2:2:106:ILE:CG2  | 2:2:110:GLU:HB2  | 2.38                     | 0.53              |
| 6:6:50:MET:C     | 6:6:52:ALA:H     | 2.16                     | 0.53              |
| 3:C:550:LEU:HD12 | 3:C:550:LEU:N    | 2.24                     | 0.53              |
| 1:1:29:LEU:HD22  | 1:1:29:LEU:O     | 2.07                     | 0.53              |
| 3:3:31:PRO:HD3   | 3:3:137:TYR:CE2  | 2.44                     | 0.53              |
| 3:3:55:PRO:HG3   | 3:3:74:GLN:HB2   | 1.90                     | 0.53              |
| 4:4:179:LYS:HE3  | 7:9:106:GLU:OE1  | 2.07                     | 0.53              |
| 5:5:42:LYS:HB2   | 5:5:108:TRP:CZ2  | 2.43                     | 0.53              |
| 6:6:138:PRO:CG   | 7:9:121:MET:HG3  | 2.38                     | 0.53              |
| 3:C:570:PHE:O    | 3:C:585:MET:HE2  | 2.09                     | 0.53              |
| 3:3:515:THR:HG23 | 3:3:683:LEU:HD12 | 1.90                     | 0.53              |
| 4:4:197:LEU:N    | 4:4:198:PRO:HD2  | 2.24                     | 0.53              |
| 4:4:210:GLU:O    | 4:4:212:PRO:HD3  | 2.08                     | 0.53              |
| 5:5:123:GLY:HA2  | 5:5:144:HIS:CE1  | 2.43                     | 0.53              |
| 6:6:104:TRP:NE1  | 6:6:158:VAL:HG12 | 2.23                     | 0.53              |
| 1:A:97:GLU:O     | 1:A:100:SER:HB3  | 2.09                     | 0.53              |
| 2:B:146:THR:HG23 | 2:B:149:ARG:HB2  | 1.91                     | 0.53              |
| 3:C:344:TYR:CD1  | 3:C:568:TYR:CE1  | 2.96                     | 0.53              |
| 4:D:70:MET:HE3   | 4:D:81:TYR:HB2   | 1.90                     | 0.53              |
| 4:D:133:LEU:HD21 | 4:D:204:TYR:CD2  | 2.43                     | 0.53              |
| 4:D:238:SER:HB2  | 4:D:275:ARG:HG2  | 1.90                     | 0.53              |
| 3:3:229:ILE:O    | 3:3:230:CYS:C    | 2.51                     | 0.53              |
| 6:6:117:MET:HE2  | 7:9:99:ILE:CG1   | 2.19                     | 0.53              |
| 1:A:41:ALA:HB2   | 1:A:116:GLU:HG3  | 1.91                     | 0.53              |
| 3:C:470:PRO:HG3  | 3:C:759:TYR:HE2  | 1.73                     | 0.53              |
| 3:C:594:ALA:O    | 3:C:598:ALA:HB3  | 2.08                     | 0.53              |
| 4:D:105:LEU:HD13 | 4:D:309:ILE:CD1  | 2.37                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:145:PRO:HA   | 5:E:150:TYR:CD2  | 2.43                     | 0.53              |
| 6:F:57:ARG:C     | 6:F:57:ARG:NE    | 2.67                     | 0.53              |
| 1:1:41:ALA:HB2   | 1:1:116:GLU:HG3  | 1.90                     | 0.53              |
| 1:1:261:PRO:HB2  | 2:2:129:HIS:HB2  | 1.91                     | 0.53              |
| 3:3:124:LYS:HE3  | 3:3:128:CYS:HA   | 1.89                     | 0.53              |
| 3:3:268:ASP:OD2  | 3:3:278:ARG:NH1  | 2.41                     | 0.53              |
| 3:3:451:PHE:HE1  | 3:3:466:GLU:HB3  | 1.74                     | 0.53              |
| 3:C:112:LEU:CD2  | 3:C:130:LEU:HD21 | 2.39                     | 0.53              |
| 3:C:216:PHE:CZ   | 8:H:128:PHE:CD2  | 2.95                     | 0.53              |
| 3:C:293:ALA:HA   | 3:C:699:TRP:CZ3  | 2.44                     | 0.53              |
| 3:C:357:ALA:HB2  | 3:C:641:LEU:HD11 | 1.90                     | 0.53              |
| 3:C:586:HIS:CE1  | 3:C:640:VAL:HG21 | 2.43                     | 0.53              |
| 3:C:707:LYS:C    | 3:C:709:GLN:H    | 2.16                     | 0.53              |
| 4:D:210:GLU:O    | 4:D:212:PRO:HD3  | 2.08                     | 0.53              |
| 5:E:144:HIS:O    | 5:E:147:ARG:HG2  | 2.08                     | 0.53              |
| 3:3:469:ARG:HB3  | 3:3:754:PRO:CB   | 2.38                     | 0.53              |
| 4:4:393:MET:C    | 4:4:396:ILE:HG22 | 2.34                     | 0.53              |
| 6:6:90:PRO:O     | 6:6:93:ARG:HB3   | 2.09                     | 0.53              |
| 6:6:128:ASP:HA   | 6:6:131:VAL:O    | 2.08                     | 0.53              |
| 1:A:118:MET:HG2  | 1:A:224:LEU:HD13 | 1.91                     | 0.53              |
| 1:A:139:ARG:HG2  | 2:B:140:PRO:HD3  | 1.90                     | 0.53              |
| 4:D:211:SER:HB2  | 4:D:214:PHE:HB3  | 1.90                     | 0.53              |
| 1:1:89:LEU:HD12  | 1:1:217:THR:HG22 | 1.90                     | 0.53              |
| 2:2:27:ILE:HG22  | 2:2:31:LEU:HD22  | 1.90                     | 0.53              |
| 3:3:294:GLY:HA3  | 9:3:786:SF4:S4   | 2.48                     | 0.53              |
| 2:B:86:LEU:O     | 2:B:89:LYS:HB3   | 2.09                     | 0.53              |
| 4:D:393:MET:O    | 4:D:396:ILE:HG22 | 2.09                     | 0.53              |
| 1:1:313:TYR:HE1  | 1:1:323:LEU:HD13 | 1.74                     | 0.53              |
| 3:3:11:VAL:CG1   | 3:3:25:HIS:CD2   | 2.92                     | 0.53              |
| 6:6:96:TRP:HA    | 6:6:99:MET:CE    | 2.34                     | 0.53              |
| 3:C:105:ALA:CB   | 3:C:140:TYR:HB2  | 2.39                     | 0.53              |
| 4:D:64:THR:HB    | 4:D:66:PHE:CE1   | 2.43                     | 0.53              |
| 2:2:116:LEU:HD23 | 2:2:116:LEU:N    | 2.25                     | 0.52              |
| 3:3:218:LEU:N    | 3:3:219:PRO:HD3  | 2.24                     | 0.52              |
| 3:3:367:PRO:HB2  | 3:3:554:LYS:CB   | 2.39                     | 0.52              |
| 4:4:261:THR:N    | 4:4:292:GLN:HE22 | 2.03                     | 0.52              |
| 3:C:183:HIS:C    | 3:C:184:CYS:O    | 2.51                     | 0.52              |
| 3:C:343:LEU:HB2  | 3:C:369:LEU:HB2  | 1.91                     | 0.52              |
| 5:E:167:PRO:HB3  | 7:G:66:TYR:CE2   | 2.44                     | 0.52              |
| 1:1:42:LYS:HG3   | 1:1:46:LYS:HE3   | 1.91                     | 0.52              |
| 2:2:139:GLU:CB   | 2:2:140:PRO:HD2  | 2.40                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:36:GLU:HG2   | 3:3:229:ILE:HG23 | 1.92                     | 0.52              |
| 3:3:232:VAL:HB   | 9:3:784:SF4:S2   | 2.49                     | 0.52              |
| 3:3:299:GLU:O    | 3:3:303:GLN:HB2  | 2.09                     | 0.52              |
| 2:B:87:SER:HB3   | 11:B:182:FES:S2  | 2.49                     | 0.52              |
| 2:B:101:THR:HG23 | 2:B:106:ILE:O    | 2.08                     | 0.52              |
| 6:F:49:GLU:OE1   | 6:F:49:GLU:HA    | 2.09                     | 0.52              |
| 1:1:312:SER:HG   | 1:1:315:HIS:HD1  | 1.55                     | 0.52              |
| 2:2:135:GLN:HB2  | 2:2:141:TYR:CD1  | 2.44                     | 0.52              |
| 3:3:282:VAL:HG22 | 3:3:282:VAL:O    | 2.08                     | 0.52              |
| 8:7:81:ARG:O     | 8:7:81:ARG:HD3   | 2.10                     | 0.52              |
| 3:C:367:PRO:HB2  | 3:C:554:LYS:CB   | 2.38                     | 0.52              |
| 3:C:545:GLU:HA   | 3:C:550:LEU:HD11 | 1.92                     | 0.52              |
| 3:C:682:GLU:OE1  | 3:C:684:ARG:NH2  | 2.37                     | 0.52              |
| 4:D:409:ARG:NH2  | 5:E:117:GLU:OE2  | 2.43                     | 0.52              |
| 1:1:60:SER:HA    | 1:1:235:ALA:HB1  | 1.91                     | 0.52              |
| 2:2:143:GLU:C    | 2:2:144:CYS:SG   | 2.92                     | 0.52              |
| 3:3:352:GLU:HG3  | 3:3:664:LEU:HD11 | 1.90                     | 0.52              |
| 3:3:591:HIS:ND1  | 3:3:592:PRO:CD   | 2.72                     | 0.52              |
| 4:4:381:LEU:H    | 4:4:382:PRO:HD2  | 1.74                     | 0.52              |
| 6:6:22:THR:HA    | 6:6:25:GLU:HG2   | 1.92                     | 0.52              |
| 8:7:117:ALA:O    | 8:7:121:ARG:HG2  | 2.10                     | 0.52              |
| 3:C:572:PRO:HD2  | 3:C:577:LEU:HD21 | 1.92                     | 0.52              |
| 3:C:616:ASN:ND2  | 3:C:622:LEU:HD11 | 2.25                     | 0.52              |
| 6:F:90:PRO:O     | 6:F:93:ARG:HB3   | 2.08                     | 0.52              |
| 3:3:261:VAL:CG2  | 9:3:786:SF4:S2   | 2.97                     | 0.52              |
| 3:3:509:ALA:HB1  | 3:3:768:GLY:CA   | 2.31                     | 0.52              |
| 4:4:85:MET:HE1   | 4:4:370:VAL:HG21 | 1.92                     | 0.52              |
| 6:6:83:ARG:HG3   | 6:6:83:ARG:NH1   | 2.25                     | 0.52              |
| 6:6:156:LYS:HA   | 6:6:159:ARG:HD2  | 1.92                     | 0.52              |
| 2:B:135:GLN:HB2  | 2:B:141:TYR:CD1  | 2.45                     | 0.52              |
| 3:C:46:ARG:O     | 3:C:107:MET:HG2  | 2.10                     | 0.52              |
| 4:D:249:ARG:HB2  | 4:D:262:PHE:HE2  | 1.74                     | 0.52              |
| 1:1:391:LEU:N    | 1:1:392:PRO:HD2  | 2.25                     | 0.52              |
| 3:3:225:ASN:HD21 | 3:3:289:TRP:HB3  | 1.74                     | 0.52              |
| 3:3:248:GLU:HG2  | 5:5:170:PHE:CE1  | 2.44                     | 0.52              |
| 3:3:481:LEU:HD22 | 3:3:527:ARG:NH1  | 2.25                     | 0.52              |
| 5:5:53:VAL:HG13  | 5:5:71:VAL:HB    | 1.91                     | 0.52              |
| 5:5:119:TYR:O    | 5:5:122:PHE:O    | 2.28                     | 0.52              |
| 1:A:18:TYR:CZ    | 1:A:263:VAL:HG11 | 2.44                     | 0.52              |
| 3:C:734:VAL:HG12 | 3:C:736:VAL:HG23 | 1.92                     | 0.52              |
| 6:F:76:ASP:O     | 6:F:77:VAL:HB    | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:101:ARG:NH1  | 3:3:140:TYR:CE1  | 2.77                     | 0.52              |
| 3:3:385:ALA:HB2  | 3:3:531:LYS:CB   | 2.40                     | 0.52              |
| 4:D:185:GLU:O    | 4:D:189:GLU:HG2  | 2.10                     | 0.52              |
| 1:1:436:LEU:HD23 | 2:2:90:LEU:HA    | 1.91                     | 0.52              |
| 3:3:20:MET:HE3   | 3:3:432:PHE:HB3  | 1.91                     | 0.52              |
| 3:3:46:ARG:O     | 3:3:107:MET:HG2  | 2.10                     | 0.52              |
| 3:3:130:LEU:HD23 | 9:3:784:SF4:S4   | 2.50                     | 0.52              |
| 4:4:85:MET:HE3   | 4:4:409:ARG:CB   | 2.40                     | 0.52              |
| 4:4:153:ARG:HH11 | 4:4:153:ARG:HG3  | 1.75                     | 0.52              |
| 4:4:367:ARG:CG   | 4:4:367:ARG:NH1  | 2.65                     | 0.52              |
| 1:A:350:HIS:O    | 3:C:205:ARG:NH1  | 2.43                     | 0.52              |
| 3:C:565:TYR:HD1  | 3:C:582:PHE:HB3  | 1.74                     | 0.52              |
| 8:H:84:LEU:HB2   | 8:H:93:LEU:HB2   | 1.91                     | 0.52              |
| 8:H:117:ALA:O    | 8:H:121:ARG:HG2  | 2.09                     | 0.52              |
| 1:1:8:GLY:C      | 1:1:10:ASP:H     | 2.17                     | 0.52              |
| 1:1:139:ARG:CG   | 2:2:140:PRO:HD3  | 2.39                     | 0.52              |
| 3:3:356:LEU:HD13 | 3:3:654:PHE:CD1  | 2.44                     | 0.52              |
| 4:4:241:ALA:HB2  | 4:4:278:VAL:HG21 | 1.92                     | 0.52              |
| 5:5:144:HIS:O    | 5:5:147:ARG:HG2  | 2.10                     | 0.52              |
| 2:B:77:LYS:HE3   | 2:B:78:TYR:CZ    | 2.45                     | 0.52              |
| 3:C:317:LEU:HD22 | 3:C:317:LEU:N    | 2.25                     | 0.52              |
| 3:C:575:GLU:OE1  | 3:C:575:GLU:HA   | 2.10                     | 0.52              |
| 4:D:91:PHE:CE1   | 4:D:120:LEU:HD12 | 2.45                     | 0.52              |
| 4:D:262:PHE:CD1  | 4:D:289:ILE:HD11 | 2.45                     | 0.52              |
| 7:G:46:HIS:HB3   | 7:G:47:PRO:CD    | 2.39                     | 0.52              |
| 8:H:121:ARG:HH11 | 8:H:121:ARG:CG   | 2.22                     | 0.52              |
| 3:3:200:LEU:HD12 | 3:3:212:GLY:O    | 2.09                     | 0.52              |
| 8:7:108:ILE:HD12 | 8:7:108:ILE:N    | 2.26                     | 0.52              |
| 1:A:6:LEU:HD12   | 1:A:240:GLN:O    | 2.10                     | 0.52              |
| 3:C:116:PRO:O    | 3:C:117:LEU:CB   | 2.57                     | 0.52              |
| 4:D:197:LEU:O    | 4:D:198:PRO:C    | 2.53                     | 0.52              |
| 6:F:16:ARG:HD3   | 6:F:17:GLU:OE1   | 2.09                     | 0.52              |
| 6:F:40:THR:HB    | 6:F:50:MET:SD    | 2.50                     | 0.52              |
| 6:F:74:GLN:OE1   | 6:F:74:GLN:HA    | 2.10                     | 0.52              |
| 6:F:104:TRP:NE1  | 6:F:158:VAL:HG12 | 2.24                     | 0.52              |
| 3:3:186:ARG:CD   | 3:3:231:PRO:HD3  | 2.37                     | 0.51              |
| 3:3:216:PHE:HZ   | 8:7:128:PHE:CD2  | 2.28                     | 0.51              |
| 3:3:701:ALA:HB2  | 3:3:763:LEU:CB   | 2.39                     | 0.51              |
| 3:C:87:VAL:CA    | 3:C:91:MET:HE1   | 2.34                     | 0.51              |
| 3:C:218:LEU:N    | 3:C:219:PRO:HD3  | 2.25                     | 0.51              |
| 3:C:282:VAL:HG22 | 3:C:282:VAL:O    | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:473:GLU:O    | 3:C:477:LEU:CD1  | 2.58                     | 0.51              |
| 4:D:44:MET:HA    | 4:D:44:MET:CE    | 2.38                     | 0.51              |
| 4:D:179:LYS:HE3  | 7:G:106:GLU:OE1  | 2.10                     | 0.51              |
| 4:D:263:ASP:O    | 4:D:285:GLU:HG3  | 2.09                     | 0.51              |
| 5:E:16:PRO:HB2   | 5:E:28:VAL:HG12  | 1.90                     | 0.51              |
| 1:1:243:THR:HG21 | 1:1:315:HIS:HE1  | 1.75                     | 0.51              |
| 6:6:74:GLN:OE1   | 6:6:74:GLN:HA    | 2.10                     | 0.51              |
| 1:A:301:PRO:HB2  | 1:A:303:THR:CG2  | 2.39                     | 0.51              |
| 3:C:130:LEU:HD23 | 9:C:784:SF4:S4   | 2.50                     | 0.51              |
| 4:D:59:ILE:HD11  | 5:E:135:ILE:HG23 | 1.91                     | 0.51              |
| 4:D:317:LEU:HD21 | 4:D:327:HIS:CD2  | 2.45                     | 0.51              |
| 6:F:92:MET:HE1   | 6:F:127:VAL:HG13 | 1.90                     | 0.51              |
| 8:H:87:PRO:O     | 8:H:88:ARG:CB    | 2.51                     | 0.51              |
| 1:1:289:ALA:HB3  | 1:1:337:MET:CE   | 2.40                     | 0.51              |
| 4:4:294:LEU:O    | 4:4:294:LEU:HD23 | 2.09                     | 0.51              |
| 3:C:299:GLU:O    | 3:C:303:GLN:HB2  | 2.11                     | 0.51              |
| 3:C:344:TYR:HD1  | 3:C:568:TYR:CE1  | 2.28                     | 0.51              |
| 4:D:85:MET:HE3   | 4:D:409:ARG:CB   | 2.40                     | 0.51              |
| 4:D:369:LYS:HG3  | 5:E:53:VAL:HG23  | 1.93                     | 0.51              |
| 8:H:92:HIS:O     | 8:H:93:LEU:HD12  | 2.09                     | 0.51              |
| 3:3:157:PHE:CZ   | 3:3:159:PHE:HB2  | 2.44                     | 0.51              |
| 3:3:575:GLU:OE1  | 3:3:575:GLU:HA   | 2.10                     | 0.51              |
| 5:5:75:VAL:HG12  | 5:5:76:SER:N     | 2.26                     | 0.51              |
| 5:5:167:PRO:CB   | 5:5:171:ARG:HH12 | 2.24                     | 0.51              |
| 6:6:50:MET:HB2   | 6:6:108:MET:CE   | 2.40                     | 0.51              |
| 8:7:15:GLU:O     | 8:7:18:SER:HB3   | 2.09                     | 0.51              |
| 8:7:92:HIS:N     | 8:7:92:HIS:CD2   | 2.78                     | 0.51              |
| 8:7:121:ARG:HG3  | 8:7:121:ARG:NH1  | 2.26                     | 0.51              |
| 1:A:214:LYS:O    | 1:A:216:THR:HG23 | 2.09                     | 0.51              |
| 1:A:241:MET:HG2  | 1:A:267:PRO:HB3  | 1.91                     | 0.51              |
| 3:C:197:ASP:OD2  | 3:C:220:SER:HB2  | 2.10                     | 0.51              |
| 4:D:101:VAL:O    | 4:D:104:LEU:N    | 2.43                     | 0.51              |
| 6:F:165:GLU:HG2  | 7:G:148:ARG:NH1  | 2.26                     | 0.51              |
| 1:A:243:THR:HG21 | 1:A:315:HIS:HE1  | 1.75                     | 0.51              |
| 3:C:352:GLU:HG3  | 3:C:664:LEU:HD11 | 1.93                     | 0.51              |
| 6:F:50:MET:C     | 6:F:52:ALA:H     | 2.19                     | 0.51              |
| 3:3:352:GLU:HG3  | 3:3:664:LEU:CD1  | 2.41                     | 0.51              |
| 4:4:263:ASP:O    | 4:4:285:GLU:HG3  | 2.11                     | 0.51              |
| 4:4:393:MET:HA   | 4:4:396:ILE:HG22 | 1.91                     | 0.51              |
| 5:5:66:GLU:CG    | 5:5:95:PRO:HA    | 2.11                     | 0.51              |
| 6:6:78:MET:O     | 6:6:78:MET:HG3   | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:157:PHE:CZ   | 3:C:159:PHE:HB2  | 2.45                     | 0.51              |
| 4:D:153:ARG:HH11 | 4:D:153:ARG:HG3  | 1.76                     | 0.51              |
| 5:E:98:ASP:OD1   | 5:E:100:ARG:HD3  | 2.11                     | 0.51              |
| 3:3:572:PRO:HD2  | 3:3:577:LEU:HD21 | 1.93                     | 0.51              |
| 3:C:205:ARG:HA   | 3:C:209:THR:CG2  | 2.39                     | 0.51              |
| 3:C:360:LEU:HD13 | 3:C:645:ALA:HB2  | 1.91                     | 0.51              |
| 3:C:684:ARG:HG2  | 3:C:684:ARG:NH1  | 2.25                     | 0.51              |
| 4:D:230:ILE:HG22 | 4:D:230:ILE:O    | 2.10                     | 0.51              |
| 3:3:101:ARG:NH1  | 3:3:140:TYR:HD1  | 2.05                     | 0.51              |
| 4:4:197:LEU:O    | 4:4:198:PRO:C    | 2.54                     | 0.51              |
| 6:6:138:PRO:HG2  | 7:9:121:MET:HG3  | 1.92                     | 0.51              |
| 3:C:261:VAL:HG21 | 9:C:786:SF4:S1   | 2.51                     | 0.51              |
| 4:D:40:VAL:HG23  | 6:F:88:MET:HE2   | 1.92                     | 0.51              |
| 8:H:15:GLU:O     | 8:H:18:SER:HB3   | 2.10                     | 0.51              |
| 3:3:344:TYR:CD1  | 3:3:568:TYR:CE1  | 2.99                     | 0.51              |
| 3:3:361:ALA:HB3  | 3:3:369:LEU:HD13 | 1.92                     | 0.51              |
| 4:4:44:MET:HA    | 4:4:44:MET:CE    | 2.41                     | 0.51              |
| 5:5:98:ASP:OD1   | 5:5:100:ARG:HD3  | 2.11                     | 0.51              |
| 5:5:157:THR:HG21 | 7:9:66:TYR:HB2   | 1.92                     | 0.51              |
| 4:D:213:ILE:HD12 | 4:D:213:ILE:H    | 1.76                     | 0.51              |
| 6:F:149:TYR:CE1  | 6:F:153:GLN:NE2  | 2.79                     | 0.51              |
| 3:3:192:GLU:HG3  | 3:3:193:GLU:HG3  | 1.93                     | 0.51              |
| 1:A:9:LEU:O      | 1:A:9:LEU:HG     | 2.10                     | 0.51              |
| 3:C:259:CYS:SG   | 3:C:261:VAL:HG22 | 2.51                     | 0.51              |
| 3:C:272:GLY:O    | 3:C:629:ILE:HA   | 2.11                     | 0.51              |
| 1:1:238:PHE:HE1  | 1:1:249:MET:HE1  | 1.75                     | 0.50              |
| 4:4:381:LEU:O    | 4:4:381:LEU:HG   | 2.11                     | 0.50              |
| 3:C:385:ALA:HB2  | 3:C:531:LYS:CB   | 2.40                     | 0.50              |
| 3:3:185:LYS:HB3  | 3:3:189:ARG:HD3  | 1.93                     | 0.50              |
| 3:3:357:ALA:HB2  | 3:3:641:LEU:HD11 | 1.92                     | 0.50              |
| 4:4:234:LEU:C    | 4:4:236:GLY:H    | 2.18                     | 0.50              |
| 4:4:249:ARG:HB2  | 4:4:262:PHE:HE2  | 1.76                     | 0.50              |
| 2:B:33:ARG:HH21  | 2:B:37:GLU:CG    | 2.24                     | 0.50              |
| 3:C:481:LEU:HD22 | 3:C:527:ARG:NH1  | 2.26                     | 0.50              |
| 4:D:234:LEU:C    | 4:D:236:GLY:H    | 2.19                     | 0.50              |
| 5:E:167:PRO:HB2  | 5:E:171:ARG:HH12 | 1.76                     | 0.50              |
| 1:1:291:ILE:O    | 1:1:328:VAL:HA   | 2.11                     | 0.50              |
| 1:1:323:LEU:C    | 1:1:323:LEU:CD2  | 2.84                     | 0.50              |
| 3:3:456:ALA:O    | 3:3:459:MET:HB2  | 2.11                     | 0.50              |
| 3:3:592:PRO:HA   | 3:3:595:GLU:HG2  | 1.93                     | 0.50              |
| 3:C:55:PRO:CD    | 3:C:74:GLN:N     | 2.75                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:136:GLU:CG   | 5:E:189:ARG:HG2  | 2.40                     | 0.50              |
| 3:3:337:ARG:HD3  | 3:3:340:GLU:HG3  | 1.93                     | 0.50              |
| 3:3:409:LEU:HD12 | 3:3:535:MET:HE2  | 1.93                     | 0.50              |
| 2:B:139:GLU:CB   | 2:B:140:PRO:HD2  | 2.41                     | 0.50              |
| 3:C:36:GLU:HG2   | 3:C:229:ILE:HG23 | 1.93                     | 0.50              |
| 3:C:360:LEU:HD13 | 3:C:645:ALA:CB   | 2.41                     | 0.50              |
| 3:C:368:HIS:CG   | 3:C:556:ALA:HB3  | 2.46                     | 0.50              |
| 1:1:359:CYS:HB3  | 9:1:439:SF4:S3   | 2.51                     | 0.50              |
| 4:4:64:THR:HB    | 4:4:66:PHE:CE1   | 2.46                     | 0.50              |
| 4:4:236:GLY:C    | 4:4:238:SER:N    | 2.65                     | 0.50              |
| 5:5:52:ILE:HG22  | 5:5:114:LEU:HB3  | 1.91                     | 0.50              |
| 3:C:550:LEU:HD21 | 3:C:680:LEU:HD11 | 1.93                     | 0.50              |
| 4:D:70:MET:HE3   | 4:D:81:TYR:HB3   | 1.94                     | 0.50              |
| 5:E:119:TYR:O    | 5:E:122:PHE:O    | 2.29                     | 0.50              |
| 3:3:168:HIS:C    | 3:3:168:HIS:CD2  | 2.89                     | 0.50              |
| 3:3:317:LEU:HD22 | 3:3:317:LEU:N    | 2.27                     | 0.50              |
| 3:3:570:PHE:O    | 3:3:585:MET:HE2  | 2.12                     | 0.50              |
| 4:4:59:ILE:HD11  | 5:5:135:ILE:HG23 | 1.93                     | 0.50              |
| 4:4:211:SER:HB2  | 4:4:214:PHE:HB3  | 1.92                     | 0.50              |
| 4:4:317:LEU:HD21 | 4:4:327:HIS:CD2  | 2.46                     | 0.50              |
| 6:6:49:GLU:OE1   | 6:6:49:GLU:HA    | 2.11                     | 0.50              |
| 8:7:16:LEU:O     | 8:7:20:MET:HG3   | 2.12                     | 0.50              |
| 3:C:451:PHE:HE1  | 3:C:466:GLU:HB3  | 1.75                     | 0.50              |
| 5:E:13:LYS:HZ3   | 5:E:33:ARG:HH21  | 1.60                     | 0.50              |
| 1:1:118:MET:HG2  | 1:1:224:LEU:HD13 | 1.92                     | 0.50              |
| 3:3:46:ARG:HG2   | 3:3:46:ARG:HH11  | 1.76                     | 0.50              |
| 3:3:169:PRO:HA   | 3:3:175:ILE:HA   | 1.94                     | 0.50              |
| 3:3:614:LEU:HD11 | 3:3:624:LEU:CD1  | 2.42                     | 0.50              |
| 6:6:77:VAL:O     | 6:6:77:VAL:HG12  | 2.10                     | 0.50              |
| 6:6:153:GLN:HG3  | 7:9:124:TYR:CZ   | 2.46                     | 0.50              |
| 1:A:233:ARG:O    | 1:A:237:TRP:HB3  | 2.12                     | 0.50              |
| 1:A:254:ILE:HD12 | 1:A:275:LEU:HD22 | 1.94                     | 0.50              |
| 1:A:367:MET:HE1  | 1:A:410:VAL:HG21 | 1.94                     | 0.50              |
| 3:C:113:LEU:HD11 | 3:C:157:PHE:CD1  | 2.46                     | 0.50              |
| 3:C:305:ARG:HG2  | 3:C:588:SER:O    | 2.11                     | 0.50              |
| 3:C:592:PRO:HA   | 3:C:595:GLU:HG2  | 1.93                     | 0.50              |
| 4:D:125:ARG:HD2  | 4:D:286:SER:OG   | 2.12                     | 0.50              |
| 1:1:145:LEU:O    | 1:1:149:ILE:HG13 | 2.12                     | 0.50              |
| 3:3:197:ASP:OD2  | 3:3:220:SER:HB2  | 2.12                     | 0.50              |
| 3:3:565:TYR:HD1  | 3:3:582:PHE:HB3  | 1.76                     | 0.50              |
| 3:3:594:ALA:O    | 3:3:598:ALA:HB3  | 2.10                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:84:ARG:CZ    | 6:6:117:MET:HE1  | 2.42                     | 0.50              |
| 6:6:104:TRP:CE2  | 6:6:173:VAL:HG22 | 2.46                     | 0.50              |
| 5:E:101:LEU:O    | 5:E:126:PHE:HA   | 2.12                     | 0.50              |
| 2:2:112:THR:OG1  | 2:2:113:PRO:HD2  | 2.12                     | 0.50              |
