



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:49 am GMT

PDB ID : 5HPW  
Title : Mode of binding of antithyroid drug, propylthiouracil to lactoperoxidase: Binding studies and structure determination  
Authors : Singh, R.P.; Singh, A.; Sharma, P.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2016-01-21  
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

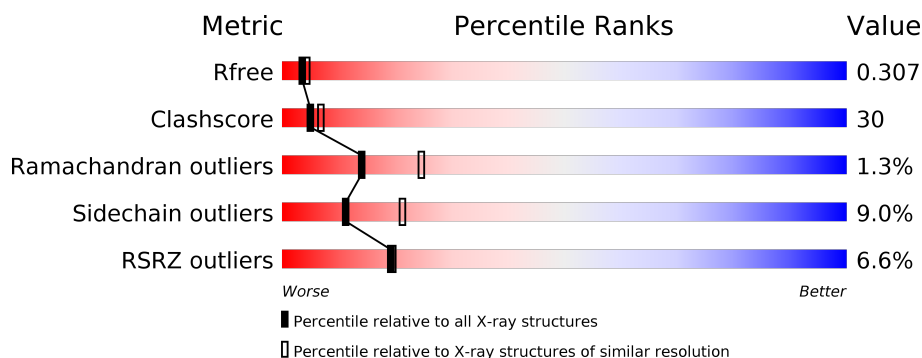
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 3846 (2.50-2.50)                                      |
| Clashscore            | 112137                      | 4554 (2.50-2.50)                                      |
| Ramachandran outliers | 110173                      | 4463 (2.50-2.50)                                      |
| Sidechain outliers    | 110143                      | 4465 (2.50-2.50)                                      |
| RSRZ outliers         | 101464                      | 3876 (2.50-2.50)                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 595    |                  |
| 1   | B     | 595    |                  |
| 1   | C     | 595    |                  |
| 1   | D     | 595    |                  |

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 crite-

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | NAG  | A     | 601 | -         | -        | -       | X                |
| 4   | NO3  | A     | 606 | -         | -        | -       | X                |
| 4   | NO3  | A     | 608 | -         | -        | -       | X                |
| 4   | NO3  | B     | 607 | -         | -        | -       | X                |
| 4   | NO3  | C     | 606 | -         | -        | -       | X                |
| 4   | NO3  | C     | 608 | -         | -        | X       | X                |
| 4   | NO3  | D     | 606 | -         | -        | X       | -                |
| 4   | NO3  | D     | 607 | -         | -        | X       | -                |
| 4   | NO3  | D     | 608 | -         | -        | X       | X                |
| 5   | 3CJ  | A     | 609 | -         | -        | X       | -                |
| 5   | 3CJ  | B     | 609 | -         | -        | X       | -                |
| 5   | 3CJ  | C     | 609 | -         | -        | X       | X                |
| 5   | 3CJ  | D     | 609 | -         | -        | X       | X                |

## 2 Entry composition [i](#)

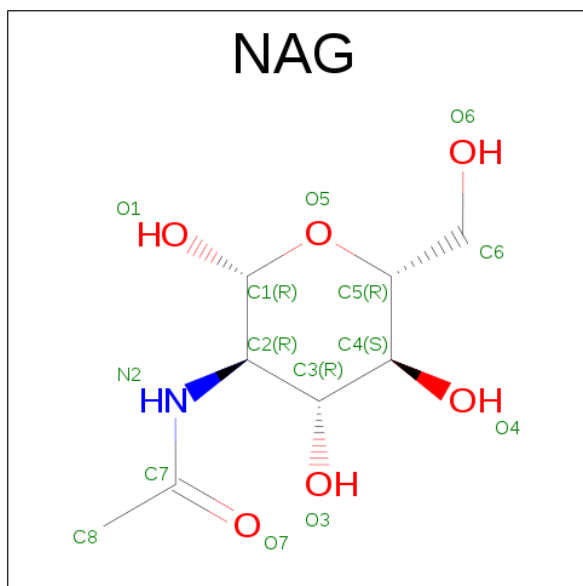
There are 7 unique types of molecules in this entry. The entry contains 20141 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lactoperoxidase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 595      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4753  | 3021 | 844 | 862 | 26 |         |         |       |
| 1   | B     | 595      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4753  | 3021 | 844 | 862 | 26 |         |         |       |
| 1   | C     | 595      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4753  | 3021 | 844 | 862 | 26 |         |         |       |
| 1   | D     | 595      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4753  | 3021 | 844 | 862 | 26 |         |         |       |

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

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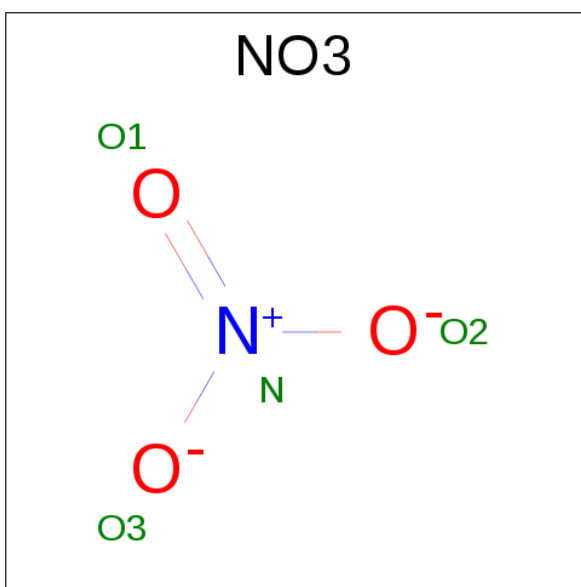
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| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

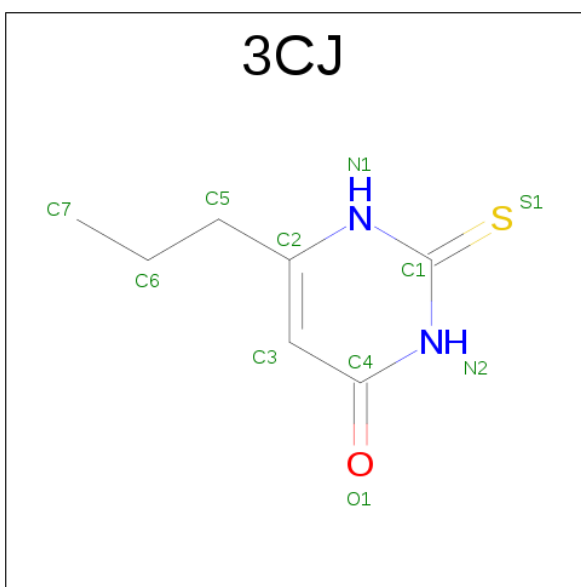
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | B     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | A     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | D     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | C     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



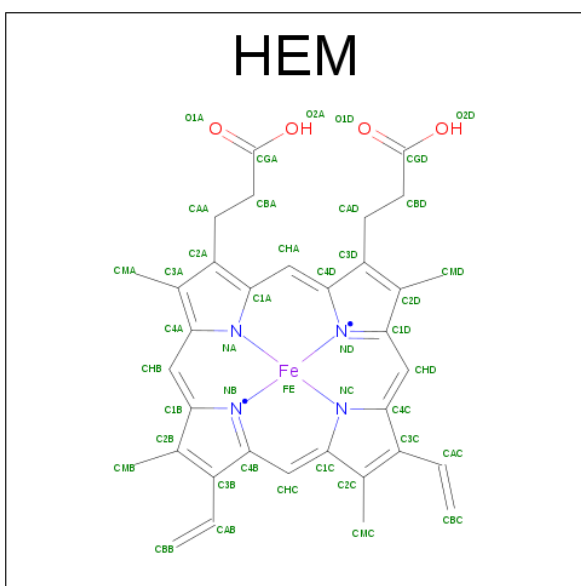
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | A     | 1        | Total | N | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 4   | A     | 1        | Total | N | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 4   | A     | 1        | Total | N | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 4   | B     | 1        | Total | N | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 4   | B     | 1        | Total | N | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 4   | B     | 1        | Total | N | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 4   | C     | 1        | Total | N | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 4   | C     | 1        | Total | N | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 4   | C     | 1        | Total | N | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 4   | D     | 1        | Total | N | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 4   | D     | 1        | Total | N | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |
| 4   | D     | 1        | Total | N | O | 0       | 0       |
|     |       |          | 4     | 1 | 3 |         |         |

- Molecule 5 is 6-propyl-2-thioxo-2,3-dihydropyrimidin-4(1H)-one (three-letter code: 3CJ) (formula: C<sub>7</sub>H<sub>10</sub>N<sub>2</sub>OS).



| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 5   | A     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 11    | 7 | 2 | 1 | 1 |         |         |
| 5   | B     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 11    | 7 | 2 | 1 | 1 |         |         |
| 5   | C     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 11    | 7 | 2 | 1 | 1 |         |         |
| 5   | D     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 11    | 7 | 2 | 1 | 1 |         |         |

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 6   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 7 is water.

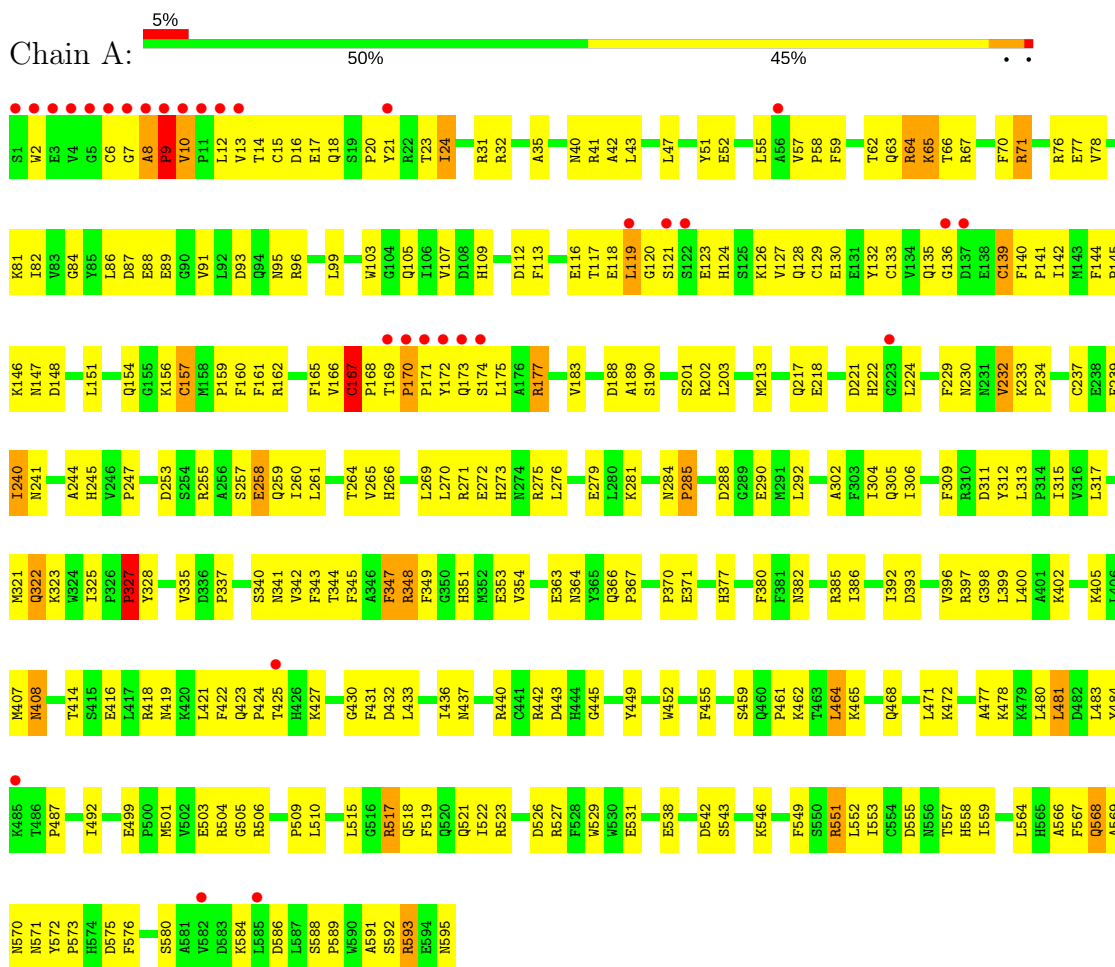
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 7   | A     | 161      | Total<br>161 | O<br>161 | 0       | 0       |
| 7   | B     | 155      | Total<br>155 | O<br>155 | 0       | 0       |
| 7   | C     | 170      | Total<br>170 | O<br>170 | 0       | 0       |
| 7   | D     | 165      | Total<br>165 | O<br>165 | 0       | 0       |



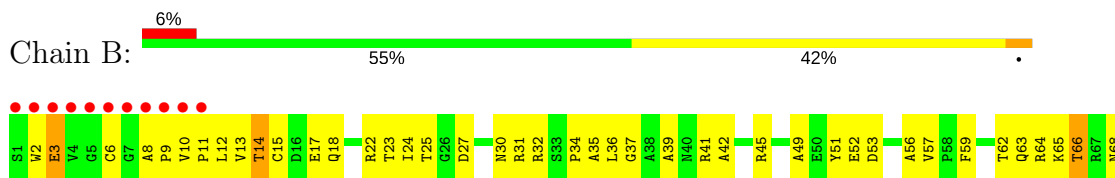
### 3 Residue-property plots

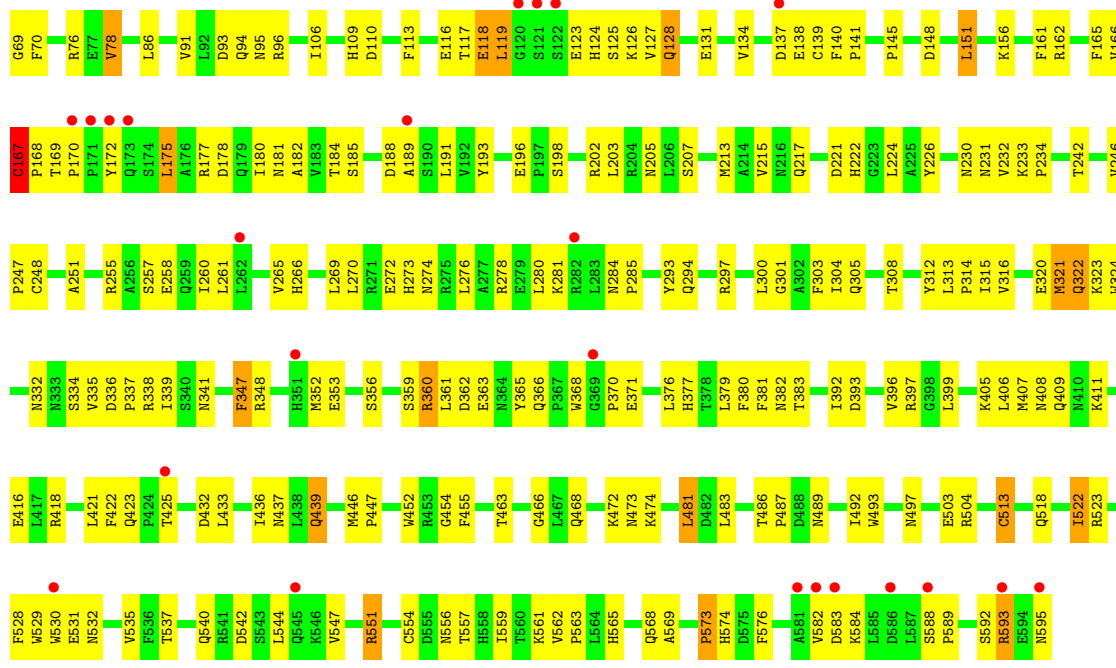
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Lactoperoxidase

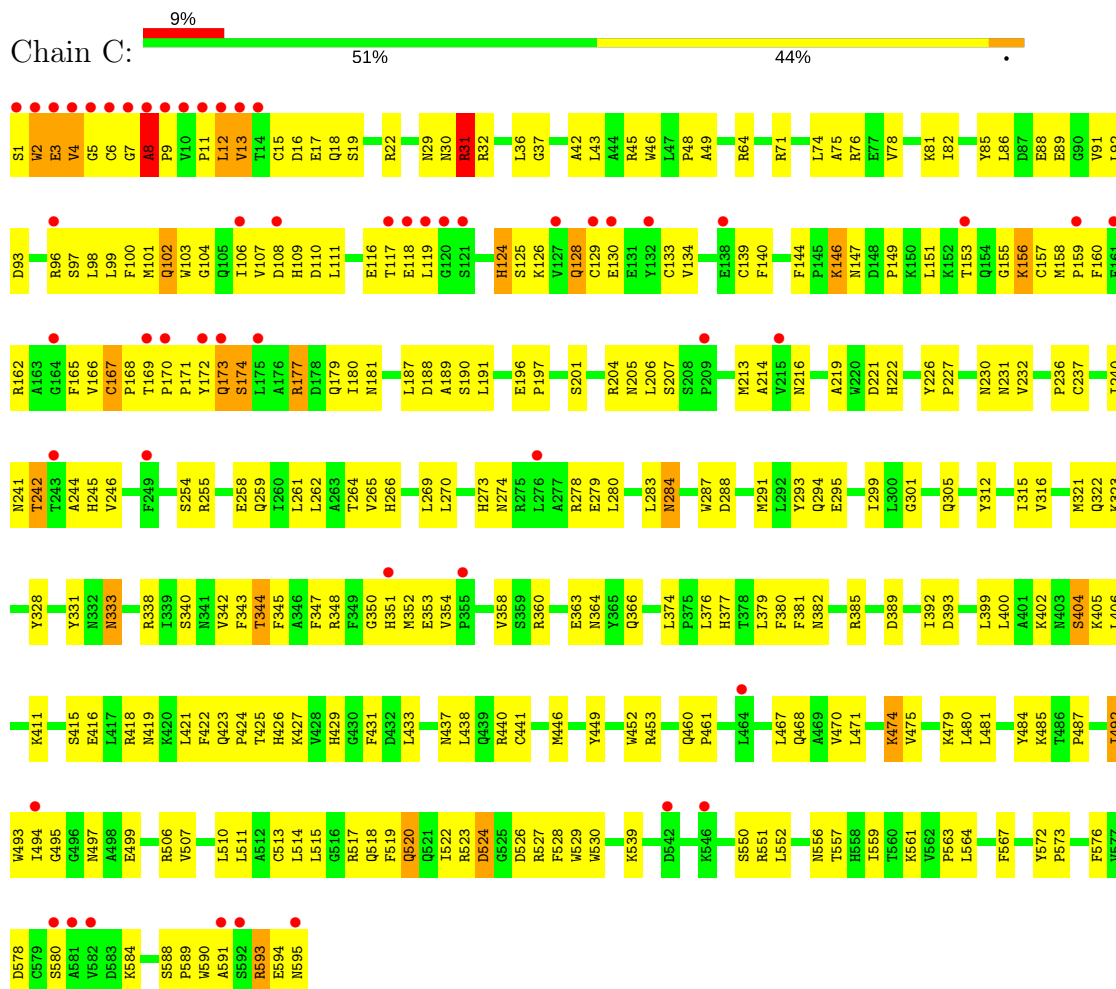


#### • Molecule 1: Lactoperoxidase



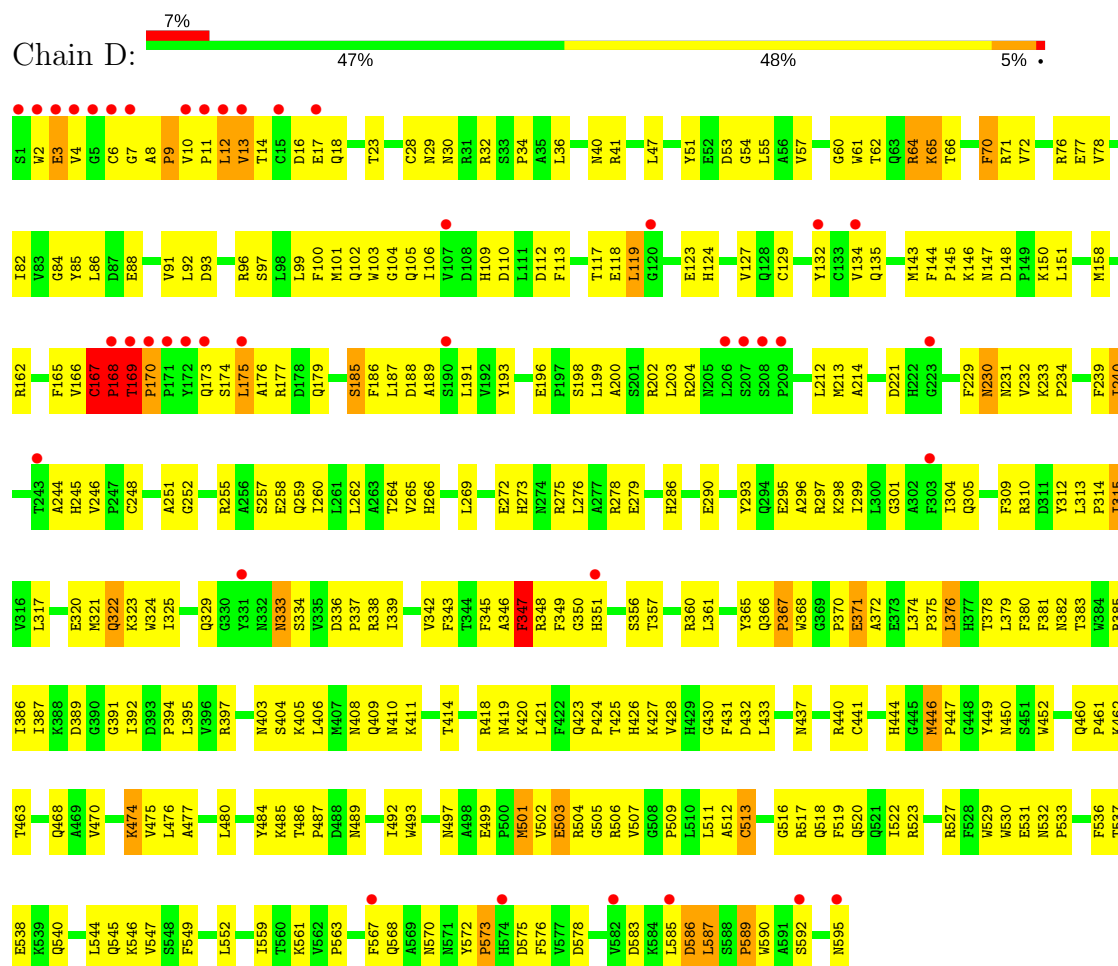


• Molecule 1: Lactoperoxidase



● Molecule 1: Lactoperoxidase

Chain D:



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 80.22Å 82.59Å 95.08Å<br>80.91° 73.71° 89.96°                | Depositor        |
| Resolution (Å)  | 42.50 – 2.50<br>42.46 – 2.50                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 91.7 (42.50-2.50)<br>87.5 (42.46-2.50)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.19 (at 2.51Å)   | Xtriage          |
| Refinement program  | REFMAC 5.7.0032   | Depositor        |
| R, $R_{free}$   | 0.260 , 0.311<br>0.254 , 0.307                              | Depositor<br>DCC |
| $R_{free}$ test set   | 3668 reflections (5.29%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 41.2  | Xtriage          |
| Anisotropy  | 0.744   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.24 , 48.9   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.91  | EDS              |
| Total number of atoms   | 20141   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 45.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.53 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.7003e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: HEM, CA, NO3, NAG, 3CJ