| 3:3:23:VAL:HG12  | 3:3:24:PHE:N     | 2.26                     | 0.50              |
| 3:3:112:LEU:CD2  | 3:3:130:LEU:HD21 | 2.42                     | 0.50              |
| 3:3:473:GLU:O    | 3:3:477:LEU:HD13 | 2.12                     | 0.50              |
| 2:B:27:ILE:HD13  | 2:B:60:VAL:HG22  | 1.93                     | 0.50              |
| 4:D:140:LEU:HD11 | 4:D:214:PHE:HB2  | 1.92                     | 0.50              |
| 8:H:16:LEU:O     | 8:H:20:MET:HG3   | 2.12                     | 0.50              |
| 1:1:367:MET:HE1  | 1:1:410:VAL:HG21 | 1.93                     | 0.49              |
| 2:2:33:ARG:HH21  | 2:2:37:GLU:CG    | 2.25                     | 0.49              |
| 3:3:515:THR:HG23 | 3:3:683:LEU:CD1  | 2.42                     | 0.49              |
| 3:3:689:LYS:HG3  | 3:3:771:VAL:CA   | 2.38                     | 0.49              |
| 4:4:185:GLU:O    | 4:4:189:GLU:HG2  | 2.12                     | 0.49              |
| 4:4:238:SER:HB2  | 4:4:275:ARG:HG2  | 1.94                     | 0.49              |
| 4:4:379:GLN:OE1  | 5:5:112:ASN:HB3  | 2.12                     | 0.49              |
| 7:9:40:ARG:NH1   | 7:9:41:HIS:O     | 2.45                     | 0.49              |
| 1:A:138:TYR:HB3  | 1:A:141:ALA:HB3  | 1.94                     | 0.49              |
| 1:A:391:LEU:N    | 1:A:392:PRO:HD2  | 2.27                     | 0.49              |
| 4:D:379:GLN:OE1  | 5:E:112:ASN:HB3  | 2.12                     | 0.49              |
| 3:3:229:ILE:HD11 | 3:3:289:TRP:HZ3  | 1.77                     | 0.49              |
| 3:3:734:VAL:HG12 | 3:3:736:VAL:HG23 | 1.94                     | 0.49              |
| 6:6:92:MET:HE1   | 6:6:127:VAL:HG13 | 1.94                     | 0.49              |
| 1:A:177:ALA:HB3  | 2:B:67:TYR:CG    | 2.47                     | 0.49              |
| 4:D:115:THR:O    | 4:D:118:VAL:HG22 | 2.12                     | 0.49              |
| 5:E:129:HIS:CD2  | 5:E:130:PRO:HD2  | 2.46                     | 0.49              |
| 1:1:350:HIS:O    | 3:3:205:ARG:NH1  | 2.45                     | 0.49              |
| 3:3:101:ARG:HB3  | 3:3:101:ARG:CZ   | 2.42                     | 0.49              |
| 3:3:272:GLY:O    | 3:3:629:ILE:HA   | 2.11                     | 0.49              |
| 3:3:472:GLU:O    | 3:3:476:ILE:HD12 | 2.12                     | 0.49              |
| 4:4:43:LEU:HD23  | 4:4:57:PRO:HA    | 1.94                     | 0.49              |
| 4:4:84:ARG:O     | 6:6:83:ARG:NH2   | 2.45                     | 0.49              |
| 5:5:123:GLY:H    | 5:5:147:ARG:HH11 | 1.60                     | 0.49              |
| 3:C:300:TRP:HB3  | 3:C:705:VAL:HG23 | 1.94                     | 0.49              |
| 3:C:546:ALA:C    | 3:C:547:MET:HE2  | 2.37                     | 0.49              |
| 3:3:29:ASP:OD2   | 5:5:187:GLY:N    | 2.38                     | 0.49              |
| 3:3:343:LEU:HB2  | 3:3:369:LEU:HB2  | 1.92                     | 0.49              |
| 3:3:550:LEU:HD21 | 3:3:680:LEU:HD11 | 1.93                     | 0.49              |
| 5:5:129:HIS:CD2  | 5:5:130:PRO:HD2  | 2.48                     | 0.49              |
| 5:5:135:ILE:HG22 | 5:5:136:LEU:HG   | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:233:GLY:HA2  | 5:E:48:PHE:CE1   | 2.48                     | 0.49              |
| 4:D:381:LEU:H    | 4:D:382:PRO:HD2  | 1.76                     | 0.49              |
| 6:F:154:LEU:O    | 6:F:158:VAL:HG13 | 2.12                     | 0.49              |
| 6:F:156:LYS:NZ   | 7:G:149:GLU:OE1  | 2.44                     | 0.49              |
| 7:G:99:ILE:O     | 7:G:100:PHE:HB2  | 2.11                     | 0.49              |
| 7:G:172:GLY:O    | 7:G:174:LYS:N    | 2.46                     | 0.49              |
| 1:1:97:GLU:O     | 1:1:100:SER:HB3  | 2.12                     | 0.49              |
| 1:1:246:SER:HB3  | 1:1:268:MET:CG   | 2.32                     | 0.49              |
| 4:4:99:LEU:O     | 4:4:103:LYS:HG2  | 2.13                     | 0.49              |
| 4:4:218:ALA:CB   | 4:4:272:VAL:HG22 | 2.43                     | 0.49              |
| 6:6:104:TRP:HB3  | 6:6:154:LEU:HD11 | 1.95                     | 0.49              |
| 8:7:68:LEU:C     | 8:7:68:LEU:HD13  | 2.38                     | 0.49              |
| 3:C:13:VAL:HG22  | 3:C:17:THR:OG1   | 2.13                     | 0.49              |
| 4:D:389:GLN:HG3  | 4:D:390:VAL:N    | 2.25                     | 0.49              |
| 5:E:40:HIS:NE2   | 5:E:44:MET:CE    | 2.75                     | 0.49              |
| 6:6:37:TRP:O     | 6:6:75:ALA:HB1   | 2.13                     | 0.49              |
| 1:A:188:LEU:HD23 | 1:A:188:LEU:O    | 2.12                     | 0.49              |
| 3:C:197:ASP:O    | 3:C:199:VAL:HG22 | 2.12                     | 0.49              |
| 5:E:25:LEU:N     | 5:E:25:LEU:CD2   | 2.76                     | 0.49              |
| 1:1:339:ASP:OD2  | 2:2:89:LYS:HE2   | 2.12                     | 0.49              |
| 3:3:55:PRO:HD3   | 3:3:74:GLN:N     | 2.23                     | 0.49              |
| 3:3:545:GLU:HA   | 3:3:550:LEU:HD11 | 1.95                     | 0.49              |
| 4:4:230:ILE:HG22 | 4:4:230:ILE:O    | 2.11                     | 0.49              |
| 4:4:346:THR:HG22 | 4:4:353:LEU:O    | 2.12                     | 0.49              |
| 5:5:20:ASN:ND2   | 5:5:26:TRP:HZ3   | 2.10                     | 0.49              |
| 1:A:339:ASP:OD2  | 2:B:89:LYS:HE2   | 2.13                     | 0.49              |
| 3:C:192:GLU:HG3  | 3:C:193:GLU:HG3  | 1.94                     | 0.49              |
| 4:D:294:LEU:O    | 4:D:294:LEU:HD23 | 2.13                     | 0.49              |
| 1:1:160:LYS:HG3  | 1:1:161:ASN:N    | 2.21                     | 0.49              |
| 3:3:368:HIS:CG   | 3:3:556:ALA:HB3  | 2.46                     | 0.49              |
| 5:5:101:LEU:O    | 5:5:126:PHE:HA   | 2.13                     | 0.49              |
| 3:C:440:ARG:HG2  | 3:C:440:ARG:NH1  | 2.06                     | 0.49              |
| 4:D:366:TYR:CZ   | 5:E:148:LYS:HE3  | 2.47                     | 0.49              |
| 1:1:185:GLU:HB2  | 1:1:218:ILE:CD1  | 2.41                     | 0.49              |
| 1:1:192:LEU:HD22 | 1:1:211:LEU:HD11 | 1.95                     | 0.49              |
| 1:1:331:ILE:HG21 | 1:1:337:MET:HE2  | 1.94                     | 0.49              |
| 3:3:202:PHE:HA   | 3:3:210:PHE:O    | 2.13                     | 0.49              |
| 6:6:82:GLY:HA2   | 9:6:182:SF4:S4   | 2.53                     | 0.49              |
| 3:C:124:LYS:HE3  | 3:C:128:CYS:HA   | 1.93                     | 0.49              |
| 4:D:190:LEU:O    | 4:D:194:LEU:HB2  | 2.13                     | 0.49              |
| 4:D:393:MET:C    | 4:D:396:ILE:HG22 | 2.37                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:108:ILE:N    | 8:H:108:ILE:HD12 | 2.27                     | 0.49              |
| 1:1:29:LEU:HD12  | 1:1:155:ARG:HG3  | 1.95                     | 0.49              |
| 1:1:32:TYR:OH    | 1:1:116:GLU:OE1  | 2.29                     | 0.49              |
| 2:2:116:LEU:HD23 | 2:2:116:LEU:H    | 1.78                     | 0.49              |
| 3:3:2:VAL:CG1    | 3:3:89:ASP:HA    | 2.39                     | 0.49              |
| 3:3:259:CYS:SG   | 3:3:261:VAL:HG22 | 2.53                     | 0.49              |
| 3:3:722:THR:CG2  | 3:3:755:LYS:HG3  | 2.42                     | 0.49              |
| 5:5:25:LEU:N     | 5:5:25:LEU:CD2   | 2.75                     | 0.49              |
| 1:A:331:ILE:HG21 | 1:A:337:MET:HE2  | 1.95                     | 0.49              |
| 1:A:342:TRP:HZ3  | 1:A:368:VAL:HG23 | 1.78                     | 0.49              |
| 2:B:112:THR:OG1  | 2:B:113:PRO:HD2  | 2.13                     | 0.49              |
| 3:C:168:HIS:C    | 3:C:168:HIS:CD2  | 2.91                     | 0.49              |
| 3:C:722:THR:CG2  | 3:C:755:LYS:HG3  | 2.42                     | 0.49              |
| 4:D:43:LEU:HD23  | 4:D:57:PRO:HA    | 1.94                     | 0.49              |
| 8:H:92:HIS:CD2   | 8:H:92:HIS:N     | 2.81                     | 0.49              |
| 1:1:177:ALA:O    | 2:2:67:TYR:HB3   | 2.13                     | 0.48              |
| 2:2:144:CYS:O    | 2:2:149:ARG:HD3  | 2.13                     | 0.48              |
| 3:3:34:CYS:HA    | 3:3:184:CYS:HB2  | 1.95                     | 0.48              |
| 3:3:225:ASN:ND2  | 3:3:289:TRP:HB3  | 2.28                     | 0.48              |
| 3:3:697:THR:HG21 | 3:3:761:SER:OG   | 2.12                     | 0.48              |
| 4:4:59:ILE:H     | 4:4:59:ILE:HD13  | 1.77                     | 0.48              |
| 4:4:363:SER:HB3  | 5:5:173:ALA:HB1  | 1.95                     | 0.48              |
| 1:A:29:LEU:HD12  | 1:A:155:ARG:HG3  | 1.95                     | 0.48              |
| 3:3:360:LEU:HD13 | 3:3:645:ALA:HB2  | 1.94                     | 0.48              |
| 4:4:125:ARG:HD2  | 4:4:286:SER:OG   | 2.14                     | 0.48              |
| 6:6:50:MET:HG3   | 6:6:108:MET:HE1  | 1.94                     | 0.48              |
| 7:9:101:CYS:SG   | 7:9:103:LEU:HD12 | 2.53                     | 0.48              |
| 3:C:185:LYS:HG3  | 3:C:202:PHE:HE2  | 1.78                     | 0.48              |
| 3:C:229:ILE:O    | 3:C:230:CYS:C    | 2.55                     | 0.48              |
| 4:D:64:THR:OG1   | 6:F:83:ARG:NH1   | 2.45                     | 0.48              |
| 1:1:128:THR:O    | 1:1:169:PHE:HA   | 2.12                     | 0.48              |
| 2:2:21:GLU:O     | 2:2:21:GLU:HG2   | 2.14                     | 0.48              |
| 3:3:101:ARG:HB3  | 3:3:101:ARG:HH11 | 1.77                     | 0.48              |
| 3:3:160:THR:OG1  | 8:7:73:SER:CB    | 2.60                     | 0.48              |
| 3:3:684:ARG:HG2  | 3:3:684:ARG:NH1  | 2.28                     | 0.48              |
| 4:4:64:THR:OG1   | 6:6:83:ARG:NH1   | 2.46                     | 0.48              |
| 4:4:381:LEU:H    | 4:4:382:PRO:CD   | 2.26                     | 0.48              |
| 5:5:145:PRO:HA   | 5:5:150:TYR:CD2  | 2.47                     | 0.48              |
| 1:A:188:LEU:HD23 | 1:A:188:LEU:C    | 2.38                     | 0.48              |
| 3:C:268:ASP:OD2  | 3:C:278:ARG:NH1  | 2.46                     | 0.48              |
| 3:C:352:GLU:HG3  | 3:C:664:LEU:CD1  | 2.42                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:646:GLU:C    | 3:C:648:LEU:H    | 2.21                     | 0.48              |
| 3:C:689:LYS:HG3  | 3:C:771:VAL:CA   | 2.37                     | 0.48              |
| 6:F:83:ARG:HG3   | 6:F:83:ARG:NH1   | 2.27                     | 0.48              |
| 6:F:106:ILE:CD1  | 6:F:151:VAL:HG12 | 2.43                     | 0.48              |
| 1:1:272:PHE:CD1  | 1:1:311:MET:HG2  | 2.47                     | 0.48              |
| 2:2:38:GLU:OE2   | 2:2:45:ARG:NH1   | 2.47                     | 0.48              |
| 4:4:47:LEU:HD13  | 4:4:52:VAL:CA    | 2.42                     | 0.48              |
| 4:4:84:ARG:NE    | 6:6:117:MET:HE1  | 2.29                     | 0.48              |
| 4:4:389:GLN:HG3  | 4:4:390:VAL:N    | 2.26                     | 0.48              |
| 5:5:13:LYS:HZ3   | 5:5:33:ARG:HH21  | 1.61                     | 0.48              |
| 1:A:341:MET:HE2  | 1:A:409:PRO:O    | 2.13                     | 0.48              |
| 2:B:116:LEU:HD23 | 2:B:116:LEU:H    | 1.78                     | 0.48              |
| 3:C:31:PRO:HD3   | 3:C:137:TYR:CE2  | 2.49                     | 0.48              |
| 3:C:34:CYS:HA    | 3:C:184:CYS:HB2  | 1.96                     | 0.48              |
| 3:C:473:GLU:O    | 3:C:477:LEU:HD13 | 2.14                     | 0.48              |
| 5:E:20:ASN:ND2   | 5:E:26:TRP:HZ3   | 2.11                     | 0.48              |
| 3:3:31:PRO:HG3   | 3:3:137:TYR:CG   | 2.48                     | 0.48              |
| 3:3:113:LEU:HD11 | 3:3:157:PHE:CD1  | 2.49                     | 0.48              |
| 3:3:522:ARG:O    | 3:3:526:GLU:HG3  | 2.14                     | 0.48              |
| 3:3:646:GLU:C    | 3:3:648:LEU:H    | 2.22                     | 0.48              |
| 4:4:205:GLU:OE1  | 4:4:284:ARG:NH2  | 2.47                     | 0.48              |
| 5:5:59:THR:O     | 5:5:59:THR:HG22  | 2.13                     | 0.48              |
| 1:A:160:LYS:HG3  | 1:A:161:ASN:N    | 2.24                     | 0.48              |
| 3:C:101:ARG:NH1  | 3:C:140:TYR:CE1  | 2.81                     | 0.48              |
| 3:C:469:ARG:HG2  | 3:C:469:ARG:HH11 | 1.78                     | 0.48              |
| 6:F:130:VAL:HG23 | 6:F:131:VAL:HG13 | 1.95                     | 0.48              |
| 1:1:395:GLU:O    | 1:1:396:GLY:C    | 2.56                     | 0.48              |
| 3:3:616:ASN:ND2  | 3:3:622:LEU:HD11 | 2.29                     | 0.48              |
| 4:4:366:TYR:CZ   | 5:5:148:LYS:HE3  | 2.49                     | 0.48              |
| 6:6:158:VAL:HA   | 6:6:172:PRO:HB3  | 1.95                     | 0.48              |
| 8:7:68:LEU:HD13  | 8:7:69:LEU:N     | 2.29                     | 0.48              |
| 1:A:185:GLU:HB2  | 1:A:218:ILE:CD1  | 2.42                     | 0.48              |
| 1:A:211:LEU:H    | 1:A:216:THR:HG21 | 1.78                     | 0.48              |
| 8:H:108:ILE:HG22 | 8:H:114:ARG:NH1  | 2.28                     | 0.48              |
| 1:1:427:GLU:O    | 1:1:428:LYS:C    | 2.57                     | 0.48              |
| 4:4:213:ILE:HD12 | 4:4:213:ILE:H    | 1.78                     | 0.48              |
| 6:6:37:TRP:CD1   | 6:6:75:ALA:HB2   | 2.49                     | 0.48              |
| 1:A:291:ILE:HD11 | 1:A:331:ILE:HD11 | 1.96                     | 0.48              |
| 3:C:116:PRO:HG3  | 3:C:180:ARG:HG2  | 1.96                     | 0.48              |
| 3:C:169:PRO:HA   | 3:C:175:ILE:HA   | 1.96                     | 0.48              |
| 3:C:515:THR:HG23 | 3:C:683:LEU:HD12 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:614:LEU:HD11 | 3:C:624:LEU:CD1  | 2.43                     | 0.48              |
| 3:C:697:THR:OG1  | 3:C:763:LEU:HD23 | 2.13                     | 0.48              |
| 4:D:47:LEU:HD13  | 4:D:52:VAL:CA    | 2.43                     | 0.48              |
| 1:1:81:LYS:HA    | 1:1:81:LYS:HE3   | 1.96                     | 0.48              |
| 1:1:114:LEU:O    | 1:1:118:MET:HG3  | 2.13                     | 0.48              |
| 4:4:83:PRO:HD3   | 4:4:94:ASP:OD1   | 2.13                     | 0.48              |
| 5:5:20:ASN:HD22  | 5:5:26:TRP:HZ3   | 1.62                     | 0.48              |
| 6:6:156:LYS:NZ   | 7:9:149:GLU:OE1  | 2.46                     | 0.48              |
| 1:A:283:PRO:HB3  | 1:A:287:ILE:CD1  | 2.44                     | 0.48              |
| 2:B:145:VAL:HG12 | 2:B:150:LEU:HB2  | 1.96                     | 0.48              |
| 3:C:202:PHE:HA   | 3:C:210:PHE:O    | 2.13                     | 0.48              |
| 3:C:413:LEU:HD13 | 3:C:448:MET:CE   | 2.39                     | 0.48              |
| 4:D:215:TYR:O    | 4:D:219:ARG:HB2  | 2.14                     | 0.48              |
| 5:E:52:ILE:HG22  | 5:E:114:LEU:HB3  | 1.91                     | 0.48              |
| 5:E:75:VAL:HG12  | 5:E:76:SER:H     | 1.77                     | 0.48              |
| 7:G:35:PRO:HD3   | 7:G:164:PRO:CG   | 2.44                     | 0.48              |
| 1:1:342:TRP:O    | 1:1:342:TRP:HE3  | 1.96                     | 0.48              |
| 4:4:350:ARG:O    | 4:4:373:PRO:HB2  | 2.14                     | 0.48              |
| 1:A:63:ARG:HD3   | 1:A:313:TYR:CD2  | 2.48                     | 0.48              |
| 3:C:6:VAL:HG12   | 3:C:7:ASN:N      | 2.29                     | 0.48              |
| 3:3:652:PRO:HA   | 3:3:653:PRO:HD3  | 1.75                     | 0.48              |
| 4:4:101:VAL:O    | 4:4:104:LEU:N    | 2.47                     | 0.48              |
| 7:9:172:GLY:O    | 7:9:174:LYS:N    | 2.47                     | 0.48              |
| 1:A:400:CYS:HB2  | 1:A:401:PRO:HD2  | 1.96                     | 0.48              |
| 4:D:138:LEU:HD11 | 4:D:146:PHE:CD1  | 2.49                     | 0.48              |
| 1:1:301:PRO:HB2  | 1:1:303:THR:CG2  | 2.44                     | 0.47              |
| 2:2:7:LYS:O      | 2:2:7:LYS:HG2    | 2.12                     | 0.47              |
| 1:A:114:LEU:O    | 1:A:118:MET:HG3  | 2.14                     | 0.47              |
| 3:C:33:PHE:CZ    | 3:C:130:LEU:HD12 | 2.49                     | 0.47              |
| 3:C:200:LEU:HD12 | 3:C:212:GLY:O    | 2.13                     | 0.47              |
| 1:1:283:PRO:HB3  | 1:1:287:ILE:CD1  | 2.43                     | 0.47              |
| 3:3:360:LEU:HD13 | 3:3:645:ALA:CB   | 2.44                     | 0.47              |
| 3:3:688:ARG:HD3  | 3:3:688:ARG:HA   | 1.71                     | 0.47              |
| 4:4:115:THR:O    | 4:4:118:VAL:HG22 | 2.14                     | 0.47              |
| 5:5:2:ARG:HG3    | 5:5:84:ASP:CG    | 2.39                     | 0.47              |
| 1:A:259:LYS:HB3  | 1:A:280:ALA:O    | 2.14                     | 0.47              |
| 3:C:50:VAL:HG12  | 3:C:95:THR:HG22  | 1.96                     | 0.47              |
| 3:C:240:ALA:CB   | 3:C:276:ARG:HB2  | 2.44                     | 0.47              |
| 6:F:82:GLY:HA2   | 9:F:182:SF4:S4   | 2.54                     | 0.47              |
| 8:H:81:ARG:O     | 8:H:81:ARG:HD3   | 2.13                     | 0.47              |
| 1:1:358:PRO:O    | 1:1:362:GLY:CA   | 2.52                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:344:TYR:HD1  | 3:3:568:TYR:CE1  | 2.31                     | 0.47              |
| 3:3:478:LEU:HD12 | 3:3:520:ARG:CZ   | 2.44                     | 0.47              |
| 3:3:478:LEU:HD12 | 3:3:520:ARG:NH2  | 2.29                     | 0.47              |
| 5:5:40:HIS:NE2   | 5:5:44:MET:CE    | 2.77                     | 0.47              |
| 3:C:101:ARG:HB3  | 3:C:101:ARG:CZ   | 2.44                     | 0.47              |
| 4:D:197:LEU:N    | 4:D:198:PRO:CD   | 2.77                     | 0.47              |
| 6:F:23:THR:O     | 6:F:23:THR:HG22  | 2.13                     | 0.47              |
| 3:3:214:MET:O    | 3:3:216:PHE:CE1  | 2.67                     | 0.47              |
| 4:4:212:PRO:CG   | 4:4:213:ILE:HD12 | 2.41                     | 0.47              |
| 6:6:149:TYR:CE1  | 6:6:153:GLN:NE2  | 2.81                     | 0.47              |
| 4:D:64:THR:CG2   | 6:F:118:PHE:CD1  | 2.97                     | 0.47              |
| 5:E:20:ASN:HD22  | 5:E:26:TRP:HZ3   | 1.62                     | 0.47              |
| 7:G:100:PHE:HA   | 9:G:183:SF4:S4   | 2.54                     | 0.47              |
| 1:1:239:ALA:C    | 1:1:241:MET:H    | 2.23                     | 0.47              |
| 3:3:31:PRO:HD3   | 3:3:137:TYR:CZ   | 2.49                     | 0.47              |
| 4:4:88:LEU:HD12  | 4:4:403:VAL:CG2  | 2.44                     | 0.47              |
| 4:4:233:GLY:HA2  | 5:5:48:PHE:CE1   | 2.49                     | 0.47              |
| 7:9:35:PRO:HD3   | 7:9:164:PRO:CG   | 2.45                     | 0.47              |
| 3:C:384:PRO:HG3  | 3:C:542:ARG:HE   | 1.80                     | 0.47              |
| 3:C:478:LEU:HD12 | 3:C:520:ARG:CZ   | 2.44                     | 0.47              |
| 3:C:689:LYS:CG   | 3:C:771:VAL:HA   | 2.38                     | 0.47              |
| 4:D:99:LEU:HA    | 4:D:99:LEU:HD13  | 1.54                     | 0.47              |
| 6:F:78:MET:HE2   | 6:F:99:MET:HE1   | 1.95                     | 0.47              |
| 1:1:188:LEU:HD23 | 1:1:188:LEU:C    | 2.40                     | 0.47              |
| 1:1:273:ARG:HB2  | 1:1:307:LEU:O    | 2.15                     | 0.47              |
| 4:4:187:VAL:HB   | 4:4:188:PRO:CD   | 2.45                     | 0.47              |
| 5:5:81:LYS:HB2   | 5:5:82:ASP:H     | 1.58                     | 0.47              |
| 3:C:29:ASP:OD1   | 3:C:29:ASP:N     | 2.47                     | 0.47              |
| 3:C:426:TYR:N    | 3:C:426:TYR:CD1  | 2.83                     | 0.47              |
| 4:D:221:VAL:HG23 | 4:D:272:VAL:CG1  | 2.45                     | 0.47              |
| 6:F:78:MET:CE    | 6:F:99:MET:HE1   | 2.45                     | 0.47              |
| 1:1:254:ILE:HD12 | 1:1:275:LEU:HD22 | 1.96                     | 0.47              |
| 1:1:342:TRP:HZ3  | 1:1:368:VAL:HG23 | 1.78                     | 0.47              |
| 1:1:400:CYS:HB2  | 1:1:401:PRO:HD2  | 1.96                     | 0.47              |
| 2:2:86:LEU:HD11  | 2:2:90:LEU:HD11  | 1.96                     | 0.47              |
| 3:3:49:LEU:HA    | 3:3:80:ALA:O     | 2.15                     | 0.47              |
| 3:3:105:ALA:CB   | 3:3:140:TYR:HB2  | 2.43                     | 0.47              |
| 3:3:185:LYS:HG3  | 3:3:202:PHE:HE2  | 1.79                     | 0.47              |
| 3:3:274:LEU:HD12 | 3:3:275:LEU:N    | 2.30                     | 0.47              |
| 3:3:300:TRP:HB3  | 3:3:705:VAL:HG23 | 1.95                     | 0.47              |
| 3:3:337:ARG:CD   | 3:3:340:GLU:HG3  | 2.45                     | 0.47              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 6:6:92:MET:O    | 6:6:92:MET:HG2   | 2.14                     | 0.47              |
| 1:A:427:GLU:O   | 1:A:428:LYS:C    | 2.57                     | 0.47              |
| 3:C:471:GLY:HA2 | 3:C:473:GLU:OE2  | 2.15                     | 0.47              |
| 4:D:106:GLY:O   | 5:E:194:SER:HB3  | 2.14                     | 0.47              |
| 4:D:218:ALA:CB  | 4:D:272:VAL:HG22 | 2.42                     | 0.47              |
| 4:D:304:ASP:HA  | 4:D:305:PRO:HD2  | 1.78                     | 0.47              |
| 1:1:83:ASP:OD1  | 1:1:83:ASP:N     | 2.48                     | 0.47              |
| 3:3:672:ALA:O   | 3:3:673:MET:HB2  | 2.15                     | 0.47              |
| 3:3:694:LEU:HB3 | 3:3:762:ALA:CB   | 2.42                     | 0.47              |
| 5:5:72:TYR:O    | 5:5:89:PHE:HA    | 2.15                     | 0.47              |
| 6:6:99:MET:CG   | 6:6:100:PRO:HD2  | 2.42                     | 0.47              |
| 1:A:332:PRO:HD2 | 2:B:90:LEU:CD2   | 2.44                     | 0.47              |
| 4:D:40:VAL:O    | 4:D:40:VAL:CG2   | 2.63                     | 0.47              |
| 1:1:92:ASN:ND2  | 10:1:440:FMN:C2  | 2.77                     | 0.47              |
| 2:2:77:LYS:HE3  | 2:2:78:TYR:CZ    | 2.50                     | 0.47              |
| 5:5:44:MET:HE3  | 5:5:44:MET:HB2   | 1.84                     | 0.47              |
| 6:6:115:GLY:HA3 | 6:6:125:GLN:OE1  | 2.15                     | 0.47              |
| 1:A:81:LYS:HA   | 1:A:81:LYS:HE3   | 1.96                     | 0.47              |
| 1:A:145:LEU:O   | 1:A:149:ILE:HG13 | 2.15                     | 0.47              |
| 1:A:342:TRP:O   | 1:A:342:TRP:HE3  | 1.97                     | 0.47              |
| 2:B:79:HIS:ND1  | 2:B:118:SER:HB2  | 2.29                     | 0.47              |
| 3:C:11:VAL:CG1  | 3:C:25:HIS:CD2   | 2.93                     | 0.47              |
| 3:C:567:TYR:HE1 | 3:C:586:HIS:HB2  | 1.80                     | 0.47              |
| 5:E:2:ARG:HG3   | 5:E:84:ASP:CG    | 2.38                     | 0.47              |
| 1:1:259:LYS:HB3 | 1:1:280:ALA:O    | 2.15                     | 0.47              |
| 3:3:309:PRO:HA  | 3:3:603:PRO:CD   | 2.45                     | 0.47              |
| 3:3:586:HIS:CE1 | 3:3:640:VAL:HG21 | 2.50                     | 0.47              |
| 1:A:272:PHE:HB3 | 1:A:276:ILE:HD11 | 1.97                     | 0.47              |
| 1:A:323:LEU:C   | 1:A:323:LEU:CD2  | 2.88                     | 0.47              |
| 3:C:20:MET:SD   | 3:C:32:LEU:CD2   | 3.03                     | 0.47              |
| 3:C:115:HIS:C   | 4:D:321:MET:HE3  | 2.39                     | 0.47              |
| 3:C:346:ALA:HA  | 3:C:372:GLN:HB2  | 1.96                     | 0.47              |
| 6:F:36:LEU:HD22 | 6:F:77:VAL:HG21  | 1.97                     | 0.47              |
| 3:3:697:THR:OG1 | 3:3:763:LEU:HD23 | 2.15                     | 0.46              |
| 6:6:23:THR:O    | 6:6:23:THR:HG22  | 2.14                     | 0.46              |
| 6:6:36:LEU:HD22 | 6:6:77:VAL:HG21  | 1.96                     | 0.46              |
| 1:A:272:PHE:CD2 | 1:A:311:MET:HE3  | 2.50                     | 0.46              |
| 3:C:55:PRO:HG3  | 3:C:74:GLN:CB    | 2.45                     | 0.46              |
| 3:C:185:LYS:HB3 | 3:C:189:ARG:HD3  | 1.97                     | 0.46              |
| 5:E:161:GLU:CG  | 5:E:163:ARG:NH2  | 2.70                     | 0.46              |
| 6:F:138:PRO:CG  | 7:G:121:MET:HG3  | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:163:TYR:CE1  | 7:G:152:ARG:HD2  | 2.50                     | 0.46              |
| 1:1:132:ILE:HG22 | 1:1:134:VAL:HG12 | 1.98                     | 0.46              |
| 3:3:47:MET:HE1   | 3:3:108:VAL:HA   | 1.96                     | 0.46              |
| 3:3:229:ILE:HD11 | 3:3:289:TRP:CZ3  | 2.49                     | 0.46              |
| 3:3:329:LEU:CD1  | 3:3:584:VAL:HG11 | 2.45                     | 0.46              |
| 3:3:474:ARG:HA   | 3:3:517:ALA:HB2  | 1.96                     | 0.46              |
| 4:4:138:LEU:HD11 | 4:4:146:PHE:CD1  | 2.50                     | 0.46              |
| 5:5:54:GLY:C     | 5:5:55:LEU:HD12  | 2.40                     | 0.46              |
| 1:A:193:GLU:HG3  | 1:A:212:TRP:NE1  | 2.30                     | 0.46              |
| 3:C:11:VAL:HG21  | 3:C:26:ALA:HB2   | 1.97                     | 0.46              |
| 3:C:237:ASP:CG   | 3:C:239:THR:HG22 | 2.41                     | 0.46              |
| 3:C:478:LEU:CD2  | 3:C:483:ASP:HB2  | 2.45                     | 0.46              |
| 5:E:123:GLY:H    | 5:E:147:ARG:HH11 | 1.63                     | 0.46              |
| 6:F:140:CYS:SG   | 7:G:99:ILE:HG13  | 2.55                     | 0.46              |
| 1:1:6:LEU:HD12   | 1:1:240:GLN:O    | 2.14                     | 0.46              |
| 1:1:135:ARG:C    | 1:1:137:GLU:H    | 2.24                     | 0.46              |
| 1:1:301:PRO:O    | 1:1:306:VAL:HG21 | 2.15                     | 0.46              |
| 3:3:33:PHE:HB2   | 3:3:45:CYS:SG    | 2.56                     | 0.46              |
| 3:3:602:LEU:HD12 | 3:3:602:LEU:N    | 2.31                     | 0.46              |
| 1:A:301:PRO:O    | 1:A:306:VAL:HG21 | 2.15                     | 0.46              |
| 3:C:240:ALA:HB2  | 3:C:276:ARG:HB2  | 1.98                     | 0.46              |
| 3:C:258:LEU:O    | 3:C:700:LYS:HE2  | 2.16                     | 0.46              |
| 3:C:260:PRO:HG3  | 3:C:536:THR:O    | 2.16                     | 0.46              |
| 3:C:592:PRO:HA   | 3:C:595:GLU:OE2  | 2.16                     | 0.46              |
| 3:C:594:ALA:C    | 3:C:596:ARG:H    | 2.23                     | 0.46              |
| 4:D:100:ALA:O    | 4:D:342:VAL:HG11 | 2.15                     | 0.46              |
| 4:D:250:LYS:HE2  | 4:D:262:PHE:CD2  | 2.50                     | 0.46              |
| 6:F:16:ARG:HG2   | 6:F:21:PHE:HE2   | 1.80                     | 0.46              |
| 8:H:29:VAL:HG22  | 8:H:60:SER:O     | 2.15                     | 0.46              |
| 2:2:179:VAL:HG12 | 2:2:180:GLU:N    | 2.29                     | 0.46              |
| 3:3:272:GLY:HA2  | 3:3:628:PRO:O    | 2.16                     | 0.46              |
| 8:H:68:LEU:HD13  | 8:H:69:LEU:N     | 2.30                     | 0.46              |
| 4:4:70:MET:C     | 4:4:72:HIS:H     | 2.23                     | 0.46              |
| 8:7:29:VAL:HG22  | 8:7:60:SER:O     | 2.16                     | 0.46              |
| 1:A:17:LEU:HD12  | 1:A:251:LEU:CD1  | 2.44                     | 0.46              |
| 1:A:291:ILE:HA   | 1:A:292:PRO:HD2  | 1.64                     | 0.46              |
| 3:C:478:LEU:HD12 | 3:C:520:ARG:NH2  | 2.31                     | 0.46              |
| 4:D:163:VAL:HG13 | 4:D:164:THR:HG23 | 1.98                     | 0.46              |
| 6:F:78:MET:O     | 6:F:78:MET:HG3   | 2.14                     | 0.46              |
| 7:G:41:HIS:CD2   | 7:G:115:LEU:HD21 | 2.51                     | 0.46              |
| 1:1:63:ARG:HD3   | 1:1:313:TYR:CD2  | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:241:ALA:HA   | 4:4:278:VAL:HG21 | 1.98                     | 0.46              |
| 5:5:150:TYR:HA   | 5:5:151:PRO:HD3  | 1.77                     | 0.46              |
| 6:6:16:ARG:NH1   | 6:6:17:GLU:OE2   | 2.48                     | 0.46              |
| 2:B:7:LYS:O      | 2:B:7:LYS:HG2    | 2.14                     | 0.46              |
| 3:C:186:ARG:CD   | 3:C:231:PRO:HD3  | 2.37                     | 0.46              |
| 3:C:272:GLY:HA2  | 3:C:628:PRO:O    | 2.15                     | 0.46              |
| 3:C:280:ARG:O    | 3:C:282:VAL:HG12 | 2.15                     | 0.46              |
| 3:C:281:GLU:HG3  | 3:C:283:PRO:HD3  | 1.96                     | 0.46              |
| 4:D:83:PRO:HD3   | 4:D:94:ASP:OD1   | 2.15                     | 0.46              |
| 4:D:187:VAL:HB   | 4:D:188:PRO:CD   | 2.45                     | 0.46              |
| 4:D:241:ALA:HA   | 4:D:278:VAL:HG21 | 1.98                     | 0.46              |
| 3:3:270:ARG:HH11 | 3:3:270:ARG:HG3  | 1.81                     | 0.46              |
| 4:4:84:ARG:HG2   | 9:6:182:SF4:S2   | 2.56                     | 0.46              |
| 4:4:215:TYR:O    | 4:4:219:ARG:HB2  | 2.15                     | 0.46              |
| 5:5:53:VAL:HG22  | 5:5:55:LEU:CD1   | 2.46                     | 0.46              |
| 6:6:78:MET:HE2   | 6:6:99:MET:HE1   | 1.97                     | 0.46              |
| 1:A:332:PRO:HD2  | 2:B:90:LEU:HD23  | 1.98                     | 0.46              |
| 1:A:436:LEU:HD23 | 2:B:90:LEU:HA    | 1.98                     | 0.46              |
| 2:B:179:VAL:HG12 | 2:B:180:GLU:N    | 2.30                     | 0.46              |
| 3:C:329:LEU:CD1  | 3:C:584:VAL:HG11 | 2.46                     | 0.46              |
| 3:C:515:THR:HG23 | 3:C:683:LEU:CD1  | 2.46                     | 0.46              |
| 3:C:672:ALA:O    | 3:C:673:MET:HB2  | 2.15                     | 0.46              |
| 5:E:157:THR:HG21 | 7:G:66:TYR:HB2   | 1.98                     | 0.46              |
| 6:F:145:GLU:HG2  | 7:G:31:VAL:CG2   | 2.32                     | 0.46              |
| 3:3:346:ALA:HA   | 3:3:372:GLN:HB2  | 1.98                     | 0.46              |
| 8:7:73:SER:OG    | 8:7:80:LYS:HA    | 2.16                     | 0.46              |
| 2:B:33:ARG:HH21  | 2:B:37:GLU:HG3   | 1.81                     | 0.46              |
| 3:C:230:CYS:HA   | 9:C:785:SF4:S2   | 2.56                     | 0.46              |
| 3:C:356:LEU:HD13 | 3:C:654:PHE:CD1  | 2.48                     | 0.46              |
| 3:C:716:LEU:CD2  | 3:C:758:LEU:HB3  | 2.45                     | 0.46              |
| 4:D:233:GLY:CA   | 5:E:48:PHE:HE1   | 2.28                     | 0.46              |
| 4:D:367:ARG:CG   | 4:D:367:ARG:NH1  | 2.69                     | 0.46              |
| 8:H:121:ARG:NH1  | 8:H:121:ARG:CG   | 2.77                     | 0.46              |
| 1:1:233:ARG:O    | 1:1:237:TRP:HB3  | 2.16                     | 0.46              |
| 1:1:291:ILE:HD11 | 1:1:331:ILE:HD11 | 1.97                     | 0.46              |
| 2:2:109:GLY:CA   | 8:7:91:ILE:HD13  | 2.44                     | 0.46              |
| 3:3:205:ARG:HA   | 3:3:209:THR:CG2  | 2.43                     | 0.46              |
| 3:3:426:TYR:N    | 3:3:426:TYR:CD1  | 2.83                     | 0.46              |
| 3:3:478:LEU:CD2  | 3:3:483:ASP:HB2  | 2.45                     | 0.46              |
| 5:5:132:LEU:HA   | 5:5:132:LEU:HD23 | 1.58                     | 0.46              |
| 7:9:99:ILE:HD12  | 7:9:99:ILE:HA    | 1.85                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:114:ASP:HB2  | 2:B:116:LEU:CD2  | 2.45                     | 0.46              |
| 3:C:394:ASP:OD2  | 3:C:502:ASN:N    | 2.49                     | 0.46              |
| 4:D:62:LEU:CD1   | 6:F:44:ALA:HB2   | 2.46                     | 0.46              |
| 4:D:108:VAL:HG23 | 4:D:108:VAL:O    | 2.16                     | 0.46              |
| 4:D:381:LEU:H    | 4:D:382:PRO:CD   | 2.28                     | 0.46              |
| 1:1:18:TYR:CZ    | 1:1:263:VAL:HG11 | 2.51                     | 0.46              |
| 2:2:145:VAL:HG12 | 2:2:150:LEU:HB2  | 1.98                     | 0.46              |
| 3:3:402:PRO:CB   | 3:3:535:MET:HE1  | 2.46                     | 0.46              |
| 6:6:100:PRO:O    | 6:6:103:LYS:HD3  | 2.16                     | 0.46              |
| 1:A:239:ALA:C    | 1:A:241:MET:H    | 2.24                     | 0.46              |
| 1:A:341:MET:HE1  | 1:A:409:PRO:CB   | 2.41                     | 0.46              |
| 3:C:47:MET:HE1   | 3:C:108:VAL:HA   | 1.97                     | 0.46              |
| 5:E:161:GLU:HG3  | 5:E:163:ARG:CZ   | 2.43                     | 0.46              |
| 1:1:132:ILE:HG21 | 1:1:145:LEU:HD11 | 1.96                     | 0.45              |
| 3:3:13:VAL:HG22  | 3:3:17:THR:OG1   | 2.15                     | 0.45              |
| 3:3:184:CYS:SG   | 3:3:186:ARG:HB2  | 2.56                     | 0.45              |
| 3:3:460:LYS:HB2  | 3:3:460:LYS:HE2  | 1.84                     | 0.45              |
| 3:3:550:LEU:N    | 3:3:550:LEU:CD1  | 2.79                     | 0.45              |
| 4:4:99:LEU:HA    | 4:4:99:LEU:HD13  | 1.55                     | 0.45              |
| 4:4:108:VAL:O    | 4:4:110:PRO:HD3  | 2.16                     | 0.45              |
| 6:6:163:TYR:CE1  | 7:9:152:ARG:HD2  | 2.51                     | 0.45              |
| 1:A:89:LEU:HD21  | 1:A:121:ALA:HB3  | 1.98                     | 0.45              |
| 1:A:357:THR:N    | 1:A:358:PRO:HD2  | 2.30                     | 0.45              |
| 3:C:29:ASP:OD2   | 5:E:187:GLY:N    | 2.46                     | 0.45              |
| 3:C:101:ARG:NH1  | 3:C:140:TYR:HD1  | 2.10                     | 0.45              |
| 4:D:182:LEU:HD22 | 4:D:186:PHE:CD2  | 2.51                     | 0.45              |
| 5:E:44:MET:HE3   | 5:E:44:MET:HB2   | 1.84                     | 0.45              |
| 6:F:50:MET:HG3   | 6:F:108:MET:HE1  | 1.98                     | 0.45              |
| 2:2:79:HIS:ND1   | 2:2:118:SER:HB2  | 2.31                     | 0.45              |
| 2:2:81:GLN:HB3   | 2:2:122:VAL:HG21 | 1.98                     | 0.45              |
| 3:3:227:THR:HG21 | 3:3:237:ASP:HB2  | 1.97                     | 0.45              |
| 3:3:256:CYS:HB2  | 3:3:265:ILE:HD13 | 1.98                     | 0.45              |
| 3:3:440:ARG:HG2  | 3:3:440:ARG:NH1  | 2.03                     | 0.45              |
| 3:3:459:MET:HG2  | 3:3:465:HIS:CB   | 2.42                     | 0.45              |
| 5:5:144:HIS:HA   | 5:5:145:PRO:HD2  | 1.86                     | 0.45              |
| 1:A:17:LEU:C     | 1:A:19:ALA:H     | 2.25                     | 0.45              |
| 1:A:135:ARG:C    | 1:A:137:GLU:H    | 2.24                     | 0.45              |
| 1:A:273:ARG:HB2  | 1:A:307:LEU:O    | 2.16                     | 0.45              |
| 3:C:36:GLU:O     | 3:C:37:LYS:C     | 2.59                     | 0.45              |
| 3:C:259:CYS:CB   | 3:C:260:PRO:CD   | 2.94                     | 0.45              |
| 2:2:33:ARG:HH21  | 2:2:37:GLU:HG3   | 1.80                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:55:PRO:CD    | 3:3:74:GLN:H     | 2.24                     | 0.45              |
| 4:4:91:PHE:CE1   | 4:4:120:LEU:HD12 | 2.51                     | 0.45              |
| 8:7:84:LEU:HB2   | 8:7:93:LEU:HB2   | 1.98                     | 0.45              |
| 1:A:272:PHE:CD1  | 1:A:311:MET:HG2  | 2.51                     | 0.45              |
| 1:A:392:PRO:O    | 1:A:397:ARG:NH1  | 2.50                     | 0.45              |
| 3:C:497:TRP:O    | 3:C:528:LYS:HE3  | 2.16                     | 0.45              |
| 3:C:571:VAL:HG11 | 3:C:591:HIS:CD2  | 2.51                     | 0.45              |
| 3:C:697:THR:HG21 | 3:C:761:SER:OG   | 2.16                     | 0.45              |
| 4:D:51:GLU:O     | 4:D:52:VAL:HG23  | 2.17                     | 0.45              |
| 6:F:104:TRP:NE1  | 6:F:173:VAL:HG22 | 2.32                     | 0.45              |
| 1:1:398:SER:HA   | 3:3:46:ARG:CD    | 2.47                     | 0.45              |
| 3:3:469:ARG:HG2  | 3:3:469:ARG:HH11 | 1.81                     | 0.45              |
| 4:4:40:VAL:HG23  | 6:6:88:MET:CE    | 2.46                     | 0.45              |
| 4:4:190:LEU:O    | 4:4:194:LEU:HB2  | 2.16                     | 0.45              |
| 4:4:221:VAL:HG23 | 4:4:272:VAL:CG1  | 2.46                     | 0.45              |
| 4:4:257:TYR:C    | 4:4:259:THR:H    | 2.25                     | 0.45              |
| 4:4:262:PHE:HD1  | 4:4:289:ILE:HD11 | 1.82                     | 0.45              |
| 1:A:211:LEU:HB2  | 1:A:216:THR:HG21 | 1.97                     | 0.45              |
| 1:A:347:PHE:C    | 1:A:347:PHE:CD2  | 2.94                     | 0.45              |
| 2:B:81:GLN:HB3   | 2:B:122:VAL:HG21 | 1.98                     | 0.45              |
| 3:C:225:ASN:HD21 | 3:C:289:TRP:HB3  | 1.81                     | 0.45              |
| 3:C:309:PRO:HA   | 3:C:603:PRO:CD   | 2.46                     | 0.45              |
| 4:D:239:LEU:HD22 | 4:D:244:VAL:HB   | 1.99                     | 0.45              |
| 5:E:49:LEU:HD13  | 5:E:74:LEU:HD23  | 1.96                     | 0.45              |
| 3:3:101:ARG:CZ   | 3:3:101:ARG:CB   | 2.94                     | 0.45              |
| 3:3:621:VAL:O    | 3:3:621:VAL:HG23 | 2.16                     | 0.45              |
| 5:5:49:LEU:HD13  | 5:5:74:LEU:HD23  | 1.97                     | 0.45              |
| 5:5:67:ARG:HD3   | 5:5:96:GLU:HG3   | 1.99                     | 0.45              |
| 1:A:132:ILE:HG21 | 1:A:145:LEU:HD11 | 1.98                     | 0.45              |
| 3:C:223:SER:O    | 3:C:226:ILE:HG12 | 2.16                     | 0.45              |
| 3:C:422:PRO:HA   | 3:C:423:PRO:HD2  | 1.89                     | 0.45              |
| 4:D:119:ILE:O    | 4:D:123:LEU:HB2  | 2.16                     | 0.45              |
| 6:F:37:TRP:CD1   | 6:F:75:ALA:HB2   | 2.51                     | 0.45              |
| 6:F:104:TRP:HB3  | 6:F:154:LEU:HD11 | 1.97                     | 0.45              |
| 3:3:583:VAL:HG23 | 3:3:598:ALA:HA   | 1.99                     | 0.45              |
| 6:6:166:ARG:HD3  | 6:6:168:GLU:OE2  | 2.16                     | 0.45              |
| 8:7:36:ASP:HB2   | 8:7:41:ILE:HD11  | 1.99                     | 0.45              |
| 3:C:117:LEU:CA   | 4:D:321:MET:HE1  | 2.43                     | 0.45              |
| 3:C:170:LEU:HD21 | 3:C:176:LEU:HD22 | 1.97                     | 0.45              |
| 3:C:270:ARG:O    | 3:C:271:SER:HB2  | 2.17                     | 0.45              |
| 4:D:88:LEU:HD12  | 4:D:403:VAL:CG2  | 2.46                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:131:VAL:HG12 | 4:D:132:PHE:N    | 2.31                     | 0.45              |
| 6:F:96:TRP:O     | 6:F:99:MET:HB2   | 2.17                     | 0.45              |
| 6:F:115:GLY:HA3  | 6:F:125:GLN:OE1  | 2.17                     | 0.45              |
| 3:3:116:PRO:HG3  | 3:3:180:ARG:HG2  | 1.99                     | 0.45              |
| 6:6:18:GLY:O     | 6:6:19:ILE:C     | 2.59                     | 0.45              |
| 1:A:6:LEU:HB2    | 1:A:241:MET:HA   | 1.99                     | 0.45              |
| 1:A:360:ARG:O    | 3:C:207:VAL:HG13 | 2.16                     | 0.45              |
| 4:D:84:ARG:CZ    | 6:F:117:MET:HE1  | 2.47                     | 0.45              |
| 4:D:153:ARG:HG3  | 4:D:153:ARG:NH1  | 2.31                     | 0.45              |
| 4:D:212:PRO:CG   | 4:D:213:ILE:HD12 | 2.41                     | 0.45              |
| 5:E:72:TYR:O     | 5:E:89:PHE:HA    | 2.17                     | 0.45              |
| 5:E:116:ARG:HB3  | 5:E:135:ILE:HG13 | 1.98                     | 0.45              |
| 6:F:37:TRP:O     | 6:F:75:ALA:HB1   | 2.17                     | 0.45              |
| 7:G:126:TYR:C    | 7:G:126:TYR:HD1  | 2.25                     | 0.45              |
| 1:1:139:ARG:HG2  | 2:2:140:PRO:HD3  | 1.99                     | 0.45              |
| 1:1:192:LEU:C    | 1:1:194:GLY:H    | 2.25                     | 0.45              |
| 3:3:370:ASP:OD2  | 3:3:558:TRP:HD1  | 2.00                     | 0.45              |
| 3:3:716:LEU:CD2  | 3:3:758:LEU:HB3  | 2.47                     | 0.45              |
| 8:7:108:ILE:HG22 | 8:7:114:ARG:NH1  | 2.32                     | 0.45              |
| 3:C:214:MET:O    | 3:C:216:PHE:CE1  | 2.70                     | 0.45              |
| 3:C:267:ALA:HA   | 3:C:277:ILE:HD13 | 1.98                     | 0.45              |
| 3:C:689:LYS:HB2  | 3:C:772:GLU:OE2  | 2.17                     | 0.45              |
| 6:F:99:MET:CG    | 6:F:100:PRO:HD2  | 2.43                     | 0.45              |
| 1:1:89:LEU:HD21  | 1:1:121:ALA:HB3  | 1.99                     | 0.45              |
| 1:1:93:ALA:O     | 1:1:134:VAL:HA   | 2.17                     | 0.45              |
| 3:3:38:HIS:CE1   | 3:3:287:GLU:HB3  | 2.52                     | 0.45              |
| 4:4:100:ALA:O    | 4:4:342:VAL:HG11 | 2.17                     | 0.45              |
| 4:4:187:VAL:N    | 4:4:188:PRO:HD2  | 2.32                     | 0.45              |
| 4:4:236:GLY:HA3  | 4:4:377:ASN:HD21 | 1.82                     | 0.45              |
| 5:5:195:LEU:O    | 5:5:196:TRP:C    | 2.60                     | 0.45              |
| 1:A:79:MET:HG3   | 1:A:125:ILE:HB   | 1.98                     | 0.45              |
| 3:C:2:VAL:CG1    | 3:C:89:ASP:HA    | 2.38                     | 0.45              |
| 3:C:194:VAL:HG12 | 3:C:411:LEU:HD22 | 1.99                     | 0.45              |
| 3:C:571:VAL:CG2  | 3:C:587:LEU:HD11 | 2.47                     | 0.45              |
| 4:D:132:PHE:CE2  | 4:D:279:ARG:HD2  | 2.52                     | 0.45              |
| 8:H:68:LEU:HD13  | 8:H:68:LEU:C     | 2.42                     | 0.45              |
| 3:3:29:ASP:OD1   | 3:3:29:ASP:N     | 2.50                     | 0.45              |
| 5:5:163:ARG:CD   | 7:9:69:TYR:CE1   | 3.00                     | 0.45              |
| 1:A:128:THR:O    | 1:A:169:PHE:HA   | 2.16                     | 0.45              |
| 4:D:144:THR:N    | 4:D:145:PRO:CD   | 2.80                     | 0.45              |
| 1:1:93:ALA:CB    | 1:1:107:LEU:HD11 | 2.43                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:357:THR:N    | 1:1:358:PRO:HD2  | 2.32                     | 0.44              |
| 3:3:546:ALA:C    | 3:3:547:MET:HE2  | 2.42                     | 0.44              |
| 6:6:78:MET:CE    | 6:6:99:MET:HE1   | 2.47                     | 0.44              |
| 3:C:269:THR:HG22 | 3:C:273:GLU:O    | 2.17                     | 0.44              |
| 3:C:616:ASN:C    | 3:C:618:GLU:H    | 2.24                     | 0.44              |
| 4:D:126:LEU:O    | 4:D:130:LEU:HB2  | 2.17                     | 0.44              |
| 5:E:59:THR:HG22  | 5:E:59:THR:O     | 2.17                     | 0.44              |
| 7:G:126:TYR:C    | 7:G:126:TYR:CD1  | 2.95                     | 0.44              |
| 1:1:10:ASP:OD1   | 1:1:11:PRO:HD2   | 2.18                     | 0.44              |
| 1:1:134:VAL:HG23 | 1:1:135:ARG:O    | 2.17                     | 0.44              |
| 1:1:193:GLU:HG3  | 1:1:212:TRP:NE1  | 2.31                     | 0.44              |
| 2:2:175:HIS:ND1  | 2:2:175:HIS:N    | 2.61                     | 0.44              |
| 3:3:55:PRO:CD    | 3:3:74:GLN:N     | 2.80                     | 0.44              |
| 3:3:202:PHE:C    | 3:3:203:ILE:HD13 | 2.41                     | 0.44              |
| 3:3:240:ALA:HB2  | 3:3:276:ARG:HB2  | 1.99                     | 0.44              |
| 4:4:126:LEU:O    | 4:4:130:LEU:HB2  | 2.17                     | 0.44              |
| 5:5:116:ARG:HB3  | 5:5:135:ILE:HG13 | 1.98                     | 0.44              |
| 7:9:41:HIS:CD2   | 7:9:115:LEU:HD21 | 2.53                     | 0.44              |
| 7:9:126:TYR:CD1  | 7:9:126:TYR:C    | 2.95                     | 0.44              |
| 2:B:38:GLU:OE2   | 2:B:45:ARG:NH1   | 2.49                     | 0.44              |
| 2:B:142:VAL:HG11 | 2:B:153:LEU:HG   | 1.99                     | 0.44              |
| 3:C:30:VAL:CG2   | 3:C:48:CYS:HA    | 2.46                     | 0.44              |
| 3:C:33:PHE:HZ    | 3:C:130:LEU:HD12 | 1.82                     | 0.44              |
| 3:C:591:HIS:CE1  | 3:C:592:PRO:HD2  | 2.52                     | 0.44              |
| 3:C:602:LEU:HD12 | 3:C:602:LEU:N    | 2.33                     | 0.44              |
| 4:D:257:TYR:C    | 4:D:259:THR:H    | 2.25                     | 0.44              |
| 7:G:127:SER:O    | 7:G:130:VAL:HG12 | 2.17                     | 0.44              |
| 8:H:81:ARG:HG3   | 8:H:94:HIS:CD2   | 2.53                     | 0.44              |
| 3:3:6:VAL:HG12   | 3:3:7:ASN:N      | 2.32                     | 0.44              |
| 3:3:20:MET:SD    | 3:3:32:LEU:CD2   | 3.05                     | 0.44              |
| 3:3:394:ASP:OD2  | 3:3:502:ASN:N    | 2.51                     | 0.44              |
| 3:3:684:ARG:HA   | 3:3:685:PRO:HD2  | 1.86                     | 0.44              |
| 4:4:51:GLU:O     | 4:4:52:VAL:HG23  | 2.16                     | 0.44              |
| 4:4:197:LEU:N    | 4:4:198:PRO:CD   | 2.80                     | 0.44              |
| 5:5:167:PRO:HB2  | 5:5:171:ARG:HH12 | 1.83                     | 0.44              |
| 2:B:74:PRO:HB2   | 8:H:121:ARG:HH21 | 1.82                     | 0.44              |
| 3:C:173:PHE:HB3  | 3:C:296:PHE:CE1  | 2.53                     | 0.44              |
| 5:E:84:ASP:OD1   | 5:E:84:ASP:N     | 2.50                     | 0.44              |
| 5:E:134:LYS:HE3  | 5:E:134:LYS:HB2  | 1.63                     | 0.44              |
| 6:F:158:VAL:HA   | 6:F:172:PRO:HB3  | 1.99                     | 0.44              |
| 3:3:194:VAL:HG12 | 3:3:411:LEU:HD22 | 1.98                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:240:ALA:CB   | 3:3:276:ARG:HB2  | 2.48                     | 0.44              |
| 3:3:707:LYS:C    | 3:3:709:GLN:N    | 2.75                     | 0.44              |
| 4:4:85:MET:HG2   | 4:4:409:ARG:HB2  | 1.98                     | 0.44              |
| 4:4:159:LEU:O    | 4:4:162:TRP:HB2  | 2.18                     | 0.44              |
| 6:6:154:LEU:O    | 6:6:158:VAL:HG13 | 2.16                     | 0.44              |
| 1:A:18:TYR:CE2   | 1:A:263:VAL:HG11 | 2.52                     | 0.44              |
| 1:A:248:GLY:O    | 1:A:268:MET:HB2  | 2.17                     | 0.44              |
| 1:A:298:PRO:HD2  | 1:A:321:SER:OG   | 2.17                     | 0.44              |
| 3:C:30:VAL:HG22  | 3:C:48:CYS:HA    | 1.99                     | 0.44              |
| 3:C:430:THR:HA   | 3:C:431:PRO:HD2  | 1.83                     | 0.44              |
| 3:C:583:VAL:HG23 | 3:C:599:HIS:H    | 1.83                     | 0.44              |
| 4:D:205:GLU:OE2  | 4:D:281:ARG:NE   | 2.28                     | 0.44              |
| 1:1:398:SER:HA   | 3:3:46:ARG:HD3   | 1.98                     | 0.44              |
| 3:3:279:ALA:HB2  | 3:3:290:ILE:CG1  | 2.35                     | 0.44              |
| 3:3:689:LYS:HB2  | 3:3:772:GLU:HG2  | 2.00                     | 0.44              |
| 4:4:85:MET:CE    | 4:4:409:ARG:HG3  | 2.43                     | 0.44              |
| 4:4:162:TRP:CE2  | 7:9:34:LYS:HD2   | 2.52                     | 0.44              |
| 6:6:76:ASP:O     | 6:6:77:VAL:CB    | 2.66                     | 0.44              |
| 3:C:337:ARG:HD3  | 3:C:340:GLU:HG3  | 1.98                     | 0.44              |
| 3:C:621:VAL:O    | 3:C:621:VAL:HG23 | 2.16                     | 0.44              |
| 4:D:85:MET:HG2   | 4:D:409:ARG:HB2  | 1.98                     | 0.44              |
| 4:D:196:VAL:O    | 4:D:200:ARG:HB2  | 2.18                     | 0.44              |
| 5:E:16:PRO:HD2   | 5:E:28:VAL:HG13  | 2.00                     | 0.44              |
| 6:F:117:MET:CE   | 7:G:99:ILE:HG12  | 2.28                     | 0.44              |