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

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$    |
| 1   | A     | 0.53         | 2/4882 (0.0%)  | 0.75        | 2/6632 (0.0%)  |
| 1   | B     | 0.47         | 0/4882         | 0.76        | 0/6632         |
| 1   | C     | 0.54         | 3/4882 (0.1%)  | 0.76        | 1/6632 (0.0%)  |
| 1   | D     | 0.51         | 1/4882 (0.0%)  | 0.79        | 3/6632 (0.0%)  |
| All | All   | 0.51         | 6/19528 (0.0%) | 0.76        | 6/26528 (0.0%) |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 10  | VAL  | C-N   | 9.65  | 1.52        | 1.34     |
| 1   | C     | 31  | ARG  | CA-C  | -5.54 | 1.38        | 1.52     |
| 1   | A     | 171 | PRO  | N-CD  | 5.39  | 1.55        | 1.47     |
| 1   | D     | 168 | PRO  | N-CD  | 5.14  | 1.55        | 1.47     |
| 1   | C     | 31  | ARG  | C-N   | -5.10 | 1.22        | 1.34     |
| 1   | C     | 9   | PRO  | N-CD  | 5.03  | 1.54        | 1.47     |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | D     | 169 | THR  | C-N-CD   | -7.76 | 103.53      | 120.60   |
| 1   | D     | 167 | CYS  | C-N-CD   | 5.57  | 140.10      | 128.40   |
| 1   | A     | 170 | PRO  | C-N-CD   | 5.51  | 139.97      | 128.40   |
| 1   | A     | 349 | PHE  | N-CA-C   | -5.38 | 96.49       | 111.00   |
| 1   | C     | 8   | ALA  | C-N-CD   | 5.32  | 139.57      | 128.40   |
| 1   | D     | 167 | CYS  | CA-CB-SG | 5.02  | 123.03      | 114.00   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4753  | 0        | 4646     | 298     | 0            |
| 1   | B     | 4753  | 0        | 4646     | 227     | 0            |
| 1   | C     | 4753  | 0        | 4649     | 313     | 0            |
| 1   | D     | 4753  | 0        | 4647     | 290     | 0            |
| 2   | A     | 56    | 0        | 51       | 1       | 0            |
| 2   | B     | 42    | 0        | 38       | 2       | 0            |
| 2   | C     | 56    | 0        | 51       | 1       | 0            |
| 2   | D     | 56    | 0        | 51       | 1       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 12    | 0        | 0        | 1       | 0            |
| 4   | B     | 12    | 0        | 0        | 1       | 0            |
| 4   | C     | 12    | 0        | 0        | 4       | 0            |
| 4   | D     | 12    | 0        | 0        | 8       | 0            |
| 5   | A     | 11    | 0        | 10       | 11      | 0            |
| 5   | B     | 11    | 0        | 10       | 12      | 0            |
| 5   | C     | 11    | 0        | 10       | 9       | 0            |
| 5   | D     | 11    | 0        | 10       | 11      | 0            |
| 6   | A     | 43    | 0        | 30       | 12      | 0            |
| 6   | B     | 43    | 0        | 30       | 14      | 0            |
| 6   | C     | 43    | 0        | 30       | 17      | 0            |
| 6   | D     | 43    | 0        | 30       | 15      | 0            |
| 7   | A     | 161   | 0        | 0        | 15      | 0            |
| 7   | B     | 155   | 0        | 0        | 10      | 0            |
| 7   | C     | 170   | 0        | 0        | 20      | 0            |
| 7   | D     | 165   | 0        | 0        | 11      | 0            |
| All | All   | 20141 | 0        | 18939    | 1151    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (1151) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:258:GLU:OE2 | 6:D:610:HEM:CMB  | 1.65                     | 1.42              |
| 1:A:167:CYS:HB2 | 1:A:168:PRO:CD   | 1.55                     | 1.32              |
| 1:D:258:GLU:OE2 | 6:D:610:HEM:HMB1 | 1.18                     | 1.30              |
| 1:B:10:VAL:HG11 | 1:B:41:ARG:NH1   | 1.48                     | 1.28              |
| 1:C:96:ARG:HD2  | 1:C:100:PHE:CD2  | 1.73                     | 1.21              |
| 1:C:167:CYS:HB3 | 1:C:168:PRO:CD   | 1.68                     | 1.17              |
| 1:C:96:ARG:HD2  | 1:C:100:PHE:CE2  | 1.79                     | 1.16              |
| 1:A:62:THR:HG21 | 1:A:65:LYS:HB2   | 1.15                     | 1.15              |
| 5:D:609:3CJ:H5  | 6:D:610:HEM:HAA1 | 1.25                     | 1.13              |
| 1:C:96:ARG:NH1  | 1:C:100:PHE:HE2  | 1.45                     | 1.12              |
| 1:D:169:THR:HB  | 1:D:170:PRO:HD3  | 1.32                     | 1.10              |
| 1:A:62:THR:HG21 | 1:A:65:LYS:CB    | 1.83                     | 1.08              |
| 1:C:167:CYS:HB3 | 1:C:168:PRO:HD2  | 1.29                     | 1.08              |
| 1:B:167:CYS:HB3 | 1:B:168:PRO:HD2  | 1.11                     | 1.07              |
| 1:A:167:CYS:HB2 | 1:A:168:PRO:HD3  | 1.24                     | 1.07              |
| 2:B:602:NAG:O4  | 2:B:603:NAG:N2   | 1.88                     | 1.06              |
| 1:A:167:CYS:CB  | 1:A:168:PRO:HD3  | 1.84                     | 1.06              |
| 1:B:167:CYS:CB  | 1:B:168:PRO:HD2  | 1.87                     | 1.04              |
| 1:C:93:ASP:OD2  | 1:C:96:ARG:NE    | 1.92                     | 1.03              |
| 1:A:169:THR:H   | 1:A:170:PRO:HD2  | 1.20                     | 1.02              |
| 1:C:42:ALA:HB2  | 1:C:166:VAL:HG11 | 1.41                     | 1.02              |
| 1:B:167:CYS:HB3 | 1:B:168:PRO:CD   | 1.89                     | 1.02              |
| 1:C:96:ARG:NH1  | 1:C:100:PHE:CE2  | 2.24                     | 1.01              |
| 1:C:423:GLN:HG2 | 7:C:733:HOH:O    | 1.59                     | 1.00              |
| 1:D:169:THR:CB  | 1:D:170:PRO:HD3  | 1.88                     | 0.99              |
| 1:A:402:LYS:HD2 | 4:A:607:NO3:O3   | 1.61                     | 0.98              |
| 1:B:42:ALA:HB2  | 1:B:166:VAL:HG11 | 1.46                     | 0.98              |
| 1:A:167:CYS:CB  | 1:A:168:PRO:CD   | 2.38                     | 0.98              |
| 1:A:169:THR:N   | 1:A:170:PRO:HD2  | 1.75                     | 0.98              |
| 1:A:557:THR:OG1 | 1:A:559:ILE:HG12 | 1.65                     | 0.97              |
| 1:C:167:CYS:CB  | 1:C:168:PRO:HD2  | 1.92                     | 0.97              |
| 5:C:609:3CJ:H2  | 6:C:610:HEM:O1D  | 1.64                     | 0.96              |
| 1:C:96:ARG:NH1  | 1:C:506:ARG:HG3  | 1.80                     | 0.95              |
| 1:C:593:ARG:NH1 | 1:C:593:ARG:HB3  | 1.81                     | 0.95              |
| 1:D:13:VAL:HG12 | 1:D:14:THR:H     | 1.29                     | 0.95              |
| 1:B:10:VAL:HG11 | 1:B:41:ARG:HH12  | 1.12                     | 0.93              |
| 1:B:10:VAL:CG1  | 1:B:41:ARG:HH12  | 1.81                     | 0.93              |
| 1:A:62:THR:CG2  | 1:A:65:LYS:HB2   | 1.98                     | 0.91              |
| 1:C:167:CYS:CB  | 1:C:168:PRO:CD   | 2.47                     | 0.91              |
| 1:C:102:GLN:OE1 | 1:C:259:GLN:NE2  | 2.03                     | 0.90              |
| 1:B:537:THR:OG1 | 1:B:540:GLN:HG3  | 1.71                     | 0.90              |
| 1:D:258:GLU:OE2 | 6:D:610:HEM:HMB2 | 1.69                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:8:ALA:HB1    | 7:A:762:HOH:O    | 1.71                     | 0.89              |
| 1:B:551:ARG:HD3  | 1:B:584:LYS:HA   | 1.53                     | 0.89              |
| 1:C:96:ARG:CD    | 1:C:100:PHE:CE2  | 2.55                     | 0.89              |
| 1:A:117:THR:HG22 | 1:A:162:ARG:O    | 1.72                     | 0.89              |
| 1:C:312:TYR:O    | 1:C:315:ILE:HG12 | 1.73                     | 0.89              |
| 1:A:129:CYS:O    | 1:A:133:CYS:HA   | 1.73                     | 0.88              |
| 1:B:10:VAL:HG11  | 1:B:41:ARG:CZ    | 2.03                     | 0.87              |
| 1:C:481:LEU:HD21 | 1:C:487:PRO:HG3  | 1.55                     | 0.87              |
| 1:B:13:VAL:O     | 1:B:13:VAL:HG12  | 1.75                     | 0.87              |
| 1:A:377:HIS:HB3  | 1:A:416:GLU:OE1  | 1.74                     | 0.87              |
| 1:C:96:ARG:HH11  | 1:C:506:ARG:HG3  | 1.40                     | 0.87              |
| 1:A:167:CYS:HB2  | 1:A:168:PRO:HD2  | 1.52                     | 0.87              |
| 1:B:167:CYS:CB   | 1:B:168:PRO:CD   | 2.51                     | 0.86              |
| 1:C:593:ARG:HB3  | 1:C:593:ARG:HH11 | 1.38                     | 0.86              |
| 1:B:537:THR:HG23 | 1:B:540:GLN:OE1  | 1.75                     | 0.86              |
| 1:D:403:ASN:HB2  | 4:D:607:NO3:O1   | 1.76                     | 0.85              |
| 1:A:42:ALA:HB2   | 1:A:166:VAL:HG11 | 1.58                     | 0.85              |
| 1:B:2:TRP:HH2    | 1:C:86:LEU:HD13  | 1.41                     | 0.84              |
| 1:D:348:ARG:HH11 | 1:D:437:ASN:ND2  | 1.75                     | 0.84              |
| 1:C:37:GLY:H     | 1:C:338:ARG:HG2  | 1.41                     | 0.84              |
| 1:C:418:ARG:HG2  | 1:C:418:ARG:HH11 | 1.41                     | 0.84              |
| 1:D:185:SER:HB3  | 1:D:339:ILE:HG12 | 1.58                     | 0.84              |
| 1:D:530:TRP:CZ2  | 4:D:608:NO3:O2   | 2.30                     | 0.84              |
| 1:C:421:LEU:HG   | 7:C:733:HOH:O    | 1.76                     | 0.84              |
| 1:C:230:ASN:HD21 | 1:C:232:VAL:HG22 | 1.42                     | 0.83              |
| 1:D:258:GLU:OE2  | 6:D:610:HEM:C2B  | 2.32                     | 0.83              |
| 1:C:11:PRO:O     | 1:C:12:LEU:HB3   | 1.78                     | 0.82              |
| 1:A:169:THR:N    | 1:A:170:PRO:CD   | 2.40                     | 0.82              |
| 1:C:146:LYS:HG3  | 1:C:147:ASN:OD1  | 1.79                     | 0.81              |
| 1:A:119:LEU:HD12 | 1:A:120:GLY:H    | 1.45                     | 0.81              |
| 1:D:572:TYR:CE1  | 1:D:573:PRO:HB3  | 2.15                     | 0.81              |
| 1:B:551:ARG:NH1  | 1:B:582:VAL:O    | 2.14                     | 0.81              |
| 1:D:92:LEU:HD13  | 4:D:607:NO3:O1   | 1.80                     | 0.81              |
| 1:D:310:ARG:O    | 1:D:314:PRO:HG2  | 1.81                     | 0.81              |
| 1:B:276:LEU:O    | 1:B:280:LEU:HG   | 1.81                     | 0.80              |
| 1:C:513:CYS:O    | 1:C:517:ARG:HG3  | 1.82                     | 0.80              |
| 2:B:602:NAG:C4   | 2:B:603:NAG:HN2  | 1.95                     | 0.79              |
| 1:B:332:ASN:OD1  | 1:B:334:SER:HB2  | 1.81                     | 0.79              |
| 5:D:609:3CJ:C6   | 6:D:610:HEM:HAA1 | 2.12                     | 0.79              |
| 1:D:333:ASN:HD22 | 1:D:333:ASN:H    | 1.29                     | 0.79              |
| 1:C:423:GLN:HB3  | 1:C:426:HIS:HD2  | 1.48                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:230:ASN:OD1  | 1:D:232:VAL:HG22 | 1.82                     | 0.79              |