| 8:H:36:ASP:HB2   | 8:H:41:ILE:HD11  | 2.00                     | 0.44              |
| 3:3:561:PRO:HG3  | 3:3:575:GLU:O    | 2.18                     | 0.44              |
| 3:3:567:TYR:HE1  | 3:3:586:HIS:HB2  | 1.82                     | 0.44              |
| 3:3:663:ALA:O    | 3:3:666:ALA:HB3  | 2.18                     | 0.44              |
| 4:4:233:GLY:CA   | 5:5:48:PHE:HE1   | 2.31                     | 0.44              |
| 1:A:134:VAL:HG23 | 1:A:135:ARG:O    | 2.17                     | 0.44              |
| 3:C:152:PRO:HG3  | 4:D:305:PRO:O    | 2.18                     | 0.44              |
| 3:C:274:LEU:HD12 | 3:C:275:LEU:N    | 2.32                     | 0.44              |
| 3:C:337:ARG:CD   | 3:C:340:GLU:HG3  | 2.48                     | 0.44              |
| 3:C:663:ALA:O    | 3:C:666:ALA:HB3  | 2.18                     | 0.44              |
| 3:C:689:LYS:HB2  | 3:C:772:GLU:HG2  | 2.00                     | 0.44              |
| 1:1:17:LEU:C     | 1:1:19:ALA:H     | 2.25                     | 0.44              |
| 1:1:291:ILE:HA   | 1:1:292:PRO:HD2  | 1.64                     | 0.44              |
| 2:2:154:LEU:O    | 2:2:158:ARG:HB2  | 2.17                     | 0.44              |
| 3:3:230:CYS:HA   | 9:3:785:SF4:S2   | 2.58                     | 0.44              |
| 3:3:334:LYS:NZ   | 3:3:334:LYS:HB3  | 2.33                     | 0.44              |
| 8:7:92:HIS:O     | 8:7:93:LEU:HD12  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:7:97:TYR:CD2   | 8:7:97:TYR:C     | 2.95                     | 0.44              |
| 1:A:177:ALA:O    | 2:B:67:TYR:HB3   | 2.17                     | 0.44              |
| 1:A:395:GLU:O    | 1:A:396:GLY:C    | 2.60                     | 0.44              |
| 2:B:106:ILE:HG22 | 2:B:110:GLU:HB2  | 1.99                     | 0.44              |
| 4:D:236:GLY:C    | 4:D:238:SER:N    | 2.64                     | 0.44              |
| 5:E:87:ARG:O     | 5:E:88:PHE:HB3   | 2.18                     | 0.44              |
| 1:1:79:MET:HG3   | 1:1:125:ILE:HB   | 1.98                     | 0.44              |
| 3:3:274:LEU:HD12 | 3:3:274:LEU:C    | 2.43                     | 0.44              |
| 4:4:131:VAL:HG12 | 4:4:132:PHE:N    | 2.33                     | 0.44              |
| 4:4:144:THR:N    | 4:4:145:PRO:CD   | 2.81                     | 0.44              |
| 4:4:211:SER:HA   | 4:4:212:PRO:HD2  | 1.89                     | 0.44              |
| 1:A:243:THR:HB   | 1:A:314:GLU:OE2  | 2.17                     | 0.44              |
| 1:A:358:PRO:O    | 1:A:362:GLY:CA   | 2.53                     | 0.44              |
| 2:B:136:VAL:HG21 | 2:B:163:LEU:CD1  | 2.43                     | 0.44              |
| 3:C:591:HIS:ND1  | 3:C:592:PRO:N    | 2.66                     | 0.44              |
| 4:D:99:LEU:O     | 4:D:103:LYS:HG2  | 2.18                     | 0.44              |
| 5:E:132:LEU:HA   | 5:E:132:LEU:HD23 | 1.62                     | 0.44              |
| 5:E:160:ARG:HH21 | 7:G:144:LYS:NZ   | 2.15                     | 0.44              |
| 3:3:277:ILE:HD13 | 3:3:277:ILE:HA   | 1.83                     | 0.44              |
| 4:4:82:THR:N     | 4:4:83:PRO:HD2   | 2.33                     | 0.44              |
| 4:4:196:VAL:O    | 4:4:196:VAL:HG22 | 2.17                     | 0.44              |
| 3:C:459:MET:HG2  | 3:C:465:HIS:CB   | 2.44                     | 0.44              |
| 4:D:65:GLY:O     | 4:D:69:THR:CG2   | 2.64                     | 0.44              |
| 1:1:18:TYR:CE2   | 1:1:263:VAL:HG11 | 2.53                     | 0.43              |
| 3:3:270:ARG:O    | 3:3:271:SER:HB2  | 2.17                     | 0.43              |
| 3:3:409:LEU:HD23 | 3:3:409:LEU:HA   | 1.72                     | 0.43              |
| 4:4:317:LEU:HD12 | 4:4:317:LEU:HA   | 1.78                     | 0.43              |
| 5:5:134:LYS:HE3  | 5:5:134:LYS:HB2  | 1.67                     | 0.43              |
| 7:9:127:SER:O    | 7:9:130:VAL:HG12 | 2.18                     | 0.43              |
| 3:C:601:VAL:C    | 3:C:602:LEU:HD12 | 2.43                     | 0.43              |
| 4:D:47:LEU:HA    | 4:D:53:LEU:HD23  | 2.00                     | 0.43              |
| 4:D:348:SER:C    | 4:D:350:ARG:H    | 2.25                     | 0.43              |
| 2:2:106:ILE:HG22 | 2:2:110:GLU:HB2  | 1.99                     | 0.43              |
| 3:3:259:CYS:CB   | 3:3:260:PRO:CD   | 2.96                     | 0.43              |
| 4:4:40:VAL:O     | 4:4:40:VAL:CG2   | 2.64                     | 0.43              |
| 4:4:61:TYR:CZ    | 6:6:87:LYS:HE2   | 2.53                     | 0.43              |
| 6:6:78:MET:HE3   | 6:6:96:TRP:HB2   | 2.00                     | 0.43              |
| 6:6:104:TRP:NE1  | 6:6:173:VAL:HG22 | 2.33                     | 0.43              |
| 8:7:16:LEU:HD13  | 8:7:16:LEU:C     | 2.43                     | 0.43              |
| 1:A:193:GLU:OE1  | 1:A:211:LEU:HD12 | 2.18                     | 0.43              |
| 3:C:707:LYS:C    | 3:C:709:GLN:N    | 2.76                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:88:LEU:HD21  | 6:F:48:ILE:HD13  | 2.00                     | 0.43              |
| 1:1:106:ILE:HG23 | 1:1:110:VAL:HG23 | 2.01                     | 0.43              |
| 3:3:497:TRP:O    | 3:3:528:LYS:HE3  | 2.18                     | 0.43              |
| 3:3:560:GLU:HA   | 3:3:561:PRO:HD2  | 1.87                     | 0.43              |
| 3:3:715:GLU:O    | 3:3:715:GLU:OE2  | 2.36                     | 0.43              |
| 4:4:153:ARG:HG3  | 4:4:153:ARG:NH1  | 2.33                     | 0.43              |
| 5:5:84:ASP:OD1   | 5:5:84:ASP:N     | 2.51                     | 0.43              |
| 6:6:16:ARG:HG2   | 6:6:21:PHE:HE2   | 1.84                     | 0.43              |
| 7:9:126:TYR:C    | 7:9:126:TYR:HD1  | 2.25                     | 0.43              |
| 8:7:121:ARG:NH1  | 8:7:121:ARG:CG   | 2.81                     | 0.43              |
| 3:C:227:THR:HG21 | 3:C:237:ASP:HB2  | 2.00                     | 0.43              |
| 3:C:716:LEU:HA   | 3:C:759:TYR:O    | 2.18                     | 0.43              |
| 4:D:83:PRO:HB2   | 4:D:169:HIS:HA   | 2.00                     | 0.43              |
| 4:D:84:ARG:NE    | 6:F:117:MET:HE1  | 2.32                     | 0.43              |
| 1:1:332:PRO:CD   | 2:2:90:LEU:HD23  | 2.47                     | 0.43              |
| 3:3:115:HIS:C    | 4:4:321:MET:HE3  | 2.43                     | 0.43              |
| 3:3:571:VAL:HG11 | 3:3:591:HIS:CD2  | 2.54                     | 0.43              |
| 6:6:37:TRP:CE3   | 6:6:37:TRP:HA    | 2.53                     | 0.43              |
| 1:A:70:PHE:CG    | 1:A:71:PRO:HD2   | 2.54                     | 0.43              |
| 1:A:93:ALA:CB    | 1:A:107:LEU:HD11 | 2.46                     | 0.43              |
| 1:A:158:LEU:HD23 | 1:A:158:LEU:HA   | 1.86                     | 0.43              |
| 2:B:106:ILE:HG23 | 2:B:110:GLU:HB2  | 2.00                     | 0.43              |
| 3:C:688:ARG:HD3  | 3:C:688:ARG:HA   | 1.71                     | 0.43              |
| 4:D:85:MET:CE    | 4:D:409:ARG:HG3  | 2.43                     | 0.43              |
| 4:D:91:PHE:CD1   | 4:D:120:LEU:HD12 | 2.53                     | 0.43              |
| 4:D:102:GLU:HG2  | 4:D:175:ILE:O    | 2.18                     | 0.43              |
| 5:E:131:ASP:OD2  | 5:E:133:ARG:NE   | 2.47                     | 0.43              |
| 1:1:110:VAL:HG23 | 1:1:110:VAL:O    | 2.18                     | 0.43              |
| 1:1:114:LEU:C    | 1:1:114:LEU:CD2  | 2.91                     | 0.43              |
| 3:3:115:HIS:HB3  | 4:4:321:MET:HE3  | 2.00                     | 0.43              |
| 3:3:471:GLY:HA2  | 3:3:473:GLU:OE2  | 2.19                     | 0.43              |
| 4:4:348:SER:C    | 4:4:350:ARG:H    | 2.27                     | 0.43              |
| 1:A:97:GLU:HB2   | 1:A:180:TYR:HE1  | 1.84                     | 0.43              |
| 1:A:246:SER:O    | 1:A:268:MET:HG2  | 2.19                     | 0.43              |
| 1:A:367:MET:HB3  | 1:A:367:MET:HE2  | 1.76                     | 0.43              |
| 1:A:438:ARG:HD2  | 1:A:438:ARG:H    | 1.83                     | 0.43              |
| 3:C:31:PRO:HG3   | 3:C:137:TYR:CG   | 2.53                     | 0.43              |
| 8:H:65:GLU:HA    | 8:H:66:PRO:HD3   | 1.86                     | 0.43              |
| 8:H:92:HIS:C     | 8:H:93:LEU:HD12  | 2.44                     | 0.43              |
| 1:1:248:GLY:O    | 1:1:268:MET:HB2  | 2.19                     | 0.43              |
| 2:2:168:LEU:HA   | 2:2:169:PRO:HD2  | 1.79                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:606:THR:O    | 3:3:610:LYS:HG3  | 2.18                     | 0.43              |
| 4:4:250:LYS:HE2  | 4:4:262:PHE:CD2  | 2.53                     | 0.43              |
| 3:C:516:VAL:O    | 3:C:520:ARG:HG3  | 2.18                     | 0.43              |
| 3:C:695:ARG:NH1  | 3:C:697:THR:HG22 | 2.33                     | 0.43              |
| 4:D:262:PHE:HD1  | 4:D:289:ILE:HD11 | 1.82                     | 0.43              |
| 5:E:67:ARG:HD3   | 5:E:96:GLU:HG3   | 1.99                     | 0.43              |
| 6:F:166:ARG:HD3  | 6:F:168:GLU:OE2  | 2.18                     | 0.43              |
| 7:G:71:GLU:HB2   | 7:G:90:VAL:HB    | 2.01                     | 0.43              |
| 1:1:211:LEU:HB2  | 1:1:216:THR:HG21 | 1.99                     | 0.43              |
| 3:3:11:VAL:HG21  | 3:3:26:ALA:HB2   | 2.00                     | 0.43              |
| 3:3:384:PRO:HG3  | 3:3:542:ARG:HE   | 1.83                     | 0.43              |
| 3:3:501:LYS:N    | 3:3:501:LYS:CD   | 2.73                     | 0.43              |
| 5:5:167:PRO:HB3  | 7:9:66:TYR:CE2   | 2.53                     | 0.43              |
| 3:C:150:GLU:O    | 3:C:151:LEU:C    | 2.62                     | 0.43              |
| 3:C:370:ASP:OD2  | 3:C:558:TRP:HD1  | 2.01                     | 0.43              |
| 4:D:288:LYS:HA   | 4:D:288:LYS:HD3  | 1.83                     | 0.43              |
| 5:E:53:VAL:HG22  | 5:E:55:LEU:CD1   | 2.48                     | 0.43              |
| 6:F:152:MET:HE2  | 6:F:152:MET:HB3  | 1.83                     | 0.43              |
| 1:1:17:LEU:HD12  | 1:1:251:LEU:CD1  | 2.49                     | 0.43              |
| 3:3:690:GLY:HA3  | 3:3:770:ARG:HH21 | 1.79                     | 0.43              |
| 3:3:695:ARG:HD2  | 3:3:717:TRP:CZ3  | 2.54                     | 0.43              |
| 4:4:119:ILE:O    | 4:4:123:LEU:HB2  | 2.19                     | 0.43              |
| 4:4:143:LEU:HD23 | 4:4:143:LEU:O    | 2.19                     | 0.43              |
| 4:4:328:PHE:C    | 4:4:328:PHE:CD2  | 2.97                     | 0.43              |
| 7:9:41:HIS:CE1   | 7:9:98:CYS:SG    | 3.12                     | 0.43              |
| 8:7:31:PHE:CD1   | 8:7:31:PHE:C     | 2.96                     | 0.43              |
| 1:A:56:GLU:HG2   | 1:A:231:MET:SD   | 2.59                     | 0.43              |
| 1:A:202:LYS:N    | 1:A:203:PRO:HD2  | 2.34                     | 0.43              |
| 1:A:211:LEU:HD12 | 1:A:211:LEU:HA   | 1.68                     | 0.43              |
| 4:D:70:MET:C     | 4:D:72:HIS:H     | 2.27                     | 0.43              |
| 1:1:5:ILE:HG22   | 1:1:6:LEU:N      | 2.34                     | 0.43              |
| 1:1:6:LEU:HB2    | 1:1:241:MET:HA   | 1.99                     | 0.43              |
| 1:1:228:VAL:HB   | 1:1:229:PRO:CD   | 2.49                     | 0.43              |
| 3:3:116:PRO:C    | 4:4:321:MET:HE1  | 2.38                     | 0.43              |
| 3:3:173:PHE:HB3  | 3:3:296:PHE:CE1  | 2.53                     | 0.43              |
| 4:4:240:ARG:HB2  | 4:4:266:LEU:HD23 | 2.01                     | 0.43              |
| 4:4:288:LYS:HD3  | 4:4:288:LYS:HA   | 1.85                     | 0.43              |
| 6:6:32:ARG:NH1   | 6:6:102:PRO:HG2  | 2.34                     | 0.43              |
| 7:9:99:ILE:HG22  | 7:9:101:CYS:SG   | 2.58                     | 0.43              |
| 1:A:63:ARG:NH1   | 1:A:313:TYR:HB3  | 2.33                     | 0.43              |
| 2:B:134:ILE:HG13 | 2:B:145:VAL:HG21 | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:412:ARG:HA   | 3:C:412:ARG:HD2  | 1.93                     | 0.43              |
| 3:C:706:GLY:O    | 3:C:709:GLN:HB2  | 2.19                     | 0.43              |
| 1:1:177:ALA:HB3  | 2:2:67:TYR:CD2   | 2.54                     | 0.43              |
| 3:3:116:PRO:O    | 3:3:117:LEU:CB   | 2.60                     | 0.43              |
| 3:3:120:PRO:HG2  | 8:7:42:TYR:CZ    | 2.53                     | 0.43              |
| 3:3:139:LEU:HD11 | 3:3:154:TYR:CD1  | 2.54                     | 0.43              |
| 3:3:513:GLN:HG2  | 3:3:769:LEU:HD23 | 2.01                     | 0.43              |
| 3:3:715:GLU:OE2  | 3:3:715:GLU:C    | 2.62                     | 0.43              |
| 5:5:87:ARG:O     | 5:5:88:PHE:HB3   | 2.19                     | 0.43              |
| 5:5:101:LEU:HA   | 5:5:102:PRO:HD2  | 1.86                     | 0.43              |
| 5:5:107:LEU:N    | 5:5:107:LEU:CD1  | 2.82                     | 0.43              |
| 3:C:17:THR:HG22  | 3:C:18:SER:O     | 2.19                     | 0.43              |
| 3:C:118:ASP:O    | 3:C:119:CYS:C    | 2.62                     | 0.43              |
| 3:C:139:LEU:HD11 | 3:C:154:TYR:CD1  | 2.54                     | 0.43              |
| 3:C:225:ASN:ND2  | 3:C:289:TRP:HB3  | 2.34                     | 0.43              |
| 3:C:474:ARG:HA   | 3:C:517:ALA:HB2  | 2.01                     | 0.43              |
| 4:D:257:TYR:C    | 4:D:259:THR:N    | 2.77                     | 0.43              |
| 4:D:363:SER:HB3  | 5:E:173:ALA:HB1  | 2.00                     | 0.43              |
| 1:1:392:PRO:O    | 1:1:397:ARG:NH1  | 2.52                     | 0.42              |
| 2:2:43:PRO:O     | 2:2:47:GLU:HG3   | 2.19                     | 0.42              |
| 3:3:55:PRO:HG3   | 3:3:74:GLN:CB    | 2.49                     | 0.42              |
| 3:3:715:GLU:CD   | 3:3:761:SER:HB2  | 2.44                     | 0.42              |
| 4:4:64:THR:N     | 4:4:409:ARG:OXT  | 2.52                     | 0.42              |
| 1:A:438:ARG:HD2  | 1:A:438:ARG:N    | 2.33                     | 0.42              |
| 2:B:45:ARG:O     | 2:B:49:ILE:HG13  | 2.19                     | 0.42              |
| 2:B:79:HIS:O     | 2:B:136:VAL:O    | 2.37                     | 0.42              |
| 4:D:236:GLY:HA3  | 4:D:377:ASN:HD21 | 1.83                     | 0.42              |
| 4:D:250:LYS:HG3  | 4:D:264:VAL:HG21 | 2.00                     | 0.42              |
| 4:D:317:LEU:HD12 | 4:D:317:LEU:HA   | 1.74                     | 0.42              |
| 5:E:13:LYS:NZ    | 5:E:33:ARG:HH21  | 2.17                     | 0.42              |
| 6:F:16:ARG:O     | 6:F:21:PHE:HD2   | 2.01                     | 0.42              |
| 3:3:267:ALA:HA   | 3:3:277:ILE:HD13 | 2.01                     | 0.42              |
| 3:3:776:LEU:N    | 3:3:776:LEU:HD23 | 2.34                     | 0.42              |
| 1:A:331:ILE:HD12 | 1:A:337:MET:CE   | 2.38                     | 0.42              |
| 3:C:109:GLU:OE2  | 3:C:156:ARG:HG3  | 2.20                     | 0.42              |
| 3:C:550:LEU:N    | 3:C:550:LEU:CD1  | 2.81                     | 0.42              |
| 3:C:571:VAL:HG23 | 3:C:587:LEU:HD11 | 2.00                     | 0.42              |
| 3:C:605:PRO:HB2  | 3:C:609:GLU:HG3  | 2.01                     | 0.42              |
| 6:F:148:ILE:O    | 6:F:152:MET:HG3  | 2.20                     | 0.42              |
| 6:F:154:LEU:O    | 6:F:154:LEU:HG   | 2.18                     | 0.42              |
| 1:1:414:LEU:O    | 1:1:418:LYS:HB2  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:2:27:ILE:HD13  | 2:2:60:VAL:HG22  | 2.01                     | 0.42              |
| 3:3:45:CYS:SG    | 3:3:47:MET:HB2   | 2.59                     | 0.42              |
| 3:3:270:ARG:HB3  | 3:3:275:LEU:HD21 | 2.00                     | 0.42              |
| 3:3:583:VAL:HG23 | 3:3:599:HIS:H    | 1.85                     | 0.42              |
| 4:4:122:GLU:CD   | 4:4:125:ARG:HE   | 2.27                     | 0.42              |
| 6:6:163:TYR:CD2  | 6:6:169:ARG:HA   | 2.54                     | 0.42              |
| 3:C:23:VAL:HG12  | 3:C:24:PHE:N     | 2.33                     | 0.42              |
| 3:C:120:PRO:O    | 3:C:245:ARG:NH1  | 2.52                     | 0.42              |
| 3:C:151:LEU:HD23 | 3:C:151:LEU:HA   | 1.85                     | 0.42              |
| 3:C:409:LEU:HD23 | 3:C:409:LEU:HA   | 1.76                     | 0.42              |
| 4:D:187:VAL:N    | 4:D:188:PRO:HD2  | 2.34                     | 0.42              |
| 4:D:197:LEU:O    | 4:D:200:ARG:HB3  | 2.19                     | 0.42              |
| 4:D:297:LEU:HD12 | 4:D:297:LEU:HA   | 1.82                     | 0.42              |
| 6:F:18:GLY:O     | 6:F:19:ILE:C     | 2.62                     | 0.42              |
| 1:1:341:MET:HE1  | 1:1:409:PRO:CB   | 2.45                     | 0.42              |
| 4:4:257:TYR:C    | 4:4:259:THR:N    | 2.77                     | 0.42              |
| 5:5:64:ARG:HB3   | 5:5:65:PRO:HD2   | 2.02                     | 0.42              |
| 2:B:26:ALA:O     | 2:B:29:PRO:HG2   | 2.19                     | 0.42              |
| 2:B:27:ILE:O     | 2:B:31:LEU:HD22  | 2.19                     | 0.42              |
| 3:C:46:ARG:HG2   | 3:C:46:ARG:NH1   | 2.34                     | 0.42              |
| 3:C:501:LYS:N    | 3:C:501:LYS:CD   | 2.75                     | 0.42              |
| 3:C:583:VAL:HG23 | 3:C:598:ALA:HA   | 1.99                     | 0.42              |
| 3:C:586:HIS:CD2  | 3:C:640:VAL:HG21 | 2.55                     | 0.42              |
| 3:C:676:LEU:O    | 3:C:676:LEU:HD13 | 2.19                     | 0.42              |
| 4:D:56:VAL:HA    | 4:D:57:PRO:HD2   | 1.94                     | 0.42              |
| 4:D:196:VAL:O    | 4:D:196:VAL:HG22 | 2.18                     | 0.42              |
| 6:F:89:ALA:N     | 6:F:90:PRO:HD2   | 2.34                     | 0.42              |
| 6:F:104:TRP:HA   | 6:F:134:ASP:OD2  | 2.19                     | 0.42              |
| 3:3:200:LEU:HD12 | 3:3:200:LEU:HA   | 1.93                     | 0.42              |
| 3:3:414:SER:OG   | 3:3:443:ARG:NH2  | 2.53                     | 0.42              |
| 3:3:451:PHE:CE1  | 3:3:466:GLU:HB3  | 2.53                     | 0.42              |
| 6:6:137:VAL:HG13 | 6:6:137:VAL:O    | 2.19                     | 0.42              |
| 1:A:238:PHE:HE1  | 1:A:249:MET:HE1  | 1.84                     | 0.42              |
| 1:A:272:PHE:HB3  | 1:A:276:ILE:CD1  | 2.50                     | 0.42              |
| 3:C:270:ARG:HB3  | 3:C:275:LEU:HD21 | 2.01                     | 0.42              |
| 3:C:334:LYS:NZ   | 3:C:334:LYS:HB3  | 2.34                     | 0.42              |
| 3:C:506:ILE:HG12 | 3:C:533:LEU:HB2  | 2.00                     | 0.42              |
| 3:C:513:GLN:HG2  | 3:C:769:LEU:HD23 | 2.01                     | 0.42              |
| 4:D:82:THR:N     | 4:D:83:PRO:HD2   | 2.34                     | 0.42              |
| 4:D:276:MET:O    | 4:D:280:ILE:HG13 | 2.19                     | 0.42              |
| 4:D:393:MET:CA   | 4:D:396:ILE:HG22 | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:41:HIS:HA    | 7:G:115:LEU:HA   | 2.02                     | 0.42              |
| 8:H:73:SER:OG    | 8:H:80:LYS:HA    | 2.19                     | 0.42              |
| 2:2:27:ILE:O     | 2:2:31:LEU:HD22  | 2.20                     | 0.42              |
| 2:2:106:ILE:HG23 | 2:2:110:GLU:HB2  | 2.02                     | 0.42              |
| 3:3:120:PRO:O    | 3:3:245:ARG:NH1  | 2.53                     | 0.42              |
| 3:3:473:GLU:O    | 3:3:477:LEU:HD12 | 2.20                     | 0.42              |
| 4:4:234:LEU:O    | 4:4:236:GLY:N    | 2.53                     | 0.42              |
| 4:4:249:ARG:HB3  | 4:4:257:TYR:CD1  | 2.40                     | 0.42              |
| 8:7:90:HIS:O     | 8:7:90:HIS:ND1   | 2.49                     | 0.42              |
| 3:C:191:PHE:CE2  | 3:C:199:VAL:HG23 | 2.55                     | 0.42              |
| 4:D:200:ARG:HA   | 4:D:200:ARG:HE   | 1.85                     | 0.42              |
| 5:E:81:LYS:HB2   | 5:E:82:ASP:H     | 1.64                     | 0.42              |
| 5:E:107:LEU:N    | 5:E:107:LEU:CD1  | 2.82                     | 0.42              |
| 1:1:438:ARG:H    | 1:1:438:ARG:HD2  | 1.85                     | 0.42              |
| 3:3:33:PHE:CE2   | 3:3:47:MET:HE3   | 2.54                     | 0.42              |
| 3:3:261:VAL:HG23 | 9:3:786:SF4:S2   | 2.60                     | 0.42              |
| 4:4:197:LEU:O    | 4:4:200:ARG:HB3  | 2.20                     | 0.42              |
| 5:5:16:PRO:HD2   | 5:5:28:VAL:HG13  | 2.01                     | 0.42              |
| 6:6:106:ILE:CD1  | 6:6:151:VAL:HG12 | 2.49                     | 0.42              |
| 7:9:41:HIS:HE1   | 7:9:98:CYS:SG    | 2.42                     | 0.42              |
| 8:7:43:ARG:HH11  | 8:7:48:TYR:CB    | 2.33                     | 0.42              |
| 1:A:37:GLY:C     | 1:A:39:GLU:H     | 2.28                     | 0.42              |
| 1:A:416:HIS:C    | 1:A:417:PHE:CD1  | 2.97                     | 0.42              |
| 3:C:120:PRO:HG2  | 8:H:42:TYR:CZ    | 2.55                     | 0.42              |
| 4:D:335:PHE:C    | 4:D:336:HIS:HD2  | 2.28                     | 0.42              |
| 4:D:383:TYR:CD1  | 4:D:383:TYR:C    | 2.96                     | 0.42              |
| 5:E:195:LEU:O    | 5:E:196:TRP:C    | 2.62                     | 0.42              |
| 1:1:367:MET:HE2  | 1:1:367:MET:HB3  | 1.74                     | 0.42              |
| 3:3:260:PRO:HG3  | 3:3:536:THR:O    | 2.19                     | 0.42              |
| 3:3:594:ALA:C    | 3:3:596:ARG:H    | 2.28                     | 0.42              |
| 4:4:182:LEU:HD22 | 4:4:186:PHE:CD2  | 2.54                     | 0.42              |
| 4:4:224:ILE:HD11 | 4:4:275:ARG:CZ   | 2.50                     | 0.42              |
| 5:5:78:PRO:HG3   | 5:5:85:GLY:CA    | 2.50                     | 0.42              |
| 7:9:96:LEU:HD21  | 7:9:129:LEU:HD13 | 2.01                     | 0.42              |
| 8:7:108:ILE:N    | 8:7:108:ILE:CD1  | 2.83                     | 0.42              |
| 2:B:154:LEU:O    | 2:B:158:ARG:HB2  | 2.20                     | 0.42              |
| 3:C:382:PHE:CD1  | 3:C:382:PHE:N    | 2.87                     | 0.42              |
| 3:C:695:ARG:HD2  | 3:C:717:TRP:CZ3  | 2.55                     | 0.42              |
| 3:C:701:ALA:N    | 3:C:763:LEU:O    | 2.51                     | 0.42              |
| 8:H:78:LYS:HA    | 8:H:78:LYS:HD3   | 1.73                     | 0.42              |
| 1:1:42:LYS:O     | 1:1:43:ARG:C     | 2.62                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:186:THR:CG2  | 1:1:200:ARG:N     | 2.69                     | 0.42              |
| 3:3:422:PRO:HA   | 3:3:423:PRO:HD2   | 1.91                     | 0.42              |
| 3:3:694:LEU:HD12 | 3:3:769:LEU:HB2   | 2.01                     | 0.42              |
| 4:4:196:VAL:O    | 4:4:200:ARG:HB2   | 2.20                     | 0.42              |
| 4:4:250:LYS:HG3  | 4:4:264:VAL:HG21  | 2.01                     | 0.42              |
| 4:4:393:MET:HE2  | 4:4:393:MET:HB3   | 1.89                     | 0.42              |
| 5:5:120:ASP:OD1  | 5:5:134:LYS:HG3   | 2.19                     | 0.42              |
| 6:6:104:TRP:HA   | 6:6:134:ASP:OD2   | 2.19                     | 0.42              |
| 1:A:10:ASP:OD1   | 1:A:11:PRO:HD2    | 2.20                     | 0.42              |
| 1:A:341:MET:HE2  | 1:A:409:PRO:C     | 2.45                     | 0.42              |
| 3:C:254:THR:OG1  | 3:C:624:LEU:HD23  | 2.19                     | 0.42              |
| 3:C:300:TRP:CD1  | 3:C:300:TRP:H     | 2.36                     | 0.42              |
| 3:C:361:ALA:CB   | 3:C:369:LEU:HD13  | 2.50                     | 0.42              |
| 5:E:137:THR:HB   | 5:E:141:LEU:HD22  | 2.02                     | 0.42              |
| 1:1:70:PHE:CG    | 1:1:71:PRO:HD2    | 2.54                     | 0.42              |
| 1:1:97:GLU:HB2   | 1:1:180:TYR:HE1   | 1.85                     | 0.42              |
| 1:1:391:LEU:N    | 1:1:392:PRO:CD    | 2.83                     | 0.42              |
| 10:1:440:FMN:C2  | 10:1:440:FMN:HO3' | 2.17                     | 0.42              |
| 3:3:397:LEU:HD21 | 3:3:480:LEU:HD13  | 2.01                     | 0.42              |
| 3:3:477:LEU:CD2  | 3:3:521:ALA:HB2   | 2.50                     | 0.42              |
| 3:3:516:VAL:O    | 3:3:520:ARG:HG3   | 2.19                     | 0.42              |
| 4:4:146:PHE:C    | 4:4:148:TYR:N     | 2.77                     | 0.42              |
| 1:A:92:ASN:HD21  | 10:A:440:FMN:C2   | 2.32                     | 0.42              |
| 4:D:211:SER:CB   | 4:D:214:PHE:HB3   | 2.50                     | 0.42              |
| 4:D:215:TYR:C    | 4:D:215:TYR:CD2   | 2.98                     | 0.42              |
| 5:E:150:TYR:HA   | 5:E:151:PRO:HD3   | 1.79                     | 0.42              |
| 6:F:138:PRO:HG3  | 7:G:121:MET:HG3   | 2.02                     | 0.42              |
| 7:G:112:ALA:HB3  | 9:G:184:SF4:S4    | 2.60                     | 0.42              |
| 1:1:28:THR:C     | 1:1:30:ASP:N      | 2.76                     | 0.41              |
| 1:1:438:ARG:HD2  | 1:1:438:ARG:N     | 2.35                     | 0.41              |
| 3:3:440:ARG:NH1  | 3:3:440:ARG:HG3   | 2.34                     | 0.41              |
| 3:3:701:ALA:N    | 3:3:763:LEU:O     | 2.51                     | 0.41              |
| 4:4:76:LEU:HD12  | 4:4:76:LEU:O      | 2.19                     | 0.41              |
| 4:4:163:VAL:HG13 | 4:4:164:THR:HG23  | 2.01                     | 0.41              |
| 6:6:96:TRP:O     | 6:6:99:MET:HB2    | 2.20                     | 0.41              |
| 2:B:79:HIS:ND1   | 2:B:118:SER:CB    | 2.83                     | 0.41              |
| 3:C:522:ARG:O    | 3:C:526:GLU:HG3   | 2.20                     | 0.41              |
| 3:C:715:GLU:C    | 3:C:715:GLU:OE2   | 2.63                     | 0.41              |
| 4:D:108:VAL:O    | 4:D:110:PRO:HD3   | 2.19                     | 0.41              |
| 4:D:140:LEU:HD13 | 4:D:208:PHE:CE2   | 2.54                     | 0.41              |
| 4:D:224:ILE:HD11 | 4:D:275:ARG:CZ    | 2.49                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:250:LYS:NZ   | 4:D:262:PHE:HB3  | 2.35                     | 0.41              |
| 5:E:30:PRO:HG2   | 5:E:33:ARG:HB2   | 2.02                     | 0.41              |
| 5:E:126:PHE:H    | 5:E:132:LEU:CD1  | 2.30                     | 0.41              |
| 8:H:6:GLU:O      | 8:H:10:TYR:CD2   | 2.73                     | 0.41              |
| 3:3:30:VAL:CG2   | 3:3:48:CYS:HA    | 2.50                     | 0.41              |
| 3:3:390:LEU:O    | 3:3:416:PHE:CD1  | 2.73                     | 0.41              |
| 3:3:547:MET:HE2  | 3:3:547:MET:HA   | 2.02                     | 0.41              |
| 6:6:147:LEU:O    | 6:6:147:LEU:HD13 | 2.20                     | 0.41              |
| 1:A:53:VAL:HG13  | 1:A:124:ALA:HB2  | 2.02                     | 0.41              |
| 1:A:249:MET:HA   | 1:A:267:PRO:HA   | 2.02                     | 0.41              |
| 3:C:270:ARG:HH11 | 3:C:270:ARG:HG3  | 1.85                     | 0.41              |
| 3:C:414:SER:OG   | 3:C:443:ARG:NH2  | 2.53                     | 0.41              |
| 5:E:146:LEU:HD22 | 5:E:146:LEU:HA   | 1.86                     | 0.41              |
| 6:F:163:TYR:CD2  | 6:F:169:ARG:HA   | 2.55                     | 0.41              |
| 7:G:141:VAL:O    | 7:G:141:VAL:HG12 | 2.20                     | 0.41              |
| 1:1:55:GLU:O     | 1:1:59:ARG:HG3   | 2.20                     | 0.41              |
| 2:2:33:ARG:O     | 2:2:34:VAL:C     | 2.63                     | 0.41              |
| 3:3:737:GLU:O    | 3:3:773:GLY:HA3  | 2.20                     | 0.41              |
| 5:5:137:THR:HB   | 5:5:141:LEU:HD22 | 2.02                     | 0.41              |
| 1:A:414:LEU:O    | 1:A:418:LYS:HB2  | 2.21                     | 0.41              |
| 6:F:100:PRO:O    | 6:F:103:LYS:HD3  | 2.20                     | 0.41              |
| 8:H:43:ARG:HH11  | 8:H:48:TYR:CB    | 2.34                     | 0.41              |
| 1:1:188:LEU:HD23 | 1:1:188:LEU:O    | 2.20                     | 0.41              |
| 1:1:272:PHE:HB3  | 1:1:276:ILE:HD11 | 2.02                     | 0.41              |
| 3:3:719:HIS:HA   | 3:3:720:PRO:HD3  | 1.89                     | 0.41              |
| 4:4:215:TYR:C    | 4:4:215:TYR:CD2  | 2.99                     | 0.41              |
| 5:5:53:VAL:HG22  | 5:5:55:LEU:HD12  | 2.02                     | 0.41              |
| 5:5:110:SER:C    | 5:5:112:ASN:H    | 2.29                     | 0.41              |
| 3:C:269:THR:HG23 | 3:C:274:LEU:HD13 | 2.03                     | 0.41              |
| 3:C:397:LEU:HD21 | 3:C:480:LEU:HD13 | 2.02                     | 0.41              |
| 3:C:616:ASN:C    | 3:C:618:GLU:N    | 2.77                     | 0.41              |
| 3:C:737:GLU:O    | 3:C:773:GLY:HA3  | 2.20                     | 0.41              |
| 4:D:205:GLU:OE1  | 4:D:284:ARG:NH2  | 2.53                     | 0.41              |
| 1:1:269:GLY:O    | 1:1:270:THR:C    | 2.60                     | 0.41              |
| 1:1:273:ARG:O    | 1:1:277:TYR:HB2  | 2.21                     | 0.41              |
| 2:2:44:GLU:CD    | 2:2:44:GLU:H     | 2.28                     | 0.41              |
| 2:2:61:MET:HB2   | 3:3:214:MET:HG3  | 2.01                     | 0.41              |
| 3:3:30:VAL:HG22  | 3:3:48:CYS:HA    | 2.03                     | 0.41              |
| 3:3:337:ARG:HD3  | 3:3:340:GLU:CG   | 2.50                     | 0.41              |
| 4:4:65:GLY:O     | 4:4:69:THR:CG2   | 2.67                     | 0.41              |
| 7:9:121:MET:HG3  | 7:9:121:MET:O    | 2.20                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:273:ARG:HA   | 1:A:307:LEU:HD22  | 2.02                     | 0.41              |
| 1:A:312:SER:C    | 1:A:314:GLU:H     | 2.28                     | 0.41              |
| 1:A:373:LYS:HE2  | 1:A:378:GLN:O     | 2.20                     | 0.41              |
| 3:C:38:HIS:CE1   | 3:C:287:GLU:HB3   | 2.56                     | 0.41              |
| 4:D:62:LEU:HD13  | 6:F:44:ALA:HB2    | 2.01                     | 0.41              |
| 5:E:78:PRO:HG3   | 5:E:85:GLY:CA     | 2.51                     | 0.41              |
| 6:F:30:TRP:CD1   | 6:F:30:TRP:C      | 2.97                     | 0.41              |
| 6:F:37:TRP:CE3   | 6:F:37:TRP:HA     | 2.55                     | 0.41              |
| 6:F:92:MET:O     | 6:F:92:MET:HG2    | 2.20                     | 0.41              |
| 6:F:163:TYR:HE1  | 7:G:152:ARG:HD2   | 1.84                     | 0.41              |
| 8:H:21:ARG:NH1   | 8:H:21:ARG:HG3    | 2.35                     | 0.41              |
| 10:1:440:FMN:H9  | 10:1:440:FMN:H1'1 | 1.64                     | 0.41              |
| 2:2:3:PHE:HB3    | 2:2:48:GLU:OE1    | 2.19                     | 0.41              |
| 3:3:246:ASN:H    | 3:3:246:ASN:ND2   | 2.18                     | 0.41              |
| 3:3:308:THR:C    | 3:3:603:PRO:HG3   | 2.45                     | 0.41              |
| 3:3:591:HIS:ND1  | 3:3:592:PRO:N     | 2.68                     | 0.41              |
| 4:4:131:VAL:HG23 | 4:4:153:ARG:NH1   | 2.36                     | 0.41              |
| 6:6:40:THR:OG1   | 6:6:50:MET:HE1    | 2.20                     | 0.41              |
| 7:9:71:GLU:HB2   | 7:9:90:VAL:HB     | 2.02                     | 0.41              |
| 7:9:136:MET:O    | 7:9:137:LEU:C     | 2.60                     | 0.41              |
| 1:A:28:THR:C     | 1:A:30:ASP:N      | 2.75                     | 0.41              |
| 1:A:42:LYS:O     | 1:A:43:ARG:C      | 2.64                     | 0.41              |
| 2:B:21:GLU:O     | 2:B:21:GLU:HG2    | 2.18                     | 0.41              |
| 3:C:101:ARG:CZ   | 3:C:101:ARG:CB    | 2.97                     | 0.41              |
| 3:C:321:THR:HG22 | 3:C:322:TRP:N     | 2.35                     | 0.41              |
| 3:C:464:ILE:H    | 3:C:464:ILE:HG12  | 1.55                     | 0.41              |
| 3:C:715:GLU:OE2  | 3:C:715:GLU:O     | 2.38                     | 0.41              |
| 3:C:753:VAL:HG13 | 3:C:759:TYR:CD1   | 2.55                     | 0.41              |
| 4:D:104:LEU:HA   | 5:E:22:LEU:HD11   | 2.02                     | 0.41              |
| 7:G:96:LEU:HD21  | 7:G:129:LEU:HD13  | 2.02                     | 0.41              |
| 8:H:16:LEU:C     | 8:H:16:LEU:HD13   | 2.45                     | 0.41              |
| 1:1:246:SER:O    | 1:1:268:MET:HG2   | 2.20                     | 0.41              |
| 1:1:249:MET:HA   | 1:1:267:PRO:HA    | 2.02                     | 0.41              |
| 2:2:79:HIS:O     | 2:2:136:VAL:O     | 2.38                     | 0.41              |
| 3:3:115:HIS:CG   | 3:3:116:PRO:CD    | 2.94                     | 0.41              |
| 3:3:150:GLU:O    | 3:3:151:LEU:C     | 2.63                     | 0.41              |
| 3:3:194:VAL:HG12 | 3:3:195:PRO:HD3   | 2.02                     | 0.41              |
| 3:3:300:TRP:CD1  | 3:3:300:TRP:H     | 2.38                     | 0.41              |
| 3:3:361:ALA:CB   | 3:3:369:LEU:HD13  | 2.50                     | 0.41              |
| 3:3:549:VAL:C    | 3:3:550:LEU:HD12  | 2.46                     | 0.41              |
| 2:B:31:LEU:HD12  | 2:B:41:ILE:HD13   | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:469:ARG:HB2  | 3:C:470:PRO:HD2  | 2.01                     | 0.41              |
| 3:C:616:ASN:HB3  | 3:C:618:GLU:HG3  | 2.01                     | 0.41              |
| 3:C:684:ARG:HA   | 3:C:685:PRO:HD2  | 1.84                     | 0.41              |
| 4:D:84:ARG:HD3   | 6:F:117:MET:CE   | 2.51                     | 0.41              |
| 4:D:164:THR:OG1  | 4:D:170:HIS:HB3  | 2.20                     | 0.41              |
| 6:F:147:LEU:O    | 6:F:147:LEU:HD13 | 2.21                     | 0.41              |
| 8:H:50:LEU:HD12  | 8:H:51:PRO:CD    | 2.49                     | 0.41              |
| 1:1:169:PHE:CE2  | 1:1:171:LEU:CD1  | 3.03                     | 0.41              |
| 3:3:281:GLU:HG3  | 3:3:283:PRO:HD3  | 2.03                     | 0.41              |
| 4:4:164:THR:OG1  | 4:4:170:HIS:HB3  | 2.21                     | 0.41              |
| 4:4:393:MET:CA   | 4:4:396:ILE:HG22 | 2.49                     | 0.41              |
| 8:7:14:VAL:O     | 8:7:17:LEU:HB2   | 2.20                     | 0.41              |
| 1:A:293:GLY:O    | 1:A:327:GLY:N    | 2.53                     | 0.41              |
| 3:C:202:PHE:C    | 3:C:203:ILE:HD13 | 2.45                     | 0.41              |
| 3:C:343:LEU:HD23 | 3:C:343:LEU:HA   | 1.86                     | 0.41              |
| 3:C:381:LEU:HD12 | 3:C:522:ARG:HD3  | 2.03                     | 0.41              |
| 3:C:390:LEU:O    | 3:C:416:PHE:CD1  | 2.74                     | 0.41              |
| 3:C:454:TYR:HB2  | 3:C:752:ASP:OD2  | 2.20                     | 0.41              |
| 4:D:143:LEU:HD23 | 4:D:143:LEU:O    | 2.21                     | 0.41              |
| 5:E:54:GLY:O     | 5:E:55:LEU:HD12  | 2.20                     | 0.41              |
| 5:E:77:LEU:HA    | 5:E:78:PRO:HD3   | 1.86                     | 0.41              |
| 6:F:106:ILE:HD12 | 6:F:151:VAL:HG12 | 2.02                     | 0.41              |
| 8:H:97:TYR:CD2   | 8:H:97:TYR:C     | 2.99                     | 0.41              |
| 8:H:112:LYS:CG   | 8:H:116:PHE:CE1  | 3.03                     | 0.41              |
| 1:1:32:TYR:O     | 1:1:37:GLY:HA2   | 2.20                     | 0.41              |
| 1:1:102:LYS:HG2  | 1:1:253:GLN:OE1  | 2.21                     | 0.41              |
| 1:1:273:ARG:HA   | 1:1:307:LEU:HD22 | 2.03                     | 0.41              |
| 1:1:364:ALA:HB3  | 3:3:207:VAL:HG13 | 2.01                     | 0.41              |
| 2:2:142:VAL:HG11 | 2:2:153:LEU:HG   | 2.02                     | 0.41              |
| 3:3:36:GLU:O     | 3:3:37:LYS:C     | 2.64                     | 0.41              |
| 3:3:118:ASP:HB2  | 9:3:784:SF4:S1   | 2.61                     | 0.41              |
| 3:3:252:THR:HA   | 3:3:253:PRO:HD2  | 1.86                     | 0.41              |
| 3:3:321:THR:HG22 | 3:3:322:TRP:N    | 2.36                     | 0.41              |
| 3:3:373:GLY:HA3  | 3:3:538:ALA:HB2  | 2.03                     | 0.41              |
| 3:3:454:TYR:HB2  | 3:3:752:ASP:OD2  | 2.20                     | 0.41              |
| 3:3:592:PRO:HA   | 3:3:595:GLU:OE2  | 2.21                     | 0.41              |
| 3:3:601:VAL:C    | 3:3:602:LEU:HD12 | 2.46                     | 0.41              |
| 3:3:692:PHE:HE1  | 3:3:773:GLY:C    | 2.28                     | 0.41              |
| 3:3:753:VAL:HG13 | 3:3:759:TYR:CD1  | 2.55                     | 0.41              |
| 4:4:62:LEU:HD13  | 6:6:44:ALA:HB2   | 2.03                     | 0.41              |
| 4:4:88:LEU:HD12  | 4:4:403:VAL:HG21 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:102:GLU:HG2  | 4:4:175:ILE:O    | 2.21                     | 0.41              |
| 4:4:276:MET:O    | 4:4:280:ILE:HG13 | 2.21                     | 0.41              |
| 5:5:2:ARG:HD2    | 5:5:84:ASP:OD1   | 2.21                     | 0.41              |
| 6:6:146:ALA:HB2  | 7:9:119:PHE:HD1  | 1.85                     | 0.41              |
| 7:9:63:CYS:HA    | 7:9:64:PRO:HD3   | 1.91                     | 0.41              |
| 7:9:108:CYS:HA   | 7:9:109:PRO:HD3  | 1.90                     | 0.41              |
| 7:9:138:VAL:HG23 | 7:9:139:ASP:N    | 2.36                     | 0.41              |
| 1:A:186:THR:HG21 | 1:A:200:ARG:H    | 1.77                     | 0.41              |
| 1:A:259:LYS:CA   | 1:A:284:LEU:HD21 | 2.48                     | 0.41              |
| 1:A:260:ARG:O    | 1:A:260:ARG:HG3  | 2.20                     | 0.41              |
| 1:A:354:GLY:HA2  | 1:A:360:ARG:HB2  | 2.03                     | 0.41              |
| 2:B:61:MET:HE1   | 8:H:88:ARG:HD3   | 2.03                     | 0.41              |
| 2:B:86:LEU:HD11  | 2:B:90:LEU:HD11  | 2.02                     | 0.41              |
| 3:C:54:LEU:N     | 3:C:55:PRO:HD3   | 2.36                     | 0.41              |
| 3:C:55:PRO:HG3   | 3:C:74:GLN:N     | 2.36                     | 0.41              |
| 3:C:129:GLU:CD   | 3:C:186:ARG:HH12 | 2.28                     | 0.41              |
| 3:C:259:CYS:HB2  | 3:C:260:PRO:CD   | 2.51                     | 0.41              |
| 3:C:454:TYR:CD2  | 3:C:454:TYR:N    | 2.88                     | 0.41              |
| 3:C:474:ARG:NH2  | 3:C:516:VAL:CG2  | 2.58                     | 0.41              |
| 3:C:560:GLU:HA   | 3:C:561:PRO:HD2  | 1.88                     | 0.41              |
| 3:C:627:ALA:HA   | 3:C:628:PRO:HD3  | 1.81                     | 0.41              |
| 3:C:695:ARG:HA   | 3:C:696:PRO:HD2  | 1.91                     | 0.41              |
| 4:D:64:THR:N     | 4:D:409:ARG:OXT  | 2.54                     | 0.41              |
| 4:D:159:LEU:O    | 4:D:162:TRP:HB2  | 2.20                     | 0.41              |
| 4:D:290:ILE:O    | 4:D:294:LEU:HB2  | 2.21                     | 0.41              |
| 4:D:316:LEU:C    | 4:D:318:GLU:H    | 2.29                     | 0.41              |
| 4:D:400:LEU:HA   | 4:D:400:LEU:HD23 | 1.83                     | 0.41              |
| 5:E:160:ARG:HG3  | 7:G:130:VAL:CG1  | 2.51                     | 0.41              |
| 6:F:30:TRP:CD1   | 6:F:30:TRP:O     | 2.73                     | 0.41              |
| 1:1:272:PHE:HB3  | 1:1:276:ILE:CD1  | 2.51                     | 0.41              |
| 3:3:469:ARG:HB2  | 3:3:470:PRO:HD2  | 2.03                     | 0.41              |
| 3:3:695:ARG:NH1  | 3:3:697:THR:HG22 | 2.36                     | 0.41              |
| 3:3:753:VAL:HA   | 3:3:754:PRO:HD2  | 1.83                     | 0.41              |
| 8:7:63:LEU:HD12  | 8:7:63:LEU:HA    | 1.85                     | 0.41              |
| 1:A:110:VAL:O    | 1:A:110:VAL:HG23 | 2.19                     | 0.41              |
| 1:A:155:ARG:H    | 1:A:155:ARG:HG2  | 1.69                     | 0.41              |
| 1:A:238:PHE:CZ   | 1:A:248:GLY:HA3  | 2.56                     | 0.41              |
| 3:C:256:CYS:HB2  | 3:C:265:ILE:HD13 | 2.03                     | 0.41              |
| 3:C:402:PRO:CB   | 3:C:535:MET:HE1  | 2.49                     | 0.41              |
| 3:C:451:PHE:CE1  | 3:C:466:GLU:HB3  | 2.55                     | 0.41              |
| 4:D:376:VAL:O    | 4:D:379:GLN:HG3  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:164:ASN:HD22 | 6:F:170:LEU:HD21 | 1.85                     | 0.41              |
| 1:1:63:ARG:NH1   | 1:1:313:TYR:HB3  | 2.36                     | 0.40              |
| 1:1:107:LEU:CD2  | 1:1:114:LEU:HD12 | 2.51                     | 0.40              |
| 1:1:211:LEU:CB   | 1:1:216:THR:HG21 | 2.50                     | 0.40              |
| 2:2:163:LEU:C    | 2:2:165:GLU:H    | 2.29                     | 0.40              |
| 3:3:129:GLU:CD   | 3:3:186:ARG:HH12 | 2.28                     | 0.40              |
| 4:4:40:VAL:CG2   | 6:6:88:MET:HE2   | 2.51                     | 0.40              |
| 4:4:200:ARG:HG3  | 4:4:204:TYR:HE1  | 1.86                     | 0.40              |
| 4:4:304:ASP:HA   | 4:4:305:PRO:HD2  | 1.81                     | 0.40              |
| 6:6:138:PRO:HG3  | 7:9:121:MET:HG3  | 2.02                     | 0.40              |
| 1:A:55:GLU:O     | 1:A:59:ARG:HG3   | 2.21                     | 0.40              |
| 1:A:273:ARG:O    | 1:A:277:TYR:HB2  | 2.22                     | 0.40              |
| 1:A:331:ILE:HA   | 1:A:332:PRO:HD2  | 1.89                     | 0.40              |
| 1:A:404:ASP:O    | 1:A:405:ALA:C    | 2.64                     | 0.40              |
| 2:B:44:GLU:N     | 2:B:44:GLU:CD    | 2.80                     | 0.40              |
| 2:B:144:CYS:O    | 2:B:149:ARG:HD3  | 2.21                     | 0.40              |
| 4:D:146:PHE:C    | 4:D:148:TYR:N    | 2.79                     | 0.40              |
| 4:D:295:GLU:C    | 4:D:297:LEU:H    | 2.29                     | 0.40              |
| 5:E:2:ARG:HD2    | 5:E:84:ASP:OD1   | 2.22                     | 0.40              |
| 6:F:101:ASP:O    | 6:F:103:LYS:N    | 2.54                     | 0.40              |
| 7:G:40:ARG:HH11  | 7:G:40:ARG:HG2   | 1.87                     | 0.40              |
| 1:1:312:SER:C    | 1:1:314:GLU:H    | 2.29                     | 0.40              |
| 4:4:383:TYR:CD1  | 4:4:383:TYR:C    | 2.99                     | 0.40              |
| 5:5:13:LYS:NZ    | 5:5:33:ARG:HH21  | 2.19                     | 0.40              |
| 1:A:181:ILE:C    | 1:A:183:GLY:H    | 2.30                     | 0.40              |
| 1:A:253:GLN:N    | 1:A:253:GLN:NE2  | 2.56                     | 0.40              |
| 2:B:3:PHE:HB3    | 2:B:48:GLU:OE1   | 2.22                     | 0.40              |
| 2:B:76:GLY:N     | 2:B:118:SER:OG   | 2.45                     | 0.40              |
| 3:C:101:ARG:HH12 | 3:C:140:TYR:HD1  | 1.54                     | 0.40              |
| 3:C:124:LYS:HG3  | 3:C:232:VAL:C    | 2.46                     | 0.40              |
| 3:C:281:GLU:HA   | 3:C:287:GLU:O    | 2.21                     | 0.40              |
| 3:C:478:LEU:HD21 | 3:C:483:ASP:HB2  | 2.03                     | 0.40              |
| 4:D:84:ARG:HG2   | 9:F:182:SF4:S2   | 2.61                     | 0.40              |
| 4:D:215:TYR:C    | 4:D:215:TYR:HD2  | 2.29                     | 0.40              |
| 4:D:275:ARG:O    | 4:D:279:ARG:HG3  | 2.20                     | 0.40              |
| 7:G:94:ASN:OD1   | 7:G:97:ARG:N     | 2.50                     | 0.40              |
| 1:1:211:LEU:HD12 | 1:1:211:LEU:HA   | 1.65                     | 0.40              |
| 2:2:42:ARG:H     | 2:2:45:ARG:HG3   | 1.86                     | 0.40              |
| 2:2:44:GLU:CD    | 2:2:44:GLU:N     | 2.78                     | 0.40              |
| 2:2:106:ILE:HD11 | 2:2:112:THR:HB   | 2.04                     | 0.40              |
| 3:3:33:PHE:CZ    | 3:3:130:LEU:HD12 | 2.56                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:118:ASP:O    | 3:3:119:CYS:C    | 2.64                     | 0.40              |
| 6:6:30:TRP:CD1   | 6:6:30:TRP:C     | 2.99                     | 0.40              |
| 6:6:148:ILE:O    | 6:6:152:MET:HG3  | 2.21                     | 0.40              |
| 8:7:43:ARG:HH11  | 8:7:48:TYR:HB2   | 1.86                     | 0.40              |
| 1:A:114:LEU:C    | 1:A:114:LEU:CD2  | 2.94                     | 0.40              |
| 2:B:44:GLU:CD    | 2:B:44:GLU:H     | 2.29                     | 0.40              |
| 3:C:160:THR:OG1  | 8:H:73:SER:CB    | 2.64                     | 0.40              |
| 3:C:274:LEU:HD12 | 3:C:274:LEU:C    | 2.46                     | 0.40              |
| 3:C:602:LEU:HA   | 3:C:603:PRO:HD2  | 1.85                     | 0.40              |
| 3:C:606:THR:O    | 3:C:610:LYS:HG3  | 2.21                     | 0.40              |
| 3:C:678:PHE:CZ   | 3:C:680:LEU:HD12 | 2.56                     | 0.40              |
| 4:D:87:TYR:CZ    | 4:D:403:VAL:HG13 | 2.56                     | 0.40              |
| 5:E:144:HIS:HA   | 5:E:145:PRO:HD2  | 1.84                     | 0.40              |
| 6:F:137:VAL:HA   | 6:F:138:PRO:HD2  | 1.95                     | 0.40              |
| 1:1:53:VAL:HG13  | 1:1:124:ALA:HB2  | 2.03                     | 0.40              |
| 1:1:202:LYS:N    | 1:1:203:PRO:HD2  | 2.36                     | 0.40              |
| 1:1:415:ARG:O    | 1:1:415:ARG:CG   | 2.63                     | 0.40              |
| 3:3:33:PHE:HZ    | 3:3:130:LEU:HD12 | 1.86                     | 0.40              |
| 3:3:50:VAL:HG12  | 3:3:95:THR:HG22  | 2.02                     | 0.40              |
| 4:4:381:LEU:HA   | 4:4:384:ALA:HB3  | 2.03                     | 0.40              |
| 5:5:75:VAL:HG12  | 5:5:76:SER:H     | 1.87                     | 0.40              |
| 6:6:127:VAL:HG12 | 6:6:131:VAL:HG22 | 2.04                     | 0.40              |
| 8:7:6:GLU:O      | 8:7:10:TYR:CD2   | 2.75                     | 0.40              |
| 1:A:242:GLY:CA   | 1:A:268:MET:O    | 2.57                     | 0.40              |
| 3:C:458:LEU:HD12 | 3:C:458:LEU:H    | 1.87                     | 0.40              |
| 4:D:73:ARG:C     | 4:D:364:MET:HG2  | 2.46                     | 0.40              |
| 4:D:240:ARG:HB2  | 4:D:266:LEU:HD23 | 2.02                     | 0.40              |
| 6:F:116:GLY:C    | 6:F:118:PHE:H    | 2.28                     | 0.40              |
| 6:F:117:MET:HE2  | 7:G:99:ILE:CG1   | 2.28                     | 0.40              |
| 3:3:381:LEU:HD12 | 3:3:522:ARG:HD3  | 2.04                     | 0.40              |
| 4:4:215:TYR:C    | 4:4:215:TYR:HD2  | 2.29                     | 0.40              |
| 4:4:234:LEU:O    | 4:4:234:LEU:HD13 | 2.22                     | 0.40              |
| 4:4:295:GLU:C    | 4:4:297:LEU:H    | 2.29                     | 0.40              |
| 4:4:318:GLU:HB2  | 8:7:39:ASP:HA    | 2.04                     | 0.40              |
| 6:6:131:VAL:HA   | 6:6:132:PRO:HD3  | 1.93                     | 0.40              |
| 6:6:154:LEU:O    | 6:6:154:LEU:HG   | 2.20                     | 0.40              |
| 1:A:211:LEU:CB   | 1:A:216:THR:HG21 | 2.51                     | 0.40              |
| 1:A:272:PHE:HD1  | 1:A:272:PHE:H    | 1.69                     | 0.40              |
| 1:A:371:PHE:HZ   | 1:A:410:VAL:HG13 | 1.86                     | 0.40              |
| 2:B:168:LEU:HA   | 2:B:169:PRO:HD2  | 1.75                     | 0.40              |
| 3:C:101:ARG:HB3  | 3:C:101:ARG:HH11 | 1.80                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 3:C:477:LEU:CD2 | 3:C:521:ALA:HB2 | 2.51                     | 0.40              |
| 4:D:168:PHE:HE1 | 6:F:141:PRO:CG  | 2.31                     | 0.40              |