| 1:B:10:VAL:CG1   | 1:B:41:ARG:NH1   | 2.38                     | 0.78              |
| 1:D:13:VAL:HG12  | 1:D:14:THR:N     | 1.98                     | 0.78              |
| 1:D:119:LEU:HD12 | 7:D:804:HOH:O    | 1.83                     | 0.78              |
| 1:C:12:LEU:HG    | 1:C:13:VAL:H     | 1.48                     | 0.77              |
| 1:A:322:GLN:H    | 1:A:322:GLN:HE21 | 1.30                     | 0.77              |
| 1:C:468:GLN:HG2  | 1:C:474:LYS:HA   | 1.66                     | 0.77              |
| 1:B:123:GLU:HB2  | 1:B:126:LYS:HG3  | 1.64                     | 0.77              |
| 1:B:117:THR:OG1  | 1:B:119:LEU:HD23 | 1.83                     | 0.77              |
| 5:C:609:3CJ:C6   | 6:C:610:HEM:HAA1 | 2.14                     | 0.77              |
| 1:A:169:THR:H    | 1:A:170:PRO:CD   | 1.95                     | 0.77              |
| 1:A:551:ARG:NH1  | 1:A:584:LYS:HG2  | 2.00                     | 0.77              |
| 1:A:351:HIS:CE1  | 1:A:433:LEU:HD21 | 2.21                     | 0.76              |
| 1:C:12:LEU:HG    | 1:C:13:VAL:N     | 1.99                     | 0.76              |
| 1:D:295:GLU:O    | 1:D:299:ILE:HG13 | 1.86                     | 0.76              |
| 1:C:125:SER:HA   | 1:C:128:GLN:HB3  | 1.67                     | 0.76              |
| 1:C:96:ARG:NH1   | 1:C:506:ARG:CG   | 2.49                     | 0.76              |
| 1:D:265:VAL:O    | 1:D:269:LEU:HG   | 1.86                     | 0.75              |
| 1:B:551:ARG:HD2  | 1:B:583:ASP:O    | 1.85                     | 0.75              |
| 1:C:146:LYS:HE3  | 1:C:147:ASN:HD21 | 1.52                     | 0.75              |
| 1:C:348:ARG:HH11 | 1:C:437:ASN:ND2  | 1.84                     | 0.75              |
| 1:C:452:TRP:HH2  | 4:C:608:NO3:O3   | 1.69                     | 0.75              |
| 1:C:167:CYS:HB3  | 1:C:168:PRO:HD3  | 1.68                     | 0.75              |
| 1:B:301:GLY:O    | 1:B:305:GLN:HG3  | 1.86                     | 0.75              |
| 2:A:604:NAG:H62  | 2:A:604:NAG:O3   | 1.87                     | 0.74              |
| 1:C:76:ARG:HH22  | 1:C:419:ASN:HD21 | 1.35                     | 0.74              |
| 1:A:261:LEU:O    | 1:A:264:THR:HB   | 1.85                     | 0.74              |
| 1:C:96:ARG:NH2   | 1:C:406:LEU:HD12 | 2.02                     | 0.74              |
| 5:C:609:3CJ:H5   | 6:C:610:HEM:HAA1 | 1.70                     | 0.74              |
| 1:C:159:PRO:HD2  | 1:C:431:PHE:HE1  | 1.50                     | 0.73              |
| 1:C:348:ARG:HB2  | 1:C:493:TRP:CD1  | 2.23                     | 0.73              |
| 1:C:96:ARG:HH21  | 1:C:406:LEU:HD12 | 1.51                     | 0.73              |
| 1:D:113:PHE:CE1  | 5:D:609:3CJ:H6   | 2.23                     | 0.73              |
| 1:C:519:PHE:HA   | 1:C:522:ILE:HG13 | 1.69                     | 0.73              |
| 1:C:146:LYS:CE   | 1:C:147:ASN:HD21 | 2.02                     | 0.73              |
| 1:C:348:ARG:HB2  | 1:C:493:TRP:NE1  | 2.02                     | 0.73              |
| 1:A:260:ILE:HG23 | 1:A:261:LEU:HD23 | 1.70                     | 0.73              |
| 1:A:588:SER:HB2  | 1:A:589:PRO:HD3  | 1.71                     | 0.73              |
| 1:B:118:GLU:HG3  | 1:B:119:LEU:H    | 1.52                     | 0.73              |
| 1:A:327:PRO:HA   | 7:A:719:HOH:O    | 1.89                     | 0.73              |
| 1:C:170:PRO:HA   | 7:C:822:HOH:O    | 1.89                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:409:GLN:NE2  | 1:B:473:ASN:HD22 | 1.87                     | 0.72              |
| 1:D:375:PRO:HG2  | 1:D:378:THR:HG23 | 1.70                     | 0.72              |
| 1:A:421:LEU:HB3  | 1:A:431:PHE:HB2  | 1.72                     | 0.72              |
| 6:B:608:HEM:HBB2 | 6:B:608:HEM:HMB1 | 1.72                     | 0.72              |
| 1:C:552:LEU:HD12 | 1:C:556:ASN:ND2  | 2.05                     | 0.72              |
| 1:C:348:ARG:CB   | 1:C:493:TRP:HE1  | 2.02                     | 0.72              |
| 1:A:239:PHE:HZ   | 1:A:427:LYS:HB3  | 1.55                     | 0.72              |
| 1:C:530:TRP:NE1  | 4:C:606:NO3:O2   | 2.22                     | 0.72              |
| 1:B:2:TRP:CZ2    | 1:C:86:LEU:HD22  | 2.25                     | 0.71              |
| 5:A:609:3CJ:H7   | 6:A:610:HEM:HBD2 | 1.73                     | 0.71              |
| 1:C:528:PHE:HB3  | 7:C:840:HOH:O    | 1.89                     | 0.71              |
| 1:C:452:TRP:CH2  | 4:C:608:NO3:O3   | 2.44                     | 0.71              |
| 1:A:119:LEU:CD1  | 1:A:120:GLY:N    | 2.53                     | 0.71              |
| 1:B:300:LEU:O    | 1:B:304:ILE:HD13 | 1.91                     | 0.71              |
| 1:C:427:LYS:N    | 1:C:427:LYS:HD2  | 2.05                     | 0.70              |
| 1:D:345:PHE:CD2  | 1:D:446:MET:SD   | 2.84                     | 0.70              |
| 1:A:105:GLN:HG3  | 5:A:609:3CJ:S1   | 2.32                     | 0.70              |
| 5:A:609:3CJ:H3   | 6:A:610:HEM:O1D  | 1.91                     | 0.70              |
| 1:C:342:VAL:HB   | 1:C:452:TRP:CZ2  | 2.27                     | 0.70              |
| 1:D:106:ILE:HG23 | 1:D:191:LEU:HD11 | 1.73                     | 0.70              |
| 1:D:322:GLN:CD   | 1:D:322:GLN:H    | 1.91                     | 0.70              |
| 1:B:213:MET:HG2  | 1:B:273:HIS:CD2  | 2.26                     | 0.70              |
| 1:A:103:TRP:O    | 1:A:107:VAL:HG23 | 1.91                     | 0.70              |
| 1:B:377:HIS:HA   | 1:B:380:PHE:CE2  | 2.26                     | 0.70              |
| 1:A:230:ASN:HD21 | 1:A:232:VAL:HG22 | 1.55                     | 0.70              |
| 1:A:340:SER:OG   | 1:A:343:PHE:HB2  | 1.92                     | 0.70              |
| 1:B:139:CYS:SG   | 1:B:141:PRO:HD3  | 2.32                     | 0.70              |
| 1:C:484:TYR:O    | 1:C:485:LYS:HB2  | 1.90                     | 0.70              |
| 1:C:519:PHE:HA   | 1:C:522:ILE:CG1  | 2.21                     | 0.70              |
| 1:A:148:ASP:O    | 1:A:151:LEU:HB2  | 1.91                     | 0.70              |
| 1:A:119:LEU:HD12 | 1:A:120:GLY:N    | 2.06                     | 0.70              |
| 1:B:39:ALA:HB1   | 1:B:182:ALA:O    | 1.92                     | 0.70              |
| 1:B:257:SER:HB2  | 7:B:729:HOH:O    | 1.91                     | 0.69              |
| 1:B:272:GLU:O    | 1:B:276:LEU:HG   | 1.93                     | 0.69              |
| 1:C:188:ASP:OD1  | 1:C:190:SER:HB3  | 1.92                     | 0.69              |
| 1:A:99:LEU:HD23  | 1:A:566:ALA:HB1  | 1.74                     | 0.69              |
| 1:B:421:LEU:HD12 | 1:B:422:PHE:H    | 1.57                     | 0.69              |
| 1:B:42:ALA:HB2   | 1:B:166:VAL:CG1  | 2.21                     | 0.69              |
| 1:D:530:TRP:HZ2  | 4:D:608:NO3:O2   | 1.72                     | 0.69              |
| 1:C:517:ARG:NH2  | 1:C:517:ARG:HB3  | 2.07                     | 0.69              |
| 1:B:273:HIS:HD2  | 1:B:274:ASN:OD1  | 1.74                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:551:ARG:CD   | 1:B:584:LYS:HA   | 2.24                     | 0.68              |
| 1:C:124:HIS:CE1  | 1:C:128:GLN:HB2  | 2.28                     | 0.68              |
| 1:C:423:GLN:HB2  | 1:C:426:HIS:HB2  | 1.75                     | 0.68              |
| 1:D:409:GLN:HB3  | 1:D:476:LEU:HD22 | 1.74                     | 0.68              |
| 1:B:463:THR:HA   | 7:B:784:HOH:O    | 1.92                     | 0.68              |
| 1:C:423:GLN:HB3  | 1:C:426:HIS:CD2  | 2.28                     | 0.68              |
| 1:B:261:LEU:HD13 | 1:B:399:LEU:HD21 | 1.73                     | 0.68              |
| 1:A:119:LEU:CD1  | 1:A:120:GLY:H    | 2.06                     | 0.68              |
| 1:D:3:GLU:HG2    | 1:D:4:VAL:H      | 1.59                     | 0.68              |
| 1:A:421:LEU:HB3  | 1:A:431:PHE:CB   | 2.24                     | 0.68              |
| 1:D:196:GLU:HB3  | 7:D:781:HOH:O    | 1.93                     | 0.68              |
| 1:B:3:GLU:HB3    | 1:B:175:LEU:HD12 | 1.74                     | 0.68              |
| 1:D:570:ASN:HB3  | 1:D:575:ASP:HB2  | 1.75                     | 0.68              |
| 1:A:367:PRO:HB2  | 1:D:64:ARG:NH2   | 2.09                     | 0.68              |
| 1:D:30:ASN:O     | 1:D:34:PRO:HA    | 1.94                     | 0.68              |
| 1:D:7:GLY:C      | 1:D:9:PRO:HD3    | 2.14                     | 0.68              |
| 1:A:88:GLU:O     | 1:A:91:VAL:HG22  | 1.93                     | 0.67              |
| 6:B:608:HEM:O1D  | 5:B:609:3CJ:H3   | 1.95                     | 0.67              |
| 1:C:96:ARG:CZ    | 1:C:506:ARG:HD2  | 2.24                     | 0.67              |
| 1:C:146:LYS:HE3  | 1:C:147:ASN:ND2  | 2.09                     | 0.67              |
| 1:A:113:PHE:CE1  | 5:A:609:3CJ:H5   | 2.30                     | 0.67              |
| 1:A:66:THR:HB    | 1:A:70:PHE:C     | 2.13                     | 0.67              |
| 6:B:608:HEM:HHA  | 5:B:609:3CJ:H7   | 1.77                     | 0.67              |
| 1:C:76:ARG:HH22  | 1:C:419:ASN:ND2  | 1.92                     | 0.67              |
| 1:D:530:TRP:NE1  | 4:D:608:NO3:O2   | 2.26                     | 0.67              |
| 1:A:464:LEU:HD12 | 1:A:464:LEU:O    | 1.94                     | 0.67              |
| 1:A:322:GLN:H    | 1:A:322:GLN:NE2  | 1.92                     | 0.67              |
| 1:C:418:ARG:NH1  | 1:C:418:ARG:HG2  | 2.02                     | 0.67              |
| 1:D:350:GLY:HA3  | 6:D:610:HEM:CBC  | 2.25                     | 0.67              |
| 1:C:316:VAL:O    | 1:C:507:VAL:HG22 | 1.95                     | 0.66              |
| 1:C:159:PRO:HD2  | 1:C:431:PHE:CE1  | 2.29                     | 0.66              |
| 1:D:166:VAL:O    | 1:D:167:CYS:CB   | 2.41                     | 0.66              |
| 1:B:118:GLU:HG3  | 1:B:119:LEU:N    | 2.08                     | 0.66              |
| 1:D:10:VAL:CG1   | 1:D:11:PRO:HD2   | 2.25                     | 0.66              |
| 1:B:2:TRP:HZ2    | 1:C:86:LEU:HD22  | 1.59                     | 0.66              |
| 1:D:385:ARG:O    | 1:D:389:ASP:HB3  | 1.95                     | 0.66              |
| 1:C:204:ARG:HA   | 1:C:213:MET:HA   | 1.78                     | 0.66              |
| 1:B:280:LEU:O    | 1:B:284:ASN:N    | 2.28                     | 0.66              |
| 1:B:113:PHE:CE1  | 5:B:609:3CJ:H5   | 2.30                     | 0.66              |
| 1:C:146:LYS:NZ   | 1:C:147:ASN:HD21 | 1.93                     | 0.66              |
| 1:C:76:ARG:NH1   | 1:C:418:ARG:HH12 | 1.94                     | 0.66              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:370:PRO:HG2 | 1:D:371:GLU:OE1  | 1.95                     | 0.66              |