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

| Atom-1        | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|------------------------|--------------------------|-------------------|
| 1:1:427:GLU:O | 3:3:316:ARG:NH1[2_545] | 2.17                     | 0.03              |

## 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   | 1     | 435/438 (99%) | 362 (83%) | 58 (13%)  | 15 (3%)  | 3           | 16 |
| 1   | A     | 435/438 (99%) | 358 (82%) | 64 (15%)  | 13 (3%)  | 3           | 19 |
| 2   | 2     | 176/181 (97%) | 156 (89%) | 16 (9%)   | 4 (2%)   | 5           | 23 |
| 2   | B     | 176/181 (97%) | 155 (88%) | 17 (10%)  | 4 (2%)   | 5           | 23 |
| 3   | 3     | 748/783 (96%) | 633 (85%) | 92 (12%)  | 23 (3%)  | 3           | 18 |
| 3   | C     | 748/783 (96%) | 625 (84%) | 103 (14%) | 20 (3%)  | 4           | 20 |
| 4   | 4     | 373/409 (91%) | 322 (86%) | 37 (10%)  | 14 (4%)  | 2           | 15 |
| 4   | D     | 373/409 (91%) | 322 (86%) | 37 (10%)  | 14 (4%)  | 2           | 15 |
| 5   | 5     | 194/207 (94%) | 165 (85%) | 23 (12%)  | 6 (3%)   | 3           | 18 |
| 5   | E     | 194/207 (94%) | 165 (85%) | 24 (12%)  | 5 (3%)   | 4           | 21 |
| 6   | 6     | 141/181 (78%) | 114 (81%) | 22 (16%)  | 5 (4%)   | 3           | 16 |
| 6   | F     | 141/181 (78%) | 117 (83%) | 19 (14%)  | 5 (4%)   | 3           | 16 |
| 7   | 9     | 152/182 (84%) | 131 (86%) | 17 (11%)  | 4 (3%)   | 4           | 21 |
| 7   | G     | 152/182 (84%) | 130 (86%) | 17 (11%)  | 5 (3%)   | 3           | 17 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 8   | 7     | 125/129 (97%)   | 112 (90%)  | 12 (10%)  | 1 (1%)   | 16          | 47 |
| 8   | H     | 125/129 (97%)   | 111 (89%)  | 13 (10%)  | 1 (1%)   | 16          | 47 |
| All | All   | 4688/5020 (93%) | 3978 (85%) | 571 (12%) | 139 (3%) | 3           | 19 |

All (139) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 4   | PRO  |
| 1   | 1     | 81  | LYS  |
| 2   | 2     | 86  | LEU  |
| 2   | 2     | 136 | VAL  |
| 2   | 2     | 140 | PRO  |
| 3   | 3     | 6   | VAL  |
| 3   | 3     | 117 | LEU  |
| 3   | 3     | 580 | LYS  |
| 7   | 9     | 173 | PHE  |
| 1   | A     | 4   | PRO  |
| 1   | A     | 81  | LYS  |
| 2   | B     | 86  | LEU  |
| 2   | B     | 136 | VAL  |
| 2   | B     | 140 | PRO  |
| 3   | C     | 6   | VAL  |
| 3   | C     | 117 | LEU  |
| 3   | C     | 580 | LYS  |
| 7   | G     | 173 | PHE  |
| 1   | 1     | 37  | GLY  |
| 1   | 1     | 160 | LYS  |
| 3   | 3     | 125 | GLY  |
| 3   | 3     | 184 | CYS  |
| 3   | 3     | 204 | GLU  |
| 3   | 3     | 285 | VAL  |
| 3   | 3     | 563 | ALA  |
| 4   | 4     | 51  | GLU  |
| 4   | 4     | 236 | GLY  |
| 4   | 4     | 258 | GLU  |
| 4   | 4     | 334 | GLY  |
| 5   | 5     | 176 | GLY  |
| 6   | 6     | 45  | CYS  |
| 6   | 6     | 77  | VAL  |
| 6   | 6     | 126 | ASN  |
| 1   | A     | 37  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 160 | LYS  |
| 3   | C     | 125 | GLY  |
| 3   | C     | 184 | CYS  |
| 3   | C     | 204 | GLU  |
| 3   | C     | 285 | VAL  |
| 3   | C     | 563 | ALA  |
| 4   | D     | 51  | GLU  |
| 4   | D     | 236 | GLY  |
| 4   | D     | 258 | GLU  |
| 4   | D     | 334 | GLY  |
| 5   | E     | 176 | GLY  |
| 6   | F     | 77  | VAL  |
| 6   | F     | 126 | ASN  |
| 1   | 1     | 18  | TYR  |
| 1   | 1     | 166 | ASP  |
| 1   | 1     | 311 | MET  |
| 3   | 3     | 220 | SER  |
| 3   | 3     | 365 | LYS  |
| 4   | 4     | 235 | THR  |
| 4   | 4     | 389 | GLN  |
| 5   | 5     | 47  | ASN  |
| 7   | 9     | 37  | PHE  |
| 7   | 9     | 48  | ASN  |
| 1   | A     | 166 | ASP  |
| 1   | A     | 311 | MET  |
| 1   | A     | 314 | GLU  |
| 3   | C     | 220 | SER  |
| 3   | C     | 365 | LYS  |
| 4   | D     | 389 | GLN  |
| 5   | E     | 47  | ASN  |
| 6   | F     | 45  | CYS  |
| 7   | G     | 48  | ASN  |
| 7   | G     | 100 | PHE  |
| 1   | 1     | 43  | ARG  |
| 1   | 1     | 314 | GLU  |
| 3   | 3     | 139 | LEU  |
| 3   | 3     | 219 | PRO  |
| 4   | 4     | 255 | SER  |
| 4   | 4     | 390 | VAL  |
| 5   | 5     | 81  | LYS  |
| 5   | 5     | 138 | PRO  |
| 1   | A     | 18  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 43  | ARG  |
| 3   | C     | 139 | LEU  |
| 3   | C     | 219 | PRO  |
| 4   | D     | 235 | THR  |
| 4   | D     | 255 | SER  |
| 4   | D     | 390 | VAL  |
| 5   | E     | 138 | PRO  |
| 7   | G     | 37  | PHE  |
| 1   | 1     | 292 | PRO  |
| 1   | 1     | 313 | TYR  |
| 2   | 2     | 48  | GLU  |
| 3   | 3     | 54  | LEU  |
| 3   | 3     | 372 | GLN  |
| 3   | 3     | 704 | ALA  |
| 4   | 4     | 211 | SER  |
| 4   | 4     | 381 | LEU  |
| 5   | 5     | 35  | LYS  |
| 5   | 5     | 111 | ALA  |
| 7   | 9     | 100 | PHE  |
| 1   | A     | 292 | PRO  |
| 2   | B     | 48  | GLU  |
| 3   | C     | 54  | LEU  |
| 3   | C     | 682 | GLU  |
| 3   | C     | 704 | ALA  |
| 5   | E     | 35  | LYS  |
| 5   | E     | 81  | LYS  |
| 1   | 1     | 193 | GLU  |
| 3   | 3     | 682 | GLU  |
| 1   | A     | 234 | GLY  |
| 3   | C     | 457 | PRO  |
| 4   | D     | 211 | SER  |
| 4   | D     | 381 | LEU  |
| 1   | 1     | 71  | PRO  |
| 3   | 3     | 457 | PRO  |
| 8   | 7     | 74  | PRO  |
| 1   | A     | 71  | PRO  |
| 8   | H     | 74  | PRO  |
| 1   | 1     | 234 | GLY  |
| 3   | 3     | 453 | PRO  |
| 3   | 3     | 529 | GLY  |
| 4   | 4     | 198 | PRO  |
| 4   | 4     | 212 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 198 | PRO  |
| 4   | D     | 212 | PRO  |
| 4   | D     | 270 | GLY  |
| 6   | F     | 100 | PRO  |
| 3   | 3     | 367 | PRO  |
| 3   | 3     | 690 | GLY  |
| 4   | 4     | 270 | GLY  |
| 3   | C     | 367 | PRO  |
| 3   | C     | 549 | VAL  |
| 1   | 1     | 3   | GLY  |
| 3   | 3     | 549 | VAL  |
| 4   | 4     | 402 | PRO  |
| 6   | 6     | 100 | PRO  |
| 6   | 6     | 101 | ASP  |
| 1   | A     | 3   | GLY  |
| 3   | C     | 508 | GLY  |
| 3   | C     | 690 | GLY  |
| 6   | F     | 101 | ASP  |
| 7   | G     | 55  | GLY  |
| 3   | 3     | 508 | GLY  |
| 4   | D     | 402 | PRO  |