| 1:A:2:TRP:HD1   | 1:A:175:LEU:HD23 | 1.60                     | 0.66              |
| 1:C:345:PHE:O   | 1:C:493:TRP:HD1  | 1.79                     | 0.66              |
| 1:A:188:ASP:OD1 | 1:A:190:SER:HB3  | 1.95                     | 0.66              |
| 1:D:570:ASN:HB3 | 1:D:575:ASP:CB   | 2.26                     | 0.66              |
| 1:C:287:TRP:HA  | 7:C:749:HOH:O    | 1.95                     | 0.66              |
| 1:D:166:VAL:O   | 1:D:167:CYS:HB2  | 1.95                     | 0.66              |
| 1:A:17:GLU:OE2  | 1:A:31:ARG:HG2   | 1.95                     | 0.66              |
| 1:C:204:ARG:CZ  | 1:C:206:LEU:HD21 | 2.25                     | 0.66              |
| 1:D:10:VAL:HG12 | 1:D:11:PRO:HD2   | 1.77                     | 0.66              |
| 1:D:530:TRP:CE2 | 4:D:608:NO3:O2   | 2.47                     | 0.66              |
| 1:B:51:TYR:HB3  | 1:B:57:VAL:O     | 1.96                     | 0.65              |
| 1:D:11:PRO:O    | 1:D:13:VAL:HG23  | 1.96                     | 0.65              |
| 1:C:348:ARG:HB2 | 1:C:493:TRP:HE1  | 1.58                     | 0.65              |
| 1:D:123:GLU:HG3 | 7:D:804:HOH:O    | 1.95                     | 0.65              |
| 1:A:167:CYS:HB3 | 1:A:168:PRO:HD3  | 1.77                     | 0.65              |
| 1:A:253:ASP:OD2 | 1:A:255:ARG:HB2  | 1.96                     | 0.65              |
| 1:A:165:PHE:CD2 | 1:A:177:ARG:HD2  | 2.32                     | 0.65              |
| 1:A:322:GLN:N   | 1:A:322:GLN:HE21 | 1.94                     | 0.65              |
| 1:C:37:GLY:N    | 1:C:338:ARG:HG2  | 2.11                     | 0.65              |
| 1:C:98:LEU:HA   | 1:C:404:SER:OG   | 1.97                     | 0.65              |
| 1:A:370:PRO:O   | 1:D:71:ARG:NH2   | 2.29                     | 0.65              |
| 1:A:99:LEU:HG   | 1:A:567:PHE:HE1  | 1.61                     | 0.65              |
| 1:B:407:MET:SD  | 1:B:408:ASN:N    | 2.69                     | 0.65              |
| 1:C:109:HIS:HA  | 1:C:255:ARG:NH2  | 2.11                     | 0.65              |
| 1:C:201:SER:HA  | 7:C:816:HOH:O    | 1.95                     | 0.65              |
| 1:A:551:ARG:NH1 | 1:A:584:LYS:CG   | 2.60                     | 0.65              |
| 1:B:94:GLN:O    | 1:B:569:ALA:HB3  | 1.96                     | 0.65              |
| 1:A:71:ARG:CZ   | 1:A:71:ARG:HB3   | 2.24                     | 0.65              |
| 1:D:463:THR:HB  | 7:D:714:HOH:O    | 1.94                     | 0.65              |
| 1:D:105:GLN:NE2 | 5:D:609:3CJ:S1   | 2.60                     | 0.65              |
| 1:A:95:ASN:O    | 1:A:96:ARG:HD3   | 1.97                     | 0.65              |
| 1:B:10:VAL:HG21 | 1:B:41:ARG:HH12  | 1.62                     | 0.65              |
| 1:B:145:PRO:O   | 1:B:148:ASP:HB2  | 1.97                     | 0.65              |
| 1:A:62:THR:HG23 | 1:A:64:ARG:H     | 1.62                     | 0.64              |
| 1:A:148:ASP:O   | 1:A:151:LEU:CB   | 2.46                     | 0.64              |
| 1:B:537:THR:OG1 | 1:B:540:GLN:CG   | 2.44                     | 0.64              |
| 1:C:48:PRO:HG2  | 7:C:720:HOH:O    | 1.98                     | 0.64              |
| 1:D:408:ASN:O   | 1:D:411:LYS:N    | 2.28                     | 0.64              |
| 1:A:123:GLU:HB2 | 1:A:126:LYS:HG3  | 1.78                     | 0.64              |
| 1:A:348:ARG:HG2 | 6:A:610:HEM:C2D  | 2.33                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:142:ILE:HD12 | 1:A:160:PHE:HB2  | 1.77                     | 0.64              |
| 1:A:546:LYS:HZ1  | 1:A:586:ASP:H    | 1.46                     | 0.64              |
| 1:C:351:HIS:CE1  | 1:C:433:LEU:HD21 | 2.32                     | 0.64              |
| 1:A:62:THR:CG2   | 1:A:65:LYS:H     | 2.10                     | 0.64              |
| 1:C:393:ASP:OD1  | 1:C:557:THR:HB   | 1.96                     | 0.64              |
| 1:D:112:ASP:OD1  | 6:D:610:HEM:O2D  | 2.16                     | 0.64              |
| 1:B:265:VAL:O    | 1:B:269:LEU:HG   | 1.98                     | 0.63              |
| 1:C:264:THR:HG23 | 1:C:392:ILE:HG23 | 1.81                     | 0.63              |
| 1:D:368:TRP:O    | 1:D:372:ALA:HB2  | 1.98                     | 0.63              |
| 1:D:424:PRO:O    | 1:D:425:THR:HB   | 1.96                     | 0.63              |
| 1:B:145:PRO:HD2  | 1:B:148:ASP:OD2  | 1.96                     | 0.63              |
| 1:A:8:ALA:HA     | 7:A:813:HOH:O    | 1.97                     | 0.63              |
| 1:B:230:ASN:OD1  | 1:B:232:VAL:HG22 | 1.98                     | 0.63              |
| 1:D:8:ALA:N      | 1:D:9:PRO:HD3    | 2.13                     | 0.63              |
| 1:B:532:ASN:O    | 1:B:535:VAL:HG23 | 1.98                     | 0.63              |
| 6:B:608:HEM:CHA  | 5:B:609:3CJ:H7   | 2.29                     | 0.63              |
| 1:A:123:GLU:CB   | 1:A:126:LYS:HG3  | 2.29                     | 0.63              |
| 1:B:167:CYS:SG   | 1:B:168:PRO:CD   | 2.87                     | 0.63              |
| 1:A:121:SER:O    | 1:A:123:GLU:N    | 2.30                     | 0.63              |
| 1:C:110:ASP:OD1  | 1:C:187:LEU:HA   | 1.99                     | 0.63              |
| 1:D:167:CYS:HB3  | 1:D:168:PRO:CD   | 2.28                     | 0.63              |
| 1:C:146:LYS:HE3  | 1:C:147:ASN:OD1  | 1.98                     | 0.62              |
| 1:B:18:GLN:HG3   | 7:B:745:HOH:O    | 1.99                     | 0.62              |
| 1:C:140:PHE:O    | 1:C:160:PHE:HB3  | 1.99                     | 0.62              |
| 1:D:10:VAL:HG12  | 1:D:11:PRO:CD    | 2.29                     | 0.62              |
| 1:D:13:VAL:CG1   | 1:D:14:THR:H     | 2.08                     | 0.62              |
| 1:D:91:VAL:O     | 1:D:406:LEU:N    | 2.28                     | 0.62              |
| 1:B:11:PRO:O     | 1:B:13:VAL:HG23  | 1.99                     | 0.62              |
| 1:D:16:ASP:O     | 1:D:18:GLN:N     | 2.30                     | 0.62              |
| 1:A:2:TRP:CD1    | 1:A:175:LEU:HD23 | 2.34                     | 0.62              |
| 1:B:353:GLU:HA   | 1:B:405:LYS:O    | 2.00                     | 0.62              |
| 1:C:468:GLN:OE1  | 1:C:474:LYS:HB3  | 1.99                     | 0.62              |
| 1:D:77:GLU:HG3   | 1:D:145:PRO:HB3  | 1.81                     | 0.62              |
| 1:C:518:GLN:HE21 | 1:C:522:ILE:HG23 | 1.63                     | 0.62              |
| 1:A:370:PRO:HG2  | 1:A:371:GLU:OE1  | 1.99                     | 0.62              |
| 1:A:136:GLY:HA2  | 1:C:124:HIS:CD2  | 2.35                     | 0.62              |
| 1:D:167:CYS:CB   | 1:D:168:PRO:CD   | 2.78                     | 0.62              |
| 1:D:425:THR:HG21 | 7:D:812:HOH:O    | 2.00                     | 0.62              |
| 1:D:446:MET:HE3  | 4:D:606:NO3:O1   | 1.99                     | 0.62              |
| 1:D:191:LEU:H    | 1:D:191:LEU:HD23 | 1.63                     | 0.61              |
| 1:A:260:ILE:HD11 | 1:A:386:ILE:HG13 | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:239:PHE:CZ   | 1:A:427:LYS:HB3  | 2.35                     | 0.61              |
| 6:B:608:HEM:C1A  | 5:B:609:3CJ:N1   | 2.68                     | 0.61              |
| 1:D:342:VAL:HB   | 1:D:446:MET:HE1  | 1.82                     | 0.61              |
| 1:D:503:GLU:O    | 1:D:504:ARG:HB2  | 2.00                     | 0.61              |
| 1:A:172:TYR:HE2  | 1:A:175:LEU:HB2  | 1.65                     | 0.61              |
| 1:B:52:GLU:HG3   | 1:B:59:PHE:HA    | 1.81                     | 0.61              |
| 1:C:425:THR:O    | 1:C:425:THR:HG22 | 2.01                     | 0.61              |
| 1:D:309:PHE:HA   | 1:D:313:LEU:HD12 | 1.82                     | 0.61              |
| 1:A:459:SER:O    | 1:A:461:PRO:HD3  | 2.01                     | 0.61              |
| 1:A:313:LEU:HD11 | 1:A:519:PHE:CG   | 2.36                     | 0.61              |
| 1:D:351:HIS:CD2  | 6:D:610:HEM:NC   | 2.69                     | 0.61              |
| 1:A:174:SER:O    | 1:A:175:LEU:HG   | 2.01                     | 0.61              |
| 1:D:240:ILE:HD13 | 1:D:382:ASN:HA   | 1.82                     | 0.61              |
| 1:B:35:ALA:HB1   | 1:B:41:ARG:NE    | 2.16                     | 0.61              |
| 1:D:101:MET:SD   | 1:D:101:MET:C    | 2.79                     | 0.61              |
| 1:D:186:PHE:O    | 1:D:188:ASP:N    | 2.33                     | 0.61              |
| 1:D:301:GLY:O    | 1:D:305:GLN:HG3  | 2.01                     | 0.61              |
| 1:D:9:PRO:HG2    | 1:D:41:ARG:HH22  | 1.66                     | 0.61              |
| 1:A:105:GLN:HB2  | 6:A:610:HEM:C2C  | 2.36                     | 0.61              |
| 1:A:62:THR:HG21  | 1:A:65:LYS:H     | 1.66                     | 0.61              |
| 1:D:325:ILE:O    | 1:D:325:ILE:HG22 | 2.01                     | 0.61              |
| 1:D:113:PHE:HE1  | 5:D:609:3CJ:H6   | 1.66                     | 0.61              |
| 1:A:165:PHE:CZ   | 1:A:169:THR:O    | 2.53                     | 0.60              |
| 1:A:272:GLU:O    | 1:A:276:LEU:HG   | 2.01                     | 0.60              |
| 1:C:168:PRO:HG3  | 1:C:172:TYR:HD2  | 1.67                     | 0.60              |
| 1:C:539:LYS:HE2  | 1:C:589:PRO:HG3  | 1.81                     | 0.60              |
| 1:C:151:LEU:HD11 | 1:C:156:LYS:HD2  | 1.82                     | 0.60              |
| 1:C:169:THR:N    | 1:C:170:PRO:CD   | 2.64                     | 0.60              |
| 1:D:144:PHE:CE1  | 1:D:158:MET:HG3  | 2.37                     | 0.60              |
| 1:A:62:THR:HG21  | 1:A:65:LYS:N     | 2.16                     | 0.60              |
| 1:B:13:VAL:CG1   | 1:B:13:VAL:O     | 2.49                     | 0.60              |
| 1:B:110:ASP:OD2  | 1:B:189:ALA:HA   | 2.02                     | 0.60              |
| 1:D:200:ALA:O    | 1:D:204:ARG:HG3  | 2.01                     | 0.60              |
| 1:D:315:ILE:O    | 1:D:505:GLY:HA2  | 2.00                     | 0.60              |
| 1:C:351:HIS:ND1  | 1:C:433:LEU:HD21 | 2.17                     | 0.60              |
| 5:C:609:3CJ:H4   | 6:C:610:HEM:HAA1 | 1.82                     | 0.60              |
| 1:D:586:ASP:O    | 1:D:589:PRO:HD2  | 2.02                     | 0.60              |
| 5:D:609:3CJ:H2   | 6:D:610:HEM:O1D  | 2.02                     | 0.60              |
| 1:A:81:LYS:HB2   | 1:A:483:LEU:HD11 | 1.84                     | 0.60              |
| 1:D:7:GLY:HA2    | 1:D:166:VAL:HB   | 1.84                     | 0.60              |
| 1:D:8:ALA:N      | 1:D:9:PRO:CD     | 2.65                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:325:ILE:O    | 1:A:325:ILE:HG22 | 2.02                     | 0.60              |
| 1:D:492:ILE:HG23 | 1:D:493:TRP:N    | 2.17                     | 0.60              |
| 1:B:258:GLU:O    | 1:B:380:PHE:HA   | 2.01                     | 0.59              |
| 1:C:191:LEU:HD23 | 1:C:191:LEU:H    | 1.67                     | 0.59              |
| 1:D:348:ARG:NH1  | 1:D:437:ASN:ND2  | 2.47                     | 0.59              |
| 1:A:396:VAL:HA   | 1:A:399:LEU:HD12 | 1.84                     | 0.59              |
| 1:A:342:VAL:HG11 | 1:A:452:TRP:CH2  | 2.37                     | 0.59              |
| 1:C:12:LEU:O     | 1:C:13:VAL:HB    | 2.01                     | 0.59              |
| 1:C:165:PHE:CG   | 1:C:177:ARG:HD2  | 2.37                     | 0.59              |
| 6:D:610:HEM:HMC1 | 6:D:610:HEM:HBC2 | 1.84                     | 0.59              |
| 1:B:409:GLN:HE22 | 1:B:473:ASN:HB2  | 1.66                     | 0.59              |
| 1:C:169:THR:N    | 1:C:170:PRO:HD3  | 2.18                     | 0.59              |
| 1:A:165:PHE:CG   | 1:A:177:ARG:HD2  | 2.37                     | 0.59              |
| 1:A:392:ILE:O    | 1:A:396:VAL:HG23 | 2.01                     | 0.59              |
| 1:C:165:PHE:CZ   | 1:C:169:THR:O    | 2.56                     | 0.59              |
| 1:D:425:THR:O    | 1:D:425:THR:HG22 | 2.02                     | 0.59              |
| 1:A:229:PHE:CD1  | 1:A:247:PRO:HG2  | 2.38                     | 0.59              |
| 1:D:168:PRO:HB2  | 1:D:170:PRO:HD2  | 1.84                     | 0.59              |
| 1:A:156:LYS:HG3  | 7:A:742:HOH:O    | 2.02                     | 0.59              |
| 1:C:522:ILE:O    | 1:C:526:ASP:HB2  | 2.03                     | 0.59              |
| 6:A:610:HEM:HMC2 | 6:A:610:HEM:HBC2 | 1.85                     | 0.59              |
| 1:A:99:LEU:HG    | 1:A:567:PHE:CE1  | 2.38                     | 0.59              |
| 1:C:557:THR:OG1  | 1:C:559:ILE:HG12 | 2.02                     | 0.59              |
| 1:D:419:ASN:O    | 1:D:430:GLY:HA2  | 2.03                     | 0.58              |
| 1:A:8:ALA:N      | 1:A:9:PRO:CD     | 2.66                     | 0.58              |
| 1:D:106:ILE:HG23 | 1:D:191:LEU:CD1  | 2.33                     | 0.58              |
| 1:D:96:ARG:HG3   | 1:D:506:ARG:HE   | 1.68                     | 0.58              |
| 1:A:9:PRO:HB2    | 1:A:41:ARG:NH2   | 2.18                     | 0.58              |
| 1:C:99:LEU:HA    | 1:C:399:LEU:HD22 | 1.85                     | 0.58              |
| 1:D:117:THR:HG22 | 1:D:162:ARG:O    | 2.04                     | 0.58              |
| 1:D:9:PRO:HG2    | 1:D:41:ARG:NH2   | 2.19                     | 0.58              |
| 1:A:146:LYS:O    | 1:A:147:ASN:HB2  | 2.04                     | 0.58              |
| 1:A:348:ARG:HG2  | 6:A:610:HEM:C3D  | 2.39                     | 0.58              |
| 1:D:486:THR:HG23 | 1:D:489:ASN:H    | 1.69                     | 0.58              |
| 1:D:501:MET:HA   | 1:D:507:VAL:O    | 2.03                     | 0.58              |
| 1:A:504:ARG:HD3  | 7:A:831:HOH:O    | 2.02                     | 0.58              |
| 1:A:66:THR:HB    | 1:A:70:PHE:O     | 2.03                     | 0.58              |
| 1:D:199:LEU:HD12 | 1:D:199:LEU:O    | 2.04                     | 0.58              |
| 1:B:348:ARG:HH11 | 1:B:437:ASN:ND2  | 2.02                     | 0.58              |
| 1:B:62:THR:HB    | 1:B:65:LYS:HB2   | 1.84                     | 0.58              |
| 1:C:124:HIS:HE1  | 1:C:128:GLN:HB2  | 1.68                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:301:GLY:O    | 1:C:305:GLN:HG3  | 2.03                     | 0.58              |
| 1:A:9:PRO:HB2    | 1:A:41:ARG:CZ    | 2.34                     | 0.58              |
| 1:B:148:ASP:HB3  | 1:B:151:LEU:HD22 | 1.85                     | 0.58              |
| 1:B:418:ARG:HG2  | 1:B:432:ASP:OD2  | 2.03                     | 0.57              |
| 1:D:10:VAL:HG12  | 1:D:11:PRO:N     | 2.19                     | 0.57              |
| 1:A:222:HIS:HB3  | 7:A:840:HOH:O    | 2.04                     | 0.57              |
| 1:A:421:LEU:HG   | 1:A:422:PHE:N    | 2.18                     | 0.57              |
| 1:D:10:VAL:CG1   | 1:D:11:PRO:CD    | 2.82                     | 0.57              |
| 1:D:342:VAL:HB   | 1:D:446:MET:CE   | 2.33                     | 0.57              |
| 1:C:196:GLU:HB3  | 7:C:707:HOH:O    | 2.03                     | 0.57              |
| 1:C:2:TRP:N      | 1:C:2:TRP:CE3    | 2.73                     | 0.57              |
| 1:D:361:LEU:HD13 | 1:D:365:TYR:O    | 2.05                     | 0.57              |
| 1:A:233:LYS:NZ   | 1:B:322:GLN:HB2  | 2.20                     | 0.57              |
| 1:C:197:PRO:HD2  | 7:C:707:HOH:O    | 2.03                     | 0.57              |
| 1:D:234:PRO:HB2  | 7:D:821:HOH:O    | 2.04                     | 0.57              |
| 1:B:66:THR:HB    | 1:B:70:PHE:O     | 2.05                     | 0.57              |
| 1:C:258:GLU:O    | 1:C:380:PHE:HA   | 2.04                     | 0.57              |
| 1:C:440:ARG:NH2  | 6:C:610:HEM:O1A  | 2.38                     | 0.57              |
| 1:D:421:LEU:HD22 | 1:D:433:LEU:HB2  | 1.86                     | 0.57              |
| 1:D:231:ASN:O    | 1:D:233:LYS:HE2  | 2.04                     | 0.57              |
| 1:B:168:PRO:CG   | 1:B:172:TYR:HB3  | 2.35                     | 0.57              |
| 1:B:392:ILE:O    | 1:B:396:VAL:HG23 | 2.05                     | 0.57              |
| 1:B:425:THR:O    | 1:B:425:THR:HG22 | 2.05                     | 0.57              |
| 1:C:167:CYS:HB2  | 1:C:168:PRO:HD2  | 1.85                     | 0.57              |
| 1:C:299:ILE:HD11 | 1:C:590:TRP:NE1  | 2.20                     | 0.57              |
| 1:A:71:ARG:HB3   | 1:A:71:ARG:NH1   | 2.20                     | 0.57              |
| 1:D:119:LEU:HD22 | 1:D:169:THR:HG21 | 1.86                     | 0.57              |
| 1:B:406:LEU:HG   | 1:B:407:MET:N    | 2.19                     | 0.56              |
| 1:A:117:THR:O    | 1:A:161:PHE:HB3  | 2.05                     | 0.56              |
| 5:A:609:3CJ:C5   | 6:A:610:HEM:HBD2 | 2.35                     | 0.56              |
| 1:C:475:VAL:HG12 | 1:C:479:LYS:HE2  | 1.88                     | 0.56              |
| 1:D:572:TYR:CD1  | 1:D:573:PRO:HB3  | 2.38                     | 0.56              |
| 1:C:168:PRO:HB2  | 1:C:170:PRO:HD2  | 1.87                     | 0.56              |
| 1:B:10:VAL:CG2   | 1:B:41:ARG:HH12  | 2.16                     | 0.56              |
| 1:C:81:LYS:HB3   | 7:C:821:HOH:O    | 2.03                     | 0.56              |
| 1:D:492:ILE:HG23 | 1:D:493:TRP:H    | 1.68                     | 0.56              |
| 1:C:173:GLN:O    | 1:C:174:SER:HB2  | 2.04                     | 0.56              |
| 1:D:109:HIS:HA   | 1:D:255:ARG:NH2  | 2.20                     | 0.56              |
| 1:A:275:ARG:HD2  | 1:A:555:ASP:HB3  | 1.88                     | 0.56              |
| 1:A:281:LYS:HD2  | 1:A:285:PRO:HA   | 1.87                     | 0.56              |
| 1:A:62:THR:CG2   | 1:A:65:LYS:N     | 2.69                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:189:ALA:HB2  | 1:A:304:ILE:HD12 | 1.87                     | 0.56              |
| 1:C:204:ARG:CZ   | 1:C:206:LEU:CD2  | 2.84                     | 0.56              |
| 1:C:517:ARG:HB3  | 1:C:517:ARG:HH21 | 1.70                     | 0.56              |
| 1:A:144:PHE:CE2  | 1:A:157:CYS:N    | 2.74                     | 0.56              |
| 1:A:367:PRO:HB2  | 1:D:64:ARG:CZ    | 2.35                     | 0.56              |
| 1:A:465:LYS:HA   | 1:A:468:GLN:HE21 | 1.71                     | 0.56              |
| 1:C:133:CYS:HB2  | 7:C:748:HOH:O    | 2.06                     | 0.56              |
| 1:B:193:TYR:CE2  | 1:B:297:ARG:HG3  | 2.41                     | 0.55              |
| 1:C:1:SER:C      | 1:C:2:TRP:CE3    | 2.80                     | 0.55              |
| 1:D:29:ASN:HD21  | 1:D:527:ARG:H    | 1.53                     | 0.55              |
| 1:D:96:ARG:HD2   | 1:D:100:PHE:CD2  | 2.40                     | 0.55              |
| 1:A:393:ASP:OD2  | 1:A:558:HIS:HB2  | 2.06                     | 0.55              |
| 1:A:169:THR:OG1  | 1:A:170:PRO:HD3  | 2.07                     | 0.55              |
| 1:A:213:MET:CB   | 1:A:270:LEU:HD11 | 2.36                     | 0.55              |
| 1:B:167:CYS:SG   | 1:B:168:PRO:HD2  | 2.46                     | 0.55              |
| 1:B:193:TYR:CD2  | 1:B:297:ARG:HG3  | 2.41                     | 0.55              |
| 1:D:529:TRP:CD1  | 1:D:531:GLU:HB2  | 2.40                     | 0.55              |
| 1:A:109:HIS:NE2  | 5:A:609:3CJ:C1   | 2.70                     | 0.55              |
| 1:A:13:VAL:HG12  | 1:A:14:THR:N     | 2.22                     | 0.55              |
| 1:A:20:PRO:O     | 1:A:21:TYR:CD1   | 2.60                     | 0.55              |
| 1:D:113:PHE:CD1  | 5:D:609:3CJ:H6   | 2.41                     | 0.55              |
| 1:D:199:LEU:O    | 1:D:203:LEU:HG   | 2.06                     | 0.55              |
| 1:D:146:LYS:O    | 1:D:147:ASN:HB2  | 2.06                     | 0.55              |
| 1:B:113:PHE:HE1  | 5:B:609:3CJ:H5   | 1.71                     | 0.55              |
| 1:C:125:SER:CA   | 1:C:128:GLN:HB3  | 2.36                     | 0.55              |
| 1:A:87:ASP:OD1   | 1:A:89:GLU:HB2   | 2.07                     | 0.55              |
| 1:B:118:GLU:HG3  | 7:B:716:HOH:O    | 2.07                     | 0.55              |
| 1:C:134:VAL:HA   | 7:C:716:HOH:O    | 2.07                     | 0.55              |
| 5:D:609:3CJ:H7   | 6:D:610:HEM:HBD2 | 1.89                     | 0.55              |
| 1:A:43:LEU:HD13  | 1:A:341:ASN:HA   | 1.88                     | 0.55              |
| 1:A:499:GLU:OE1  | 1:A:509:PRO:HG2  | 2.07                     | 0.55              |
| 1:B:123:GLU:CB   | 1:B:126:LYS:HG3  | 2.34                     | 0.55              |
| 1:C:381:PHE:CZ   | 1:C:424:PRO:HG3  | 2.43                     | 0.54              |
| 6:C:610:HEM:HMB1 | 6:C:610:HEM:HBB2 | 1.88                     | 0.54              |
| 1:D:167:CYS:CB   | 1:D:168:PRO:HD2  | 2.37                     | 0.54              |
| 1:A:367:PRO:HB2  | 1:D:64:ARG:HH21  | 1.70                     | 0.54              |
| 1:B:377:HIS:ND1  | 1:B:416:GLU:OE1  | 2.40                     | 0.54              |
| 1:C:97:SER:O     | 1:C:98:LEU:C     | 2.46                     | 0.54              |
| 1:D:333:ASN:HD22 | 1:D:333:ASN:N    | 2.03                     | 0.54              |
| 1:A:284:ASN:OD1  | 1:A:592:SER:N    | 2.39                     | 0.54              |