### 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   | 1     | 355/356 (100%) | 316 (89%) | 39 (11%) | 6           | 24 |
| 1   | A     | 355/356 (100%) | 316 (89%) | 39 (11%) | 6           | 24 |
| 2   | 2     | 150/152 (99%)  | 126 (84%) | 24 (16%) | 2           | 12 |
| 2   | B     | 150/152 (99%)  | 125 (83%) | 25 (17%) | 2           | 10 |
| 3   | 3     | 607/628 (97%)  | 535 (88%) | 72 (12%) | 5           | 21 |
| 3   | C     | 607/628 (97%)  | 532 (88%) | 75 (12%) | 4           | 19 |
| 4   | 4     | 325/355 (92%)  | 288 (89%) | 37 (11%) | 5           | 23 |
| 4   | D     | 325/355 (92%)  | 291 (90%) | 34 (10%) | 6           | 26 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 5   | 5     | 167/175 (95%)   | 151 (90%)  | 16 (10%)  | 8           | 30 |
| 5   | E     | 167/175 (95%)   | 151 (90%)  | 16 (10%)  | 8           | 30 |
| 6   | 6     | 118/149 (79%)   | 100 (85%)  | 18 (15%)  | 3           | 12 |
| 6   | F     | 118/149 (79%)   | 98 (83%)   | 20 (17%)  | 2           | 10 |
| 7   | 9     | 126/150 (84%)   | 112 (89%)  | 14 (11%)  | 6           | 24 |
| 7   | G     | 126/150 (84%)   | 112 (89%)  | 14 (11%)  | 6           | 24 |
| 8   | 7     | 104/106 (98%)   | 92 (88%)   | 12 (12%)  | 5           | 23 |
| 8   | H     | 104/106 (98%)   | 92 (88%)   | 12 (12%)  | 5           | 23 |
| All | All   | 3904/4142 (94%) | 3437 (88%) | 467 (12%) | 5           | 21 |

All (467) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 10  | ASP  |
| 1   | 1     | 29  | LEU  |
| 1   | 1     | 49  | THR  |
| 1   | 1     | 104 | ARG  |
| 1   | 1     | 114 | LEU  |
| 1   | 1     | 128 | THR  |
| 1   | 1     | 134 | VAL  |
| 1   | 1     | 144 | ARG  |
| 1   | 1     | 155 | ARG  |
| 1   | 1     | 161 | ASN  |
| 1   | 1     | 168 | SER  |
| 1   | 1     | 171 | LEU  |
| 1   | 1     | 186 | THR  |
| 1   | 1     | 217 | THR  |
| 1   | 1     | 241 | MET  |
| 1   | 1     | 243 | THR  |
| 1   | 1     | 249 | MET  |
| 1   | 1     | 253 | GLN  |
| 1   | 1     | 255 | SER  |
| 1   | 1     | 270 | THR  |
| 1   | 1     | 271 | THR  |
| 1   | 1     | 278 | GLU  |
| 1   | 1     | 290 | ILE  |
| 1   | 1     | 291 | ILE  |
| 1   | 1     | 295 | SER  |
| 1   | 1     | 309 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 316 | LEU  |
| 1   | 1     | 323 | LEU  |
| 1   | 1     | 342 | TRP  |
| 1   | 1     | 346 | ARG  |
| 1   | 1     | 357 | THR  |
| 1   | 1     | 363 | VAL  |
| 1   | 1     | 368 | VAL  |
| 1   | 1     | 374 | ILE  |
| 1   | 1     | 388 | GLU  |
| 1   | 1     | 397 | ARG  |
| 1   | 1     | 414 | LEU  |
| 1   | 1     | 419 | ASP  |
| 1   | 1     | 437 | TRP  |
| 2   | 2     | 5   | ASP  |
| 2   | 2     | 7   | LYS  |
| 2   | 2     | 24  | ARG  |
| 2   | 2     | 31  | LEU  |
| 2   | 2     | 35  | GLN  |
| 2   | 2     | 45  | ARG  |
| 2   | 2     | 53  | VAL  |
| 2   | 2     | 61  | MET  |
| 2   | 2     | 87  | SER  |
| 2   | 2     | 89  | LYS  |
| 2   | 2     | 96  | LEU  |
| 2   | 2     | 106 | ILE  |
| 2   | 2     | 114 | ASP  |
| 2   | 2     | 122 | VAL  |
| 2   | 2     | 139 | GLU  |
| 2   | 2     | 140 | PRO  |
| 2   | 2     | 144 | CYS  |
| 2   | 2     | 146 | THR  |
| 2   | 2     | 150 | LEU  |
| 2   | 2     | 153 | LEU  |
| 2   | 2     | 162 | ARG  |
| 2   | 2     | 163 | LEU  |
| 2   | 2     | 172 | CYS  |
| 2   | 2     | 176 | VAL  |
| 3   | 3     | 11  | VAL  |
| 3   | 3     | 23  | VAL  |
| 3   | 3     | 32  | LEU  |
| 3   | 3     | 42  | ILE  |
| 3   | 3     | 55  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 3     | 73  | ILE  |
| 3   | 3     | 94  | ASP  |
| 3   | 3     | 121 | THR  |
| 3   | 3     | 123 | ASP  |
| 3   | 3     | 124 | LYS  |
| 3   | 3     | 133 | ARG  |
| 3   | 3     | 135 | VAL  |
| 3   | 3     | 150 | GLU  |
| 3   | 3     | 153 | VAL  |
| 3   | 3     | 168 | HIS  |
| 3   | 3     | 188 | VAL  |
| 3   | 3     | 189 | ARG  |
| 3   | 3     | 192 | GLU  |
| 3   | 3     | 207 | VAL  |
| 3   | 3     | 209 | THR  |
| 3   | 3     | 214 | MET  |
| 3   | 3     | 218 | LEU  |
| 3   | 3     | 219 | PRO  |
| 3   | 3     | 220 | SER  |
| 3   | 3     | 238 | LEU  |
| 3   | 3     | 269 | THR  |
| 3   | 3     | 274 | LEU  |
| 3   | 3     | 275 | LEU  |
| 3   | 3     | 282 | VAL  |
| 3   | 3     | 284 | GLU  |
| 3   | 3     | 303 | GLN  |
| 3   | 3     | 306 | LEU  |
| 3   | 3     | 317 | LEU  |
| 3   | 3     | 337 | ARG  |
| 3   | 3     | 369 | LEU  |
| 3   | 3     | 381 | LEU  |
| 3   | 3     | 399 | LEU  |
| 3   | 3     | 408 | ILE  |
| 3   | 3     | 412 | ARG  |
| 3   | 3     | 417 | VAL  |
| 3   | 3     | 419 | ASP  |
| 3   | 3     | 425 | ARG  |
| 3   | 3     | 435 | LEU  |
| 3   | 3     | 440 | ARG  |
| 3   | 3     | 448 | MET  |
| 3   | 3     | 450 | LEU  |
| 3   | 3     | 464 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 3     | 473 | GLU  |
| 3   | 3     | 501 | LYS  |
| 3   | 3     | 507 | LEU  |
| 3   | 3     | 512 | LEU  |
| 3   | 3     | 514 | ASP  |
| 3   | 3     | 515 | THR  |
| 3   | 3     | 523 | LEU  |
| 3   | 3     | 542 | ARG  |
| 3   | 3     | 550 | LEU  |
| 3   | 3     | 587 | LEU  |
| 3   | 3     | 593 | LEU  |
| 3   | 3     | 617 | LEU  |
| 3   | 3     | 644 | LEU  |
| 3   | 3     | 655 | ARG  |
| 3   | 3     | 676 | LEU  |
| 3   | 3     | 683 | LEU  |
| 3   | 3     | 684 | ARG  |
| 3   | 3     | 705 | VAL  |
| 3   | 3     | 715 | GLU  |
| 3   | 3     | 716 | LEU  |
| 3   | 3     | 738 | THR  |
| 3   | 3     | 747 | VAL  |
| 3   | 3     | 771 | VAL  |
| 3   | 3     | 776 | LEU  |
| 3   | 3     | 777 | VAL  |
| 4   | 4     | 40  | VAL  |
| 4   | 4     | 44  | MET  |
| 4   | 4     | 59  | ILE  |
| 4   | 4     | 69  | THR  |
| 4   | 4     | 74  | THR  |
| 4   | 4     | 99  | LEU  |
| 4   | 4     | 104 | LEU  |
| 4   | 4     | 105 | LEU  |
| 4   | 4     | 120 | LEU  |
| 4   | 4     | 129 | HIS  |
| 4   | 4     | 131 | VAL  |
| 4   | 4     | 143 | LEU  |
| 4   | 4     | 152 | GLU  |
| 4   | 4     | 163 | VAL  |
| 4   | 4     | 168 | PHE  |
| 4   | 4     | 170 | HIS  |
| 4   | 4     | 187 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 4     | 200 | ARG  |
| 4   | 4     | 201 | ILE  |
| 4   | 4     | 213 | ILE  |
| 4   | 4     | 219 | ARG  |
| 4   | 4     | 230 | ILE  |
| 4   | 4     | 234 | LEU  |
| 4   | 4     | 239 | LEU  |
| 4   | 4     | 262 | PHE  |
| 4   | 4     | 272 | VAL  |
| 4   | 4     | 290 | ILE  |
| 4   | 4     | 296 | ARG  |
| 4   | 4     | 297 | LEU  |
| 4   | 4     | 314 | ARG  |
| 4   | 4     | 317 | LEU  |
| 4   | 4     | 319 | THR  |
| 4   | 4     | 342 | VAL  |
| 4   | 4     | 367 | ARG  |
| 4   | 4     | 369 | LYS  |
| 4   | 4     | 396 | ILE  |
| 4   | 4     | 407 | VAL  |
| 5   | 5     | 5   | ARG  |
| 5   | 5     | 25  | LEU  |
| 5   | 5     | 27  | VAL  |
| 5   | 5     | 38  | MET  |
| 5   | 5     | 52  | ILE  |
| 5   | 5     | 80  | TRP  |
| 5   | 5     | 84  | ASP  |
| 5   | 5     | 90  | VAL  |
| 5   | 5     | 104 | VAL  |
| 5   | 5     | 107 | LEU  |
| 5   | 5     | 141 | LEU  |
| 5   | 5     | 146 | LEU  |
| 5   | 5     | 147 | ARG  |
| 5   | 5     | 154 | GLU  |
| 5   | 5     | 157 | THR  |
| 5   | 5     | 161 | GLU  |
| 6   | 6     | 16  | ARG  |
| 6   | 6     | 19  | ILE  |
| 6   | 6     | 27  | LEU  |
| 6   | 6     | 33  | SER  |
| 6   | 6     | 37  | TRP  |
| 6   | 6     | 40  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 6     | 45  | CYS  |
| 6   | 6     | 57  | ARG  |
| 6   | 6     | 74  | GLN  |
| 6   | 6     | 83  | ARG  |
| 6   | 6     | 84  | LEU  |
| 6   | 6     | 114 | SER  |
| 6   | 6     | 123 | ILE  |
| 6   | 6     | 131 | VAL  |
| 6   | 6     | 141 | PRO  |
| 6   | 6     | 151 | VAL  |
| 6   | 6     | 153 | GLN  |
| 6   | 6     | 156 | LYS  |
| 7   | 9     | 31  | VAL  |
| 7   | 9     | 33  | LEU  |
| 7   | 9     | 36  | ARG  |
| 7   | 9     | 42  | VAL  |
| 7   | 9     | 50  | LEU  |
| 7   | 9     | 58  | LEU  |
| 7   | 9     | 85  | GLU  |
| 7   | 9     | 97  | ARG  |
| 7   | 9     | 99  | ILE  |
| 7   | 9     | 101 | CYS  |
| 7   | 9     | 139 | ASP  |
| 7   | 9     | 140 | VAL  |
| 7   | 9     | 157 | VAL  |
| 7   | 9     | 159 | VAL  |
| 8   | 7     | 21  | ARG  |
| 8   | 7     | 39  | ASP  |
| 8   | 7     | 43  | ARG  |
| 8   | 7     | 44  | MET  |
| 8   | 7     | 50  | LEU  |
| 8   | 7     | 52  | THR  |
| 8   | 7     | 54  | ILE  |
| 8   | 7     | 63  | LEU  |
| 8   | 7     | 78  | LYS  |
| 8   | 7     | 82  | ILE  |
| 8   | 7     | 85  | ARG  |
| 8   | 7     | 92  | HIS  |
| 1   | A     | 10  | ASP  |
| 1   | A     | 29  | LEU  |
| 1   | A     | 49  | THR  |
| 1   | A     | 104 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 114 | LEU  |
| 1   | A     | 128 | THR  |
| 1   | A     | 134 | VAL  |
| 1   | A     | 144 | ARG  |
| 1   | A     | 155 | ARG  |
| 1   | A     | 161 | ASN  |
| 1   | A     | 168 | SER  |
| 1   | A     | 171 | LEU  |
| 1   | A     | 186 | THR  |
| 1   | A     | 217 | THR  |
| 1   | A     | 241 | MET  |
| 1   | A     | 243 | THR  |
| 1   | A     | 249 | MET  |
| 1   | A     | 253 | GLN  |
| 1   | A     | 255 | SER  |
| 1   | A     | 270 | THR  |
| 1   | A     | 271 | THR  |
| 1   | A     | 290 | ILE  |
| 1   | A     | 291 | ILE  |
| 1   | A     | 295 | SER  |
| 1   | A     | 309 | THR  |
| 1   | A     | 316 | LEU  |
| 1   | A     | 323 | LEU  |
| 1   | A     | 342 | TRP  |
| 1   | A     | 346 | ARG  |
| 1   | A     | 357 | THR  |
| 1   | A     | 363 | VAL  |
| 1   | A     | 368 | VAL  |
| 1   | A     | 374 | ILE  |
| 1   | A     | 388 | GLU  |
| 1   | A     | 397 | ARG  |
| 1   | A     | 400 | CYS  |
| 1   | A     | 414 | LEU  |
| 1   | A     | 419 | ASP  |
| 1   | A     | 437 | TRP  |
| 2   | B     | 5   | ASP  |
| 2   | B     | 7   | LYS  |
| 2   | B     | 24  | ARG  |
| 2   | B     | 28  | MET  |
| 2   | B     | 31  | LEU  |
| 2   | B     | 35  | GLN  |
| 2   | B     | 45  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 53  | VAL  |
| 2   | B     | 61  | MET  |
| 2   | B     | 87  | SER  |
| 2   | B     | 89  | LYS  |
| 2   | B     | 96  | LEU  |
| 2   | B     | 106 | ILE  |
| 2   | B     | 114 | ASP  |
| 2   | B     | 122 | VAL  |
| 2   | B     | 139 | GLU  |
| 2   | B     | 140 | PRO  |
| 2   | B     | 144 | CYS  |
| 2   | B     | 146 | THR  |
| 2   | B     | 150 | LEU  |
| 2   | B     | 153 | LEU  |
| 2   | B     | 162 | ARG  |
| 2   | B     | 163 | LEU  |
| 2   | B     | 172 | CYS  |
| 2   | B     | 176 | VAL  |
| 3   | C     | 11  | VAL  |
| 3   | C     | 23  | VAL  |
| 3   | C     | 32  | LEU  |
| 3   | C     | 42  | ILE  |
| 3   | C     | 55  | PRO  |
| 3   | C     | 73  | ILE  |
| 3   | C     | 94  | ASP  |
| 3   | C     | 121 | THR  |
| 3   | C     | 123 | ASP  |
| 3   | C     | 124 | LYS  |
| 3   | C     | 133 | ARG  |
| 3   | C     | 135 | VAL  |
| 3   | C     | 142 | LYS  |
| 3   | C     | 150 | GLU  |
| 3   | C     | 153 | VAL  |
| 3   | C     | 188 | VAL  |
| 3   | C     | 189 | ARG  |
| 3   | C     | 192 | GLU  |
| 3   | C     | 200 | LEU  |
| 3   | C     | 207 | VAL  |
| 3   | C     | 209 | THR  |
| 3   | C     | 214 | MET  |
| 3   | C     | 218 | LEU  |
| 3   | C     | 219 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 220 | SER  |
| 3   | C     | 238 | LEU  |
| 3   | C     | 269 | THR  |
| 3   | C     | 274 | LEU  |
| 3   | C     | 275 | LEU  |
| 3   | C     | 277 | ILE  |
| 3   | C     | 282 | VAL  |
| 3   | C     | 284 | GLU  |
| 3   | C     | 303 | GLN  |
| 3   | C     | 306 | LEU  |
| 3   | C     | 317 | LEU  |
| 3   | C     | 337 | ARG  |
| 3   | C     | 369 | LEU  |
| 3   | C     | 381 | LEU  |
| 3   | C     | 399 | LEU  |
| 3   | C     | 408 | ILE  |
| 3   | C     | 412 | ARG  |
| 3   | C     | 417 | VAL  |
| 3   | C     | 419 | ASP  |
| 3   | C     | 425 | ARG  |
| 3   | C     | 435 | LEU  |
| 3   | C     | 440 | ARG  |
| 3   | C     | 448 | MET  |
| 3   | C     | 450 | LEU  |
| 3   | C     | 455 | ARG  |
| 3   | C     | 464 | ILE  |
| 3   | C     | 473 | GLU  |
| 3   | C     | 501 | LYS  |
| 3   | C     | 507 | LEU  |
| 3   | C     | 512 | LEU  |
| 3   | C     | 514 | ASP  |
| 3   | C     | 515 | THR  |
| 3   | C     | 523 | LEU  |
| 3   | C     | 542 | ARG  |
| 3   | C     | 550 | LEU  |
| 3   | C     | 587 | LEU  |
| 3   | C     | 593 | LEU  |
| 3   | C     | 617 | LEU  |
| 3   | C     | 644 | LEU  |
| 3   | C     | 655 | ARG  |
| 3   | C     | 676 | LEU  |
| 3   | C     | 683 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 684 | ARG  |
| 3   | C     | 705 | VAL  |
| 3   | C     | 715 | GLU  |
| 3   | C     | 716 | LEU  |
| 3   | C     | 738 | THR  |
| 3   | C     | 747 | VAL  |
| 3   | C     | 771 | VAL  |
| 3   | C     | 776 | LEU  |
| 3   | C     | 777 | VAL  |
| 4   | D     | 40  | VAL  |
| 4   | D     | 44  | MET  |
| 4   | D     | 59  | ILE  |
| 4   | D     | 62  | LEU  |
| 4   | D     | 69  | THR  |
| 4   | D     | 74  | THR  |
| 4   | D     | 99  | LEU  |
| 4   | D     | 104 | LEU  |
| 4   | D     | 105 | LEU  |
| 4   | D     | 120 | LEU  |
| 4   | D     | 129 | HIS  |
| 4   | D     | 131 | VAL  |
| 4   | D     | 143 | LEU  |
| 4   | D     | 152 | GLU  |
| 4   | D     | 163 | VAL  |
| 4   | D     | 168 | PHE  |
| 4   | D     | 170 | HIS  |
| 4   | D     | 187 | VAL  |
| 4   | D     | 219 | ARG  |
| 4   | D     | 230 | ILE  |
| 4   | D     | 234 | LEU  |
| 4   | D     | 239 | LEU  |
| 4   | D     | 262 | PHE  |
| 4   | D     | 272 | VAL  |
| 4   | D     | 290 | ILE  |
| 4   | D     | 296 | ARG  |
| 4   | D     | 297 | LEU  |
| 4   | D     | 314 | ARG  |
| 4   | D     | 317 | LEU  |
| 4   | D     | 319 | THR  |
| 4   | D     | 342 | VAL  |
| 4   | D     | 367 | ARG  |
| 4   | D     | 369 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 396 | ILE  |
| 5   | E     | 5   | ARG  |
| 5   | E     | 25  | LEU  |
| 5   | E     | 27  | VAL  |
| 5   | E     | 38  | MET  |
| 5   | E     | 52  | ILE  |
| 5   | E     | 80  | TRP  |
| 5   | E     | 84  | ASP  |
| 5   | E     | 90  | VAL  |
| 5   | E     | 104 | VAL  |
| 5   | E     | 107 | LEU  |
| 5   | E     | 141 | LEU  |
| 5   | E     | 146 | LEU  |
| 5   | E     | 147 | ARG  |
| 5   | E     | 154 | GLU  |
| 5   | E     | 157 | THR  |
| 5   | E     | 161 | GLU  |
| 6   | F     | 16  | ARG  |
| 6   | F     | 17  | GLU  |
| 6   | F     | 19  | ILE  |
| 6   | F     | 27  | LEU  |
| 6   | F     | 33  | SER  |
| 6   | F     | 37  | TRP  |
| 6   | F     | 40  | THR  |
| 6   | F     | 45  | CYS  |
| 6   | F     | 57  | ARG  |
| 6   | F     | 74  | GLN  |
| 6   | F     | 83  | ARG  |
| 6   | F     | 84  | LEU  |
| 6   | F     | 107 | SER  |
| 6   | F     | 114 | SER  |
| 6   | F     | 123 | ILE  |
| 6   | F     | 131 | VAL  |
| 6   | F     | 141 | PRO  |
| 6   | F     | 151 | VAL  |
| 6   | F     | 153 | GLN  |
| 6   | F     | 156 | LYS  |
| 7   | G     | 31  | VAL  |
| 7   | G     | 33  | LEU  |
| 7   | G     | 36  | ARG  |
| 7   | G     | 42  | VAL  |
| 7   | G     | 50  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 58  | LEU  |
| 7   | G     | 85  | GLU  |
| 7   | G     | 97  | ARG  |
| 7   | G     | 99  | ILE  |
| 7   | G     | 101 | CYS  |
| 7   | G     | 139 | ASP  |
| 7   | G     | 140 | VAL  |
| 7   | G     | 157 | VAL  |
| 7   | G     | 159 | VAL  |
| 8   | H     | 21  | ARG  |
| 8   | H     | 39  | ASP  |
| 8   | H     | 43  | ARG  |
| 8   | H     | 44  | MET  |
| 8   | H     | 50  | LEU  |
| 8   | H     | 52  | THR  |
| 8   | H     | 54  | ILE  |
| 8   | H     | 63  | LEU  |
| 8   | H     | 78  | LYS  |
| 8   | H     | 82  | ILE  |
| 8   | H     | 85  | ARG  |
| 8   | H     | 92  | HIS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 92  | ASN  |
| 1   | 1     | 220 | ASN  |
| 2   | 2     | 120 | GLN  |
| 3   | 3     | 38  | HIS  |
| 3   | 3     | 168 | HIS  |
| 3   | 3     | 208 | HIS  |
| 3   | 3     | 246 | ASN  |
| 3   | 3     | 368 | HIS  |
| 3   | 3     | 410 | HIS  |
| 3   | 3     | 661 | GLN  |
| 3   | 3     | 702 | HIS  |
| 3   | 3     | 733 | GLN  |
| 3   | 3     | 749 | HIS  |
| 4   | 4     | 292 | GLN  |
| 4   | 4     | 327 | HIS  |
| 4   | 4     | 336 | HIS  |
| 4   | 4     | 377 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | 5     | 129 | HIS  |
| 6   | 6     | 98  | GLN  |
| 6   | 6     | 153 | GLN  |
| 7   | 9     | 38  | HIS  |
| 8   | 7     | 92  | HIS  |
| 1   | A     | 92  | ASN  |
| 1   | A     | 220 | ASN  |
| 2   | B     | 120 | GLN  |
| 2   | B     | 177 | HIS  |
| 3   | C     | 38  | HIS  |
| 3   | C     | 168 | HIS  |
| 3   | C     | 246 | ASN  |
| 3   | C     | 368 | HIS  |
| 3   | C     | 410 | HIS  |
| 3   | C     | 586 | HIS  |
| 3   | C     | 661 | GLN  |
| 3   | C     | 733 | GLN  |
| 3   | C     | 749 | HIS  |
| 4   | D     | 292 | GLN  |
| 4   | D     | 327 | HIS  |
| 4   | D     | 330 | HIS  |
| 4   | D     | 336 | HIS  |
| 4   | D     | 377 | ASN  |
| 5   | E     | 129 | HIS  |
| 6   | F     | 153 | GLN  |
| 7   | G     | 38  | HIS  |
| 8   | H     | 92  | HIS  |

### 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

Of 34 ligands modelled in this entry, 14 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | SF4  | G     | 183 | 7    | 0,12,12      | -    | -        | -           |      |          |
| 10  | FMN  | 1     | 440 | -    | 33,33,33     | 1.33 | 3 (9%)   | 48,50,50    | 1.61 | 15 (31%) |
| 9   | SF4  | 1     | 439 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | 3     | 786 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 10  | FMN  | A     | 440 | -    | 33,33,33     | 1.14 | 3 (9%)   | 48,50,50    | 1.40 | 9 (18%)  |
| 9   | SF4  | 9     | 183 | 7    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | F     | 182 | 6    | 0,12,12      | -    | -        | -           |      |          |
| 11  | FES  | B     | 182 | 2    | 0,4,4        | -    | -        | -           |      |          |
| 9   | SF4  | 9     | 184 | 7    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | C     | 784 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | 3     | 784 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | G     | 184 | 7    | 0,12,12      | -    | -        | -           |      |          |
| 11  | FES  | 2     | 182 | 2    | 0,4,4        | -    | -        | -           |      |          |
| 9   | SF4  | C     | 785 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 11  | FES  | C     | 787 | 3    | 0,4,4        | -    | -        | -           |      |          |
| 9   | SF4  | C     | 786 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 11  | FES  | 3     | 787 | 3    | 0,4,4        | -    | -        | -           |      |          |
| 9   | SF4  | 3     | 785 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | 6     | 182 | 6    | 0,12,12      | -    | -        | -           |      |          |
| 9   | SF4  | A     | 439 | 1    | 0,12,12      | -    | -        | -           |      |          |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 9   | SF4  | G     | 183 | 7    | -       | -           | 0/6/5/5 |
| 10  | FMN  | 1     | 440 | -    | -       | 10/18/18/18 | 0/3/3/3 |
| 9   | SF4  | 1     | 439 | 1    | -       | -           | 0/6/5/5 |
| 10  | FMN  | A     | 440 | -    | -       | 4/18/18/18  | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 9   | SF4  | 3     | 786 | 3    | -       | -        | 0/6/5/5 |
| 9   | SF4  | 9     | 183 | 7    | -       | -        | 0/6/5/5 |
| 9   | SF4  | F     | 182 | 6    | -       | -        | 0/6/5/5 |
| 11  | FES  | B     | 182 | 2    | -       | -        | 0/1/1/1 |
| 9   | SF4  | 9     | 184 | 7    | -       | -        | 0/6/5/5 |
| 9   | SF4  | C     | 784 | 3    | -       | -        | 0/6/5/5 |
| 9   | SF4  | 3     | 784 | 3    | -       | -        | 0/6/5/5 |
| 9   | SF4  | G     | 184 | 7    | -       | -        | 0/6/5/5 |
| 11  | FES  | 2     | 182 | 2    | -       | -        | 0/1/1/1 |
| 9   | SF4  | C     | 785 | 3    | -       | -        | 0/6/5/5 |
| 11  | FES  | C     | 787 | 3    | -       | -        | 0/1/1/1 |
| 9   | SF4  | C     | 786 | 3    | -       | -        | 0/6/5/5 |
| 11  | FES  | 3     | 787 | 3    | -       | -        | 0/1/1/1 |
| 9   | SF4  | 3     | 785 | 3    | -       | -        | 0/6/5/5 |
| 9   | SF4  | 6     | 182 | 6    | -       | -        | 0/6/5/5 |
| 9   | SF4  | A     | 439 | 1    | -       | -        | 0/6/5/5 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 10  | A     | 440 | FMN  | C4A-N5  | 3.85  | 1.39        | 1.30     |
| 10  | 1     | 440 | FMN  | C4A-N5  | 3.58  | 1.38        | 1.30     |
| 10  | 1     | 440 | FMN  | C9A-N10 | -3.16 | 1.35        | 1.41     |
| 10  | A     | 440 | FMN  | C10-N1  | 2.38  | 1.38        | 1.33     |
| 10  | A     | 440 | FMN  | C5'-C4' | 2.28  | 1.54        | 1.51     |
| 10  | 1     | 440 | FMN  | C4A-C10 | -2.17 | 1.37        | 1.44     |

All (24) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10  | A     | 440 | FMN  | C4-N3-C2    | -3.07 | 120.18      | 125.64   |
| 10  | 1     | 440 | FMN  | O4'-C4'-C3' | -3.00 | 102.22      | 109.25   |
| 10  | 1     | 440 | FMN  | C4-N3-C2    | -2.98 | 120.34      | 125.64   |
| 10  | A     | 440 | FMN  | C4A-C10-N10 | 2.92  | 120.66      | 116.48   |
| 10  | 1     | 440 | FMN  | O4'-C4'-C5' | -2.71 | 104.00      | 109.99   |
| 10  | 1     | 440 | FMN  | O2'-C2'-C3' | 2.70  | 115.57      | 109.25   |
| 10  | 1     | 440 | FMN  | C9-C9A-N10  | -2.69 | 118.24      | 121.85   |
| 10  | A     | 440 | FMN  | C10-C4A-N5  | -2.62 | 119.46      | 124.81   |
| 10  | 1     | 440 | FMN  | C9A-C5A-N5  | -2.60 | 119.69      | 122.45   |
| 10  | 1     | 440 | FMN  | C4A-C4-N3   | 2.57  | 119.79      | 113.25   |
| 10  | 1     | 440 | FMN  | C4A-C10-N10 | 2.51  | 120.08      | 116.48   |
| 10  | 1     | 440 | FMN  | O4-C4-C4A   | -2.50 | 119.92      | 126.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10  | 1     | 440 | FMN  | C5A-C9A-N10 | 2.48  | 120.21      | 117.97   |
| 10  | A     | 440 | FMN  | C4A-C4-N3   | 2.46  | 119.50      | 113.25   |
| 10  | 1     | 440 | FMN  | C10-C4A-N5  | -2.42 | 119.87      | 124.81   |
| 10  | 1     | 440 | FMN  | C4-C4A-N5   | 2.36  | 121.47      | 118.21   |
| 10  | 1     | 440 | FMN  | O2-C2-N1    | -2.35 | 117.90      | 121.80   |
| 10  | A     | 440 | FMN  | C4'-C3'-C2' | 2.35  | 117.47      | 113.57   |
| 10  | A     | 440 | FMN  | C5'-C4'-C3' | -2.34 | 107.80      | 112.22   |
| 10  | A     | 440 | FMN  | C9A-C5A-N5  | -2.22 | 120.10      | 122.45   |
| 10  | A     | 440 | FMN  | O4-C4-C4A   | -2.21 | 120.69      | 126.53   |
| 10  | A     | 440 | FMN  | C4A-C10-N1  | -2.15 | 119.32      | 124.59   |
| 10  | 1     | 440 | FMN  | C5'-C4'-C3' | 2.06  | 116.10      | 112.22   |
| 10  | 1     | 440 | FMN  | O3'-C3'-C4' | 2.04  | 113.56      | 108.93   |

There are no chirality outliers.