| 1:C:107:VAL:O    | 1:C:111:LEU:HG   | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:272:GLU:O    | 1:D:276:LEU:HG   | 2.07                     | 0.54              |
| 1:B:409:GLN:HE21 | 1:B:473:ASN:HD22 | 1.55                     | 0.54              |
| 1:C:342:VAL:HG21 | 1:C:452:TRP:CE2  | 2.42                     | 0.54              |
| 1:C:96:ARG:CZ    | 1:C:506:ARG:CD   | 2.85                     | 0.54              |
| 1:D:544:LEU:O    | 1:D:547:VAL:HG22 | 2.07                     | 0.54              |
| 1:D:97:SER:O     | 1:D:404:SER:OG   | 2.26                     | 0.54              |
| 1:B:138:GLU:OE1  | 1:B:162:ARG:HB2  | 2.06                     | 0.54              |
| 1:C:348:ARG:NH1  | 1:C:437:ASN:ND2  | 2.54                     | 0.54              |
| 1:A:203:LEU:HD13 | 1:A:213:MET:HE1  | 1.89                     | 0.54              |
| 1:B:593:ARG:HG3  | 1:B:595:ASN:H    | 1.72                     | 0.54              |
| 1:B:341:ASN:HB3  | 1:B:446:MET:HE1  | 1.89                     | 0.54              |
| 6:B:608:HEM:HMC2 | 6:B:608:HEM:HBC2 | 1.89                     | 0.54              |
| 1:C:7:GLY:O      | 1:C:8:ALA:HB3    | 2.07                     | 0.54              |
| 1:A:62:THR:O     | 1:A:63:GLN:HB3   | 2.07                     | 0.54              |
| 1:C:280:LEU:O    | 1:C:284:ASN:ND2  | 2.41                     | 0.54              |
| 1:D:96:ARG:NH2   | 1:D:315:ILE:HB   | 2.23                     | 0.54              |
| 1:C:1:SER:C      | 1:C:2:TRP:HE3    | 2.10                     | 0.54              |
| 1:D:9:PRO:CG     | 1:D:41:ARG:NH2   | 2.71                     | 0.54              |
| 1:A:408:ASN:C    | 1:A:408:ASN:OD1  | 2.46                     | 0.53              |
| 1:C:213:MET:HG2  | 1:C:273:HIS:NE2  | 2.24                     | 0.53              |
| 1:C:259:GLN:OE1  | 1:C:261:LEU:HB2  | 2.08                     | 0.53              |
| 1:D:193:TYR:OH   | 1:D:297:ARG:HA   | 2.07                     | 0.53              |
| 1:D:96:ARG:CZ    | 1:D:315:ILE:HB   | 2.38                     | 0.53              |
| 1:C:82:ILE:HD12  | 1:C:480:LEU:HD23 | 1.91                     | 0.53              |
| 1:D:103:TRP:O    | 1:D:106:ILE:N    | 2.36                     | 0.53              |
| 1:D:9:PRO:HG3    | 1:D:41:ARG:CZ    | 2.39                     | 0.53              |
| 1:A:367:PRO:HB2  | 1:D:64:ARG:NE    | 2.24                     | 0.53              |
| 1:B:117:THR:HG22 | 1:B:161:PHE:HB3  | 1.89                     | 0.53              |
| 1:B:30:ASN:O     | 1:B:34:PRO:HA    | 2.07                     | 0.53              |
| 1:C:551:ARG:O    | 1:C:552:LEU:C    | 2.45                     | 0.53              |
| 1:D:589:PRO:HB2  | 1:D:590:TRP:CE3  | 2.43                     | 0.53              |
| 1:D:214:ALA:HA   | 2:D:602:NAG:O7   | 2.08                     | 0.53              |
| 1:D:446:MET:CE   | 4:D:606:NO3:O1   | 2.56                     | 0.53              |
| 1:A:15:CYS:HB3   | 7:A:747:HOH:O    | 2.09                     | 0.53              |
| 1:A:99:LEU:CD2   | 1:A:566:ALA:HB1  | 2.39                     | 0.53              |
| 1:A:62:THR:HG21  | 1:A:65:LYS:CA    | 2.37                     | 0.53              |
| 1:B:117:THR:CG2  | 1:B:161:PHE:HB3  | 2.39                     | 0.53              |
| 6:B:608:HEM:CHA  | 5:B:609:3CJ:N1   | 2.71                     | 0.53              |
| 1:C:452:TRP:CD1  | 1:C:492:ILE:HG12 | 2.43                     | 0.53              |
| 1:D:563:PRO:HD3  | 1:D:576:PHE:CE2  | 2.44                     | 0.53              |
| 1:A:142:ILE:CD1  | 1:A:160:PHE:HB2  | 2.38                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:128:GLN:HG3  | 1:B:134:VAL:HG21 | 1.91                     | 0.53              |
| 1:B:165:PHE:CZ   | 1:B:169:THR:O    | 2.62                     | 0.53              |
| 1:B:522:ILE:HG13 | 1:B:523:ARG:N    | 2.22                     | 0.53              |
| 1:C:205:ASN:HB2  | 1:C:214:ALA:HA   | 1.90                     | 0.53              |
| 1:A:16:ASP:O     | 1:A:18:GLN:N     | 2.37                     | 0.53              |
| 1:A:233:LYS:HZ2  | 1:B:322:GLN:HB2  | 1.73                     | 0.53              |
| 1:C:237:CYS:HA   | 1:C:381:PHE:O    | 2.09                     | 0.53              |
| 1:C:385:ARG:NH1  | 1:C:389:ASP:OD2  | 2.42                     | 0.53              |
| 1:D:376:LEU:HD21 | 1:D:380:PHE:HE1  | 1.74                     | 0.53              |
| 1:C:523:ARG:HG3  | 1:C:529:TRP:CE2  | 2.43                     | 0.52              |
| 1:D:119:LEU:CD2  | 1:D:169:THR:HG21 | 2.39                     | 0.52              |
| 1:C:11:PRO:O     | 1:C:12:LEU:CB    | 2.51                     | 0.52              |
| 1:C:204:ARG:HB2  | 1:C:206:LEU:HG   | 1.91                     | 0.52              |
| 1:D:6:CYS:O      | 1:D:167:CYS:SG   | 2.67                     | 0.52              |
| 1:A:241:ASN:ND2  | 1:A:244:ALA:HB2  | 2.24                     | 0.52              |
| 1:B:167:CYS:SG   | 1:B:168:PRO:HD3  | 2.49                     | 0.52              |
| 1:C:144:PHE:HE1  | 1:C:158:MET:HG3  | 1.74                     | 0.52              |
| 1:C:437:ASN:O    | 1:C:440:ARG:N    | 2.40                     | 0.52              |
| 1:B:2:TRP:CH2    | 1:C:86:LEU:HD13  | 2.31                     | 0.52              |
| 1:C:97:SER:O     | 1:C:99:LEU:N     | 2.42                     | 0.52              |
| 1:A:13:VAL:HG12  | 1:A:14:THR:H     | 1.74                     | 0.52              |
| 1:A:492:ILE:HD11 | 1:A:510:LEU:HD21 | 1.90                     | 0.52              |
| 1:B:93:ASP:OD2   | 1:B:406:LEU:HD12 | 2.09                     | 0.52              |
| 1:C:125:SER:O    | 1:C:128:GLN:HB3  | 2.08                     | 0.52              |
| 1:D:397:ARG:HG3  | 1:D:559:ILE:HD12 | 1.91                     | 0.52              |
| 1:D:424:PRO:O    | 1:D:425:THR:CB   | 2.58                     | 0.52              |
| 1:D:513:CYS:O    | 1:D:517:ARG:HG2  | 2.09                     | 0.52              |
| 1:C:96:ARG:CZ    | 1:C:100:PHE:CE2  | 2.92                     | 0.52              |
| 1:C:400:LEU:HD13 | 1:C:563:PRO:HD2  | 1.91                     | 0.52              |
| 1:D:348:ARG:HH22 | 1:D:440:ARG:HG2  | 1.73                     | 0.52              |
| 1:A:168:PRO:HB2  | 1:A:170:PRO:O    | 2.10                     | 0.52              |
| 1:C:117:THR:HG22 | 1:C:162:ARG:O    | 2.09                     | 0.52              |
| 1:C:29:ASN:HD21  | 1:C:527:ARG:H    | 1.57                     | 0.52              |
| 1:C:552:LEU:HD12 | 1:C:556:ASN:HD22 | 1.74                     | 0.52              |
| 1:A:52:GLU:OE2   | 1:A:62:THR:HG22  | 2.09                     | 0.52              |
| 1:B:352:MET:O    | 1:B:405:LYS:HD3  | 2.10                     | 0.52              |
| 1:C:64:ARG:HA    | 1:C:71:ARG:NH2   | 2.25                     | 0.52              |
| 1:A:128:GLN:HA   | 1:A:132:TYR:HD1  | 1.75                     | 0.52              |
| 1:C:221:ASP:HB2  | 1:C:226:TYR:CZ   | 2.44                     | 0.52              |
| 1:D:143:MET:HG2  | 7:D:725:HOH:O    | 2.09                     | 0.52              |
| 1:B:418:ARG:HH11 | 1:B:418:ARG:HG2  | 1.75                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:244:ALA:O    | 1:D:245:HIS:HB2  | 2.10                     | 0.52              |
| 1:A:113:PHE:HE1  | 5:A:609:3CJ:H5   | 1.75                     | 0.52              |
| 1:B:42:ALA:CB    | 1:B:166:VAL:HG11 | 2.30                     | 0.52              |
| 1:B:551:ARG:CD   | 1:B:583:ASP:O    | 2.57                     | 0.52              |
| 6:B:608:HEM:HAA1 | 5:B:609:3CJ:H4   | 1.92                     | 0.52              |
| 1:C:29:ASN:HD21  | 1:C:527:ARG:N    | 2.08                     | 0.52              |
| 1:D:16:ASP:O     | 1:D:17:GLU:HB3   | 2.10                     | 0.52              |
| 1:C:288:ASP:OD1  | 1:C:291:MET:HB3  | 2.10                     | 0.51              |
| 1:D:102:GLN:OE1  | 1:D:259:GLN:NE2  | 2.35                     | 0.51              |
| 1:A:258:GLU:O    | 1:A:380:PHE:HA   | 2.09                     | 0.51              |
| 1:A:343:PHE:CD1  | 1:A:518:GLN:HG2  | 2.46                     | 0.51              |
| 1:B:10:VAL:CB    | 1:B:41:ARG:HH12  | 2.23                     | 0.51              |
| 1:B:169:THR:N    | 1:B:170:PRO:HD2  | 2.26                     | 0.51              |
| 1:D:257:SER:O    | 1:D:381:PHE:HA   | 2.11                     | 0.51              |
| 1:A:340:SER:HG   | 1:A:343:PHE:HB2  | 1.75                     | 0.51              |
| 1:A:551:ARG:HD2  | 1:A:584:LYS:HA   | 1.91                     | 0.51              |
| 1:B:397:ARG:NH2  | 1:B:559:ILE:HD13 | 2.25                     | 0.51              |
| 1:C:561:LYS:HD3  | 1:C:576:PHE:HB3  | 1.92                     | 0.51              |
| 1:D:379:LEU:HA   | 1:D:382:ASN:HB2  | 1.91                     | 0.51              |
| 1:A:8:ALA:N      | 1:A:9:PRO:HD2    | 2.26                     | 0.51              |
| 1:C:146:LYS:HE3  | 1:C:147:ASN:CG   | 2.30                     | 0.51              |
| 1:C:287:TRP:CZ3  | 1:C:295:GLU:HG3  | 2.45                     | 0.51              |
| 1:C:75:ALA:HB1   | 1:C:438:LEU:HB2  | 1.92                     | 0.51              |
| 1:B:25:THR:O     | 1:B:184:THR:HG22 | 2.10                     | 0.51              |
| 1:B:37:GLY:H     | 1:B:338:ARG:HG2  | 1.76                     | 0.51              |
| 1:C:348:ARG:CB   | 1:C:493:TRP:NE1  | 2.68                     | 0.51              |
| 1:A:593:ARG:HD2  | 1:A:595:ASN:H    | 1.75                     | 0.51              |
| 1:A:7:GLY:O      | 1:A:8:ALA:HB3    | 2.10                     | 0.51              |
| 1:B:180:ILE:HG22 | 1:B:181:ASN:N    | 2.25                     | 0.51              |
| 1:C:76:ARG:NH1   | 1:C:418:ARG:NH1  | 2.59                     | 0.51              |
| 1:A:315:ILE:O    | 1:A:505:GLY:HA2  | 2.11                     | 0.51              |
| 1:C:441:CYS:O    | 1:C:446:MET:HB2  | 2.10                     | 0.51              |
| 1:D:349:PHE:CD1  | 1:D:349:PHE:C    | 2.84                     | 0.51              |
| 1:D:499:GLU:OE1  | 1:D:509:PRO:HG2  | 2.11                     | 0.51              |
| 1:C:116:GLU:O    | 1:C:117:THR:HB   | 2.10                     | 0.51              |
| 1:D:349:PHE:CD1  | 1:D:350:GLY:N    | 2.78                     | 0.51              |
| 1:B:447:PRO:HG2  | 1:B:452:TRP:NE1  | 2.25                     | 0.51              |
| 1:B:503:GLU:O    | 1:B:504:ARG:HB2  | 2.10                     | 0.51              |
| 1:B:530:TRP:CG   | 1:B:531:GLU:N    | 2.79                     | 0.51              |