All (14) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | 1     | 440 | FMN  | N10-C1'-C2'-O2' |
| 10  | 1     | 440 | FMN  | N10-C1'-C2'-C3' |
| 10  | 1     | 440 | FMN  | C3'-C4'-C5'-O5' |
| 10  | 1     | 440 | FMN  | O4'-C4'-C5'-O5' |
| 10  | A     | 440 | FMN  | N10-C1'-C2'-O2' |
| 10  | A     | 440 | FMN  | N10-C1'-C2'-C3' |
| 10  | A     | 440 | FMN  | C3'-C4'-C5'-O5' |
| 10  | A     | 440 | FMN  | O4'-C4'-C5'-O5' |
| 10  | 1     | 440 | FMN  | O2'-C2'-C3'-C4' |
| 10  | 1     | 440 | FMN  | C2'-C3'-C4'-O4' |
| 10  | 1     | 440 | FMN  | O2'-C2'-C3'-O3' |
| 10  | 1     | 440 | FMN  | C4'-C5'-O5'-P   |
| 10  | 1     | 440 | FMN  | O3'-C3'-C4'-O4' |
| 10  | 1     | 440 | FMN  | C1'-C2'-C3'-O3' |

There are no ring outliers.

17 monomers are involved in 40 short contacts:

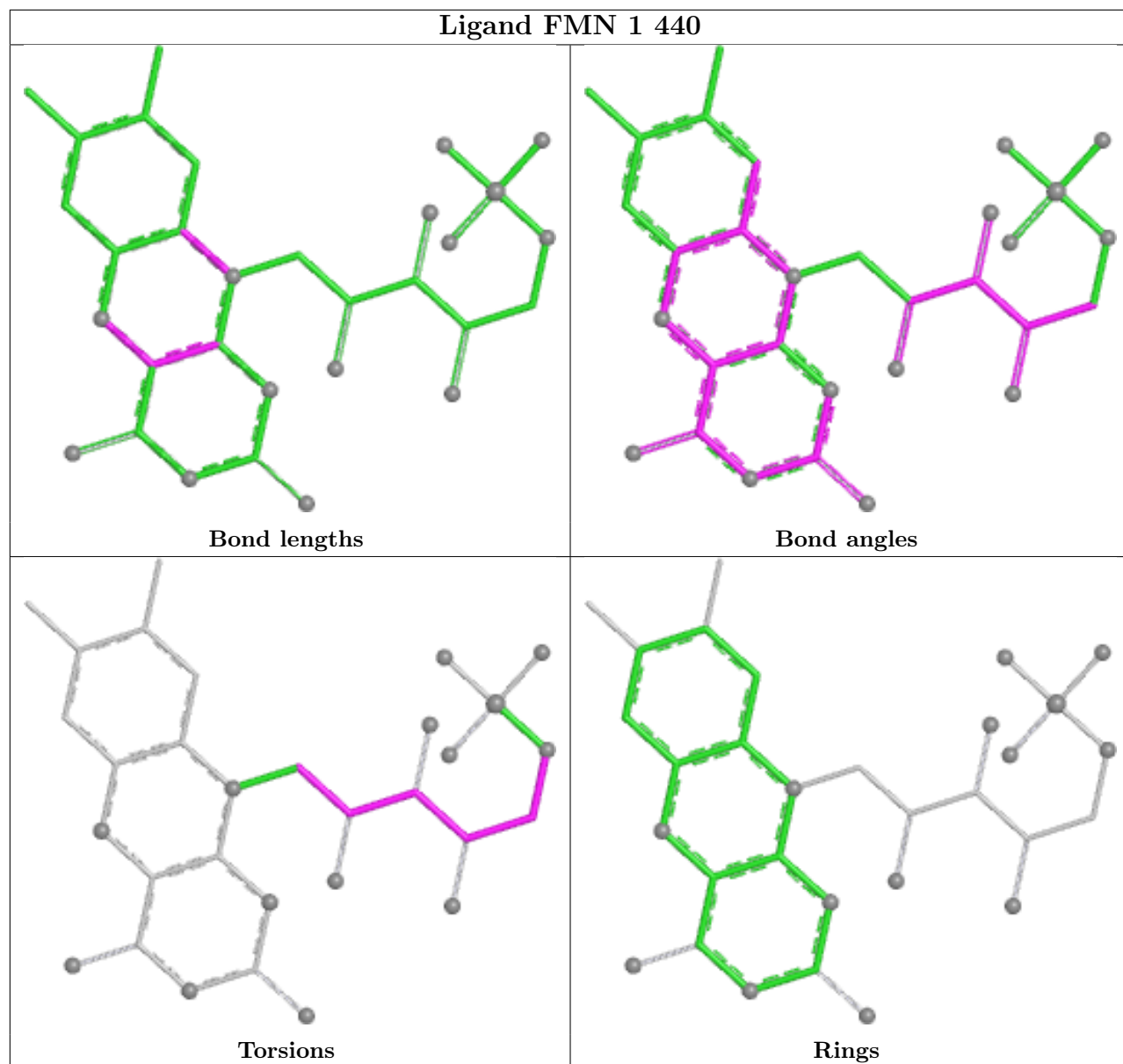
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 9   | G     | 183 | SF4  | 1       | 0            |
| 10  | 1     | 440 | FMN  | 8       | 0            |
| 9   | 1     | 439 | SF4  | 2       | 0            |
| 9   | 3     | 786 | SF4  | 3       | 0            |
| 10  | A     | 440 | FMN  | 4       | 0            |

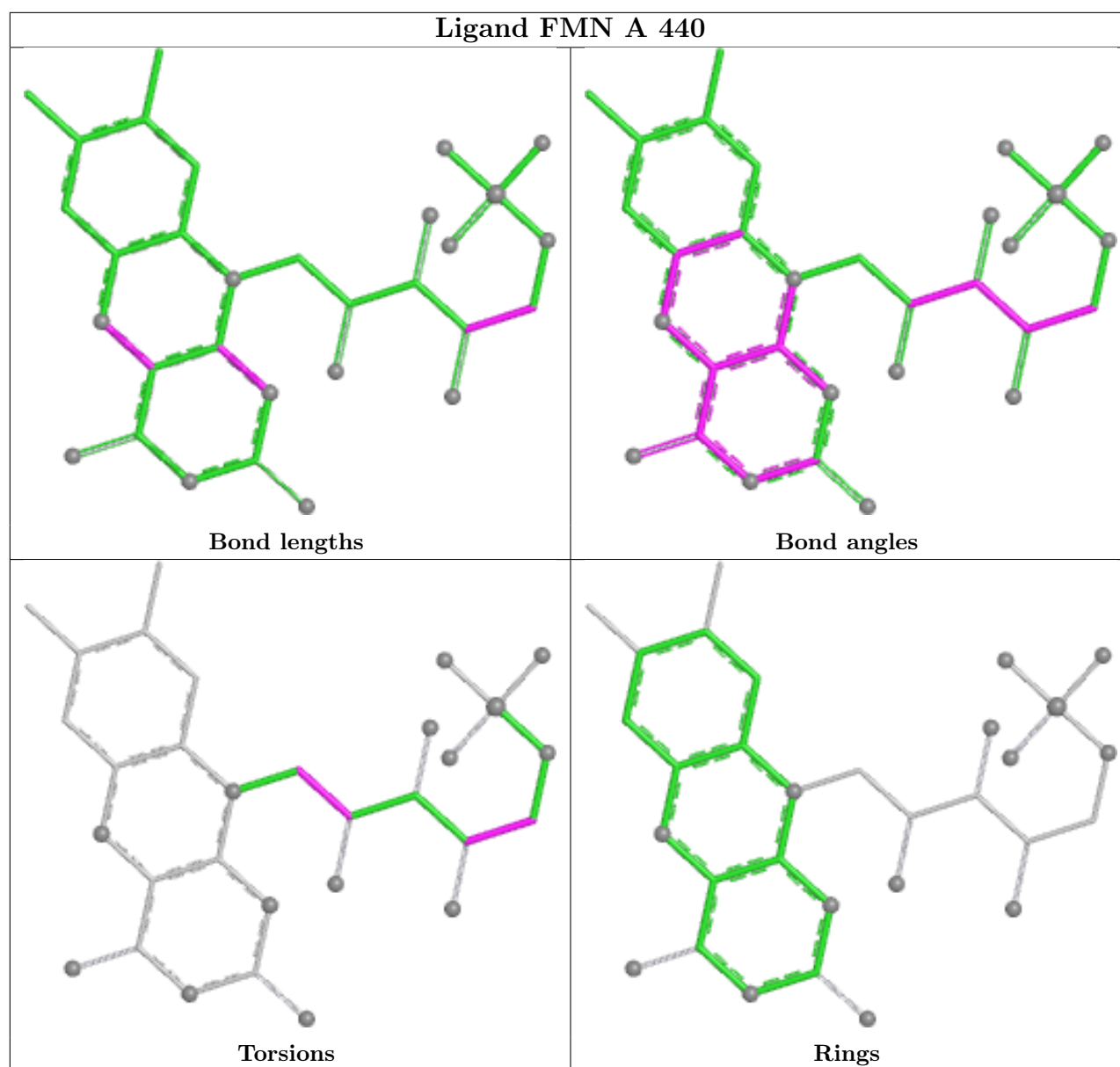
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 9   | F     | 182 | SF4  | 4       | 0            |
| 11  | B     | 182 | FES  | 1       | 0            |
| 9   | C     | 784 | SF4  | 2       | 0            |
| 9   | 3     | 784 | SF4  | 3       | 0            |
| 9   | G     | 184 | SF4  | 1       | 0            |
| 9   | C     | 785 | SF4  | 1       | 0            |
| 11  | C     | 787 | FES  | 1       | 0            |
| 9   | C     | 786 | SF4  | 2       | 0            |
| 11  | 3     | 787 | FES  | 1       | 0            |
| 9   | 3     | 785 | SF4  | 1       | 0            |
| 9   | 6     | 182 | SF4  | 4       | 0            |
| 9   | A     | 439 | SF4  | 1       | 0            |

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | 1     | 437/438 (99%)   | -0.30  | 0 100 100     | 26, 49, 76, 109       | 0     |
| 1   | A     | 437/438 (99%)   | -0.30  | 1 (0%) 91 83  | 29, 49, 77, 111       | 0     |
| 2   | 2     | 178/181 (98%)   | -0.27  | 0 100 100     | 28, 51, 84, 124       | 0     |
| 2   | B     | 178/181 (98%)   | -0.28  | 0 100 100     | 30, 51, 84, 125       | 0     |
| 3   | 3     | 754/783 (96%)   | 0.18   | 12 (1%) 70 49 | 26, 69, 107, 130      | 0     |
| 3   | C     | 754/783 (96%)   | 0.19   | 14 (1%) 66 45 | 28, 70, 108, 130      | 0     |
| 4   | 4     | 377/409 (92%)   | 0.10   | 11 (2%) 53 32 | 34, 68, 103, 124      | 0     |
| 4   | D     | 377/409 (92%)   | 0.05   | 4 (1%) 78 59  | 35, 69, 106, 124      | 0     |
| 5   | 5     | 196/207 (94%)   | 0.37   | 5 (2%) 57 36  | 40, 74, 106, 122      | 0     |
| 5   | E     | 196/207 (94%)   | 0.23   | 3 (1%) 72 52  | 42, 76, 107, 122      | 0     |
| 6   | 6     | 145/181 (80%)   | 0.32   | 2 (1%) 73 53  | 39, 64, 91, 122       | 0     |
| 6   | F     | 145/181 (80%)   | 0.33   | 3 (2%) 63 42  | 40, 66, 92, 122       | 0     |
| 7   | 9     | 154/182 (84%)   | -0.06  | 4 (2%) 57 36  | 31, 51, 94, 128       | 0     |
| 7   | G     | 154/182 (84%)   | 0.02   | 0 100 100     | 34, 52, 94, 130       | 0     |
| 8   | 7     | 127/129 (98%)   | -0.17  | 1 (0%) 82 65  | 43, 57, 93, 117       | 0     |
| 8   | H     | 127/129 (98%)   | -0.12  | 1 (0%) 82 65  | 43, 58, 94, 115       | 0     |
| All | All   | 4736/5020 (94%) | 0.03   | 61 (1%) 75 56 | 26, 61, 103, 130      | 0     |

All (61) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C     | 566 | ALA  | 4.6  |
| 3   | C     | 652 | PRO  | 3.6  |
| 5   | 5     | 48  | PHE  | 3.5  |
| 7   | 9     | 177 | THR  | 3.4  |
| 3   | C     | 654 | PHE  | 3.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | 5     | 143 | GLY  | 3.4  |
| 4   | 4     | 211 | SER  | 3.1  |
| 4   | 4     | 39  | GLY  | 3.0  |
| 3   | 3     | 680 | LEU  | 2.9  |
| 4   | 4     | 238 | SER  | 2.9  |
| 4   | 4     | 47  | LEU  | 2.9  |
| 1   | A     | 4   | PRO  | 2.8  |
| 3   | C     | 772 | GLU  | 2.8  |
| 7   | 9     | 176 | PRO  | 2.8  |
| 3   | 3     | 577 | LEU  | 2.8  |
| 3   | 3     | 723 | ALA  | 2.8  |
| 6   | 6     | 160 | GLY  | 2.7  |
| 3   | 3     | 485 | GLU  | 2.7  |
| 5   | 5     | 194 | SER  | 2.7  |
| 3   | C     | 143 | TYR  | 2.7  |
| 3   | 3     | 448 | MET  | 2.6  |
| 3   | C     | 364 | LEU  | 2.5  |
| 7   | 9     | 160 | GLY  | 2.5  |
| 3   | 3     | 339 | GLU  | 2.5  |
| 4   | 4     | 215 | TYR  | 2.5  |
| 6   | F     | 55  | ASP  | 2.4  |
| 4   | 4     | 236 | GLY  | 2.4  |
| 8   | 7     | 3   | ALA  | 2.4  |
| 4   | D     | 236 | GLY  | 2.3  |
| 6   | F     | 76  | ASP  | 2.3  |
| 5   | E     | 51  | ASP  | 2.3  |
| 7   | 9     | 48  | ASN  | 2.3  |
| 3   | 3     | 143 | TYR  | 2.3  |
| 3   | 3     | 654 | PHE  | 2.3  |
| 3   | 3     | 687 | GLU  | 2.3  |
| 4   | 4     | 140 | LEU  | 2.3  |
| 8   | H     | 3   | ALA  | 2.2  |
| 5   | 5     | 86  | SER  | 2.2  |
| 4   | 4     | 46  | THR  | 2.2  |
| 3   | C     | 318 | VAL  | 2.2  |
| 3   | C     | 487 | SER  | 2.2  |
| 3   | C     | 577 | LEU  | 2.2  |
| 5   | E     | 173 | ALA  | 2.2  |
| 6   | 6     | 101 | ASP  | 2.1  |
| 3   | 3     | 2   | VAL  | 2.1  |
| 3   | 3     | 556 | ALA  | 2.1  |
| 4   | D     | 270 | GLY  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C     | 696 | PRO  | 2.1  |
| 5   | E     | 68  | PHE  | 2.1  |
| 6   | F     | 113 | SER  | 2.1  |
| 3   | 3     | 559 | ASP  | 2.1  |
| 5   | 5     | 51  | ASP  | 2.1  |
| 4   | D     | 230 | ILE  | 2.1  |
| 4   | 4     | 199 | HIS  | 2.1  |
| 3   | C     | 604 | ALA  | 2.1  |
| 4   | D     | 147 | PHE  | 2.1  |
| 4   | 4     | 48  | SER  | 2.0  |
| 4   | 4     | 209 | ALA  | 2.0  |
| 3   | C     | 378 | PRO  | 2.0  |
| 3   | C     | 727 | ALA  | 2.0  |
| 3   | C     | 290 | ILE  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 10  | FMN  | A     | 440 | 31/31 | 0.93 | 0.10 | 35,47,59,63                 | 0     |
| 10  | FMN  | 1     | 440 | 31/31 | 0.94 | 0.10 | 28,37,46,59                 | 0     |
| 12  | MN   | 3     | 789 | 1/1   | 0.94 | 0.07 | 61,61,61,61                 | 0     |
| 12  | MN   | H     | 202 | 1/1   | 0.94 | 0.08 | 68,68,68,68                 | 0     |
| 12  | MN   | E     | 208 | 1/1   | 0.95 | 0.08 | 93,93,93,93                 | 0     |
| 12  | MN   | 5     | 208 | 1/1   | 0.96 | 0.07 | 67,67,67,67                 | 0     |
| 12  | MN   | C     | 789 | 1/1   | 0.97 | 0.05 | 61,61,61,61                 | 0     |
| 12  | MN   | D     | 410 | 1/1   | 0.97 | 0.07 | 63,63,63,63                 | 0     |
| 12  | MN   | 2     | 206 | 1/1   | 0.98 | 0.07 | 64,64,64,64                 | 0     |

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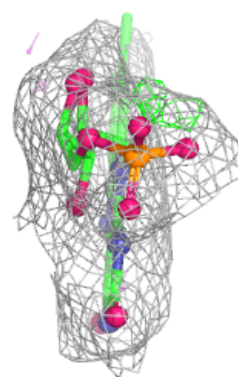
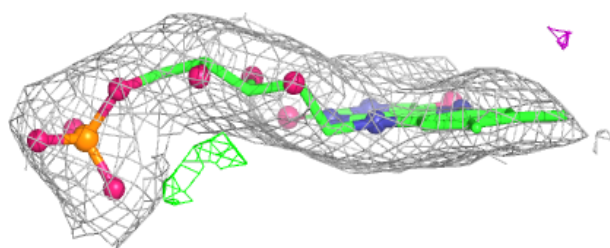
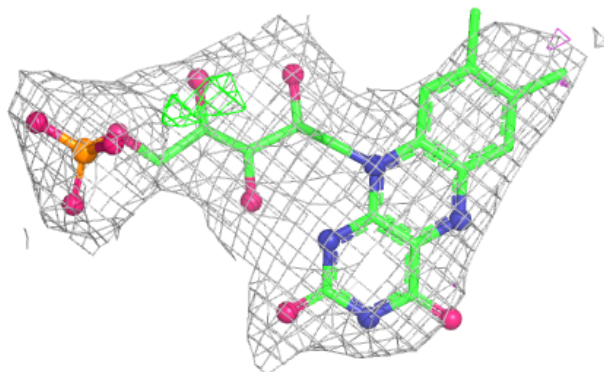
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 12  | MN   | C     | 788 | 1/1   | 0.98 | 0.04 | 47,47,47,47                 | 0     |
| 12  | MN   | 4     | 411 | 1/1   | 0.98 | 0.04 | 61,61,61,61                 | 0     |
| 13  | CA   | C     | 790 | 1/1   | 0.98 | 0.14 | 39,39,39,39                 | 0     |
| 11  | FES  | C     | 787 | 4/4   | 0.99 | 0.03 | 33,39,42,42                 | 0     |
| 9   | SF4  | 9     | 183 | 8/8   | 0.99 | 0.05 | 18,28,30,33                 | 0     |
| 12  | MN   | 3     | 788 | 1/1   | 0.99 | 0.07 | 32,32,32,32                 | 0     |
| 9   | SF4  | A     | 439 | 8/8   | 0.99 | 0.04 | 29,32,37,42                 | 0     |
| 12  | MN   | 4     | 410 | 1/1   | 0.99 | 0.04 | 65,65,65,65                 | 0     |
| 9   | SF4  | C     | 786 | 8/8   | 0.99 | 0.04 | 37,50,59,64                 | 0     |
| 9   | SF4  | F     | 182 | 8/8   | 0.99 | 0.05 | 40,50,61,73                 | 0     |
| 12  | MN   | 7     | 202 | 1/1   | 0.99 | 0.09 | 63,63,63,63                 | 0     |
| 9   | SF4  | G     | 183 | 8/8   | 0.99 | 0.04 | 32,39,44,47                 | 0     |
| 9   | SF4  | G     | 184 | 8/8   | 0.99 | 0.04 | 36,43,45,48                 | 0     |
| 9   | SF4  | 3     | 784 | 8/8   | 0.99 | 0.04 | 25,27,32,34                 | 0     |
| 9   | SF4  | 6     | 182 | 8/8   | 0.99 | 0.04 | 23,34,48,49                 | 0     |
| 11  | FES  | 2     | 182 | 4/4   | 0.99 | 0.03 | 29,34,35,36                 | 0     |
| 13  | CA   | 3     | 790 | 1/1   | 0.99 | 0.12 | 30,30,30,30                 | 0     |
| 11  | FES  | B     | 182 | 4/4   | 0.99 | 0.04 | 38,41,49,51                 | 0     |
| 9   | SF4  | 3     | 786 | 8/8   | 1.00 | 0.03 | 27,34,37,39                 | 0     |
| 9   | SF4  | C     | 784 | 8/8   | 1.00 | 0.03 | 30,35,41,42                 | 0     |
| 9   | SF4  | C     | 785 | 8/8   | 1.00 | 0.03 | 30,32,39,46                 | 0     |
| 9   | SF4  | 1     | 439 | 8/8   | 1.00 | 0.04 | 21,24,37,40                 | 0     |
| 11  | FES  | 3     | 787 | 4/4   | 1.00 | 0.03 | 35,36,37,38                 | 0     |
| 9   | SF4  | 3     | 785 | 8/8   | 1.00 | 0.02 | 22,23,28,34                 | 0     |
| 9   | SF4  | 9     | 184 | 8/8   | 1.00 | 0.03 | 23,26,28,32                 | 0     |

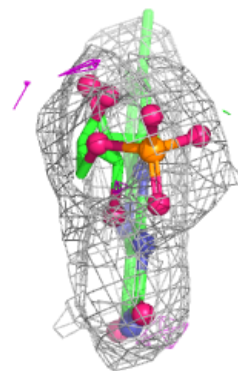
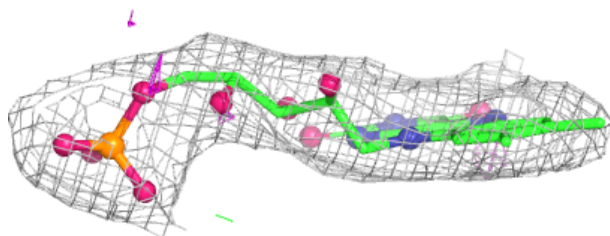
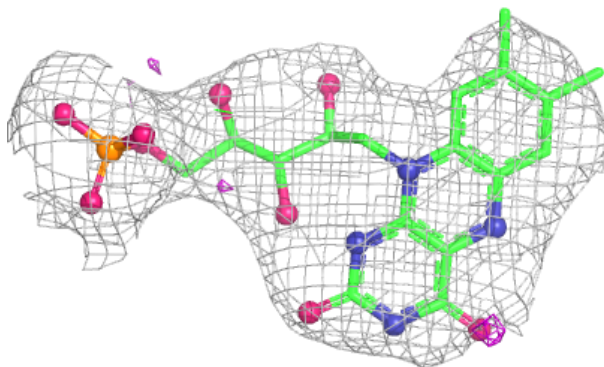
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FMN A 440:**

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

**Electron density around FMN 1 440:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.