| 1:B:556:ASN:O    | 1:B:557:THR:HG23 | 2.10                     | 0.51              |
| 1:B:56:ALA:O     | 1:B:162:ARG:NH1  | 2.40                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:321:MET:C    | 1:B:323:LYS:H    | 2.13                     | 0.50              |
| 1:D:169:THR:HB   | 1:D:170:PRO:CD   | 2.22                     | 0.50              |
| 1:D:474:LYS:HB3  | 1:D:474:LYS:NZ   | 2.26                     | 0.50              |
| 1:A:245:HIS:CG   | 1:A:245:HIS:O    | 2.65                     | 0.50              |
| 1:A:63:GLN:O     | 1:A:63:GLN:HG3   | 2.11                     | 0.50              |
| 1:B:409:GLN:NE2  | 1:B:473:ASN:ND2  | 2.59                     | 0.50              |
| 1:B:78:VAL:HA    | 1:B:483:LEU:HD13 | 1.93                     | 0.50              |
| 1:C:358:VAL:HB   | 1:C:379:LEU:CD1  | 2.41                     | 0.50              |
| 1:C:415:SER:HB2  | 7:C:800:HOH:O    | 2.11                     | 0.50              |
| 1:D:167:CYS:HB2  | 1:D:168:PRO:HD2  | 1.91                     | 0.50              |
| 1:A:312:TYR:O    | 1:A:315:ILE:HG12 | 2.12                     | 0.50              |
| 1:D:221:ASP:OD1  | 1:D:221:ASP:C    | 2.50                     | 0.50              |
| 1:D:312:TYR:N    | 1:D:567:PHE:HE2  | 2.09                     | 0.50              |
| 1:C:125:SER:HA   | 1:C:128:GLN:CB   | 2.40                     | 0.50              |
| 1:D:255:ARG:HH11 | 5:D:609:3CJ:H7   | 1.77                     | 0.50              |
| 1:B:166:VAL:HG22 | 1:B:178:ASP:O    | 2.11                     | 0.50              |
| 1:C:124:HIS:HD1  | 1:C:125:SER:N    | 2.09                     | 0.50              |
| 1:C:259:GLN:HG3  | 1:C:262:LEU:HB3  | 1.94                     | 0.50              |
| 1:D:204:ARG:HH22 | 1:D:290:GLU:HA   | 1.77                     | 0.50              |
| 1:D:298:LYS:HG2  | 1:D:536:PHE:CZ   | 2.47                     | 0.50              |
| 1:D:376:LEU:O    | 1:D:379:LEU:N    | 2.39                     | 0.50              |
| 1:C:342:VAL:HB   | 1:C:452:TRP:HZ2  | 1.75                     | 0.50              |
| 1:D:248:CYS:HA   | 1:D:383:THR:HG21 | 1.94                     | 0.50              |
| 1:A:234:PRO:HB2  | 7:A:776:HOH:O    | 2.12                     | 0.49              |
| 1:B:294:GLN:OE1  | 1:B:294:GLN:HA   | 2.12                     | 0.49              |
| 1:B:341:ASN:HB3  | 4:B:605:NO3:O1   | 2.12                     | 0.49              |
| 1:C:227:PRO:HG3  | 1:C:270:LEU:HD22 | 1.93                     | 0.49              |
| 1:C:481:LEU:O    | 1:C:485:LYS:N    | 2.36                     | 0.49              |
| 5:C:609:3CJ:S1   | 6:C:610:HEM:ND   | 2.85                     | 0.49              |
| 1:C:98:LEU:CD1   | 1:C:101:MET:HE2  | 2.42                     | 0.49              |
| 1:D:84:GLY:HA2   | 7:D:775:HOH:O    | 2.11                     | 0.49              |
| 1:A:139:CYS:SG   | 1:A:141:PRO:HD3  | 2.52                     | 0.49              |
| 1:B:205:ASN:OD1  | 1:B:207:SER:OG   | 2.30                     | 0.49              |
| 1:B:274:ASN:O    | 1:B:278:ARG:HG3  | 2.12                     | 0.49              |
| 1:C:527:ARG:HH11 | 1:C:527:ARG:HG2  | 1.77                     | 0.49              |
| 1:A:313:LEU:HD11 | 1:A:519:PHE:CD2  | 2.48                     | 0.49              |
| 1:A:442:ARG:O    | 1:A:445:GLY:N    | 2.45                     | 0.49              |
| 1:C:331:TYR:CE2  | 1:C:333:ASN:HB3  | 2.47                     | 0.49              |
| 1:D:346:ALA:O    | 1:D:348:ARG:N    | 2.44                     | 0.49              |
| 1:D:502:VAL:O    | 1:D:502:VAL:HG23 | 2.13                     | 0.49              |
| 1:A:31:ARG:NH2   | 1:A:527:ARG:NH1  | 2.61                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:74:LEU:O     | 1:C:78:VAL:CG1   | 2.60                     | 0.49              |
| 1:D:240:ILE:CD1  | 1:D:382:ASN:HA   | 2.42                     | 0.49              |
| 1:D:346:ALA:C    | 1:D:348:ARG:H    | 2.16                     | 0.49              |
| 1:D:449:TYR:OH   | 1:D:470:VAL:HG11 | 2.12                     | 0.49              |
| 1:A:229:PHE:CG   | 1:A:247:PRO:HG2  | 2.47                     | 0.49              |
| 1:C:342:VAL:CB   | 1:C:452:TRP:CZ2  | 2.94                     | 0.49              |
| 1:D:502:VAL:O    | 1:D:503:GLU:C    | 2.50                     | 0.49              |
| 1:A:347:PHE:CE1  | 6:A:610:HEM:HBC1 | 2.48                     | 0.49              |
| 1:D:343:PHE:CD1  | 1:D:518:GLN:HG2  | 2.47                     | 0.49              |
| 1:D:450:ASN:HD21 | 1:D:487:PRO:HB2  | 1.78                     | 0.49              |
| 1:A:168:PRO:HB3  | 1:A:170:PRO:HG2  | 1.95                     | 0.49              |
| 1:A:284:ASN:HD21 | 1:A:591:ALA:HA   | 1.77                     | 0.49              |
| 1:C:363:GLU:CD   | 1:C:363:GLU:H    | 2.15                     | 0.49              |
| 1:D:246:VAL:HG11 | 1:D:387:ILE:HD12 | 1.95                     | 0.49              |
| 1:D:317:LEU:HD12 | 1:D:321:MET:HA   | 1.95                     | 0.49              |
| 1:D:62:THR:HB    | 1:D:65:LYS:HB2   | 1.95                     | 0.49              |
| 1:A:551:ARG:CZ   | 1:A:584:LYS:HG2  | 2.41                     | 0.49              |
| 1:C:1:SER:H2     | 1:C:2:TRP:HZ3    | 1.49                     | 0.49              |
| 1:D:314:PRO:HD3  | 1:D:321:MET:HE1  | 1.94                     | 0.49              |
| 1:D:110:ASP:OD2  | 1:D:189:ALA:N    | 2.45                     | 0.49              |
| 1:A:42:ALA:HB2   | 1:A:166:VAL:CG1  | 2.37                     | 0.48              |
| 1:A:347:PHE:O    | 1:A:347:PHE:HD1  | 1.95                     | 0.48              |
| 1:A:62:THR:O     | 1:A:63:GLN:CB    | 2.61                     | 0.48              |
| 1:B:554:CYS:SG   | 1:B:562:VAL:HG21 | 2.52                     | 0.48              |
| 1:C:30:ASN:HD21  | 1:C:333:ASN:HB2  | 1.78                     | 0.48              |
| 1:A:144:PHE:HD2  | 1:A:156:LYS:C    | 2.17                     | 0.48              |
| 1:A:503:GLU:O    | 1:A:504:ARG:HB2  | 2.13                     | 0.48              |
| 1:A:76:ARG:NH1   | 1:A:432:ASP:OD2  | 2.46                     | 0.48              |
| 1:B:113:PHE:CD1  | 5:B:609:3CJ:H5   | 2.48                     | 0.48              |
| 1:B:312:TYR:CE2  | 1:B:316:VAL:HG21 | 2.48                     | 0.48              |
| 1:C:125:SER:O    | 1:C:126:LYS:C    | 2.51                     | 0.48              |
| 1:C:151:LEU:HA   | 1:C:155:GLY:O    | 2.13                     | 0.48              |
| 1:C:347:PHE:HB3  | 6:C:610:HEM:HMD3 | 1.95                     | 0.48              |
| 1:C:43:LEU:HD12  | 1:C:179:GLN:HB2  | 1.95                     | 0.48              |
| 1:D:119:LEU:CD2  | 1:D:169:THR:CG2  | 2.91                     | 0.48              |
| 1:A:464:LEU:O    | 1:A:468:GLN:HG3  | 2.12                     | 0.48              |
| 1:A:51:TYR:HB3   | 1:A:57:VAL:O     | 2.13                     | 0.48              |
| 1:B:10:VAL:HG11  | 1:B:41:ARG:NH2   | 2.28                     | 0.48              |
| 1:B:8:ALA:HB1    | 1:B:9:PRO:HD2    | 1.96                     | 0.48              |
| 1:C:180:ILE:HG22 | 1:C:181:ASN:N    | 2.29                     | 0.48              |
| 1:C:22:ARG:CZ    | 1:C:528:PHE:HB2  | 2.43                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:593:ARG:HB3  | 1:C:593:ARG:CZ   | 2.43                     | 0.48              |
| 1:D:144:PHE:HE1  | 1:D:158:MET:HG3  | 1.75                     | 0.48              |
| 1:D:380:PHE:HE2  | 1:D:420:LYS:O    | 1.96                     | 0.48              |
| 1:A:244:ALA:O    | 1:A:245:HIS:HB3  | 2.14                     | 0.48              |
| 1:A:275:ARG:CD   | 1:A:555:ASP:HB3  | 2.43                     | 0.48              |
| 1:C:377:HIS:ND1  | 1:C:416:GLU:OE1  | 2.43                     | 0.48              |
| 1:A:58:PRO:HG3   | 1:A:162:ARG:CZ   | 2.43                     | 0.48              |
| 1:B:213:MET:HB3  | 1:B:270:LEU:HD11 | 1.94                     | 0.48              |
| 1:B:140:PHE:CE2  | 1:B:439:GLN:HG3  | 2.48                     | 0.48              |
| 1:C:102:GLN:HB2  | 1:C:399:LEU:HD21 | 1.96                     | 0.48              |
| 1:D:150:LYS:HE2  | 1:D:419:ASN:HD22 | 1.78                     | 0.48              |
| 1:A:317:LEU:HD12 | 1:A:321:MET:SD   | 2.53                     | 0.48              |
| 1:A:481:LEU:HA   | 1:A:484:TYR:O    | 2.14                     | 0.48              |
| 6:A:610:HEM:CMC  | 6:A:610:HEM:HBC2 | 2.43                     | 0.48              |
| 1:B:137:ASP:CG   | 1:B:138:GLU:H    | 2.17                     | 0.48              |
| 1:D:187:LEU:HD21 | 1:D:304:ILE:HG22 | 1.95                     | 0.48              |
| 1:A:91:VAL:HA    | 7:A:777:HOH:O    | 2.12                     | 0.48              |
| 5:C:609:3CJ:S1   | 6:C:610:HEM:C1D  | 3.07                     | 0.48              |
| 1:D:193:TYR:CZ   | 1:D:297:ARG:HA   | 2.49                     | 0.48              |
| 1:D:93:ASP:OD2   | 1:D:96:ARG:HG3   | 2.13                     | 0.48              |
| 1:A:146:LYS:HB3  | 7:A:823:HOH:O    | 2.12                     | 0.48              |
| 1:C:17:GLU:HB3   | 1:C:18:GLN:OE1   | 2.14                     | 0.48              |
| 1:C:204:ARG:NE   | 1:C:206:LEU:HD21 | 2.29                     | 0.48              |
| 1:D:275:ARG:O    | 1:D:279:GLU:HG2  | 2.14                     | 0.48              |
| 1:D:408:ASN:HB3  | 1:D:411:LYS:HB2  | 1.95                     | 0.48              |
| 1:A:165:PHE:CZ   | 1:A:169:THR:C    | 2.87                     | 0.47              |
| 1:B:113:PHE:HB2  | 1:B:255:ARG:NH2  | 2.29                     | 0.47              |
| 1:B:91:VAL:CG1   | 1:B:411:LYS:HD3  | 2.44                     | 0.47              |
| 1:B:418:ARG:O    | 1:B:432:ASP:CB   | 2.62                     | 0.47              |
| 1:D:357:THR:HB   | 1:D:374:LEU:O    | 2.14                     | 0.47              |
| 1:A:130:GLU:HG3  | 1:A:159:PRO:HD3  | 1.95                     | 0.47              |
| 1:A:109:HIS:NE2  | 5:A:609:3CJ:S1   | 2.87                     | 0.47              |
| 1:B:124:HIS:O    | 1:B:127:VAL:HB   | 2.14                     | 0.47              |
| 1:A:367:PRO:CB   | 1:D:64:ARG:NE    | 2.77                     | 0.47              |
| 1:C:17:GLU:O     | 1:C:18:GLN:NE2   | 2.46                     | 0.47              |
| 1:C:36:LEU:HD23  | 1:C:338:ARG:HD3  | 1.96                     | 0.47              |
| 1:A:67:ARG:N     | 1:A:70:PHE:O     | 2.45                     | 0.47              |
| 1:A:84:GLY:CA    | 1:A:418:ARG:NE   | 2.78                     | 0.47              |
| 1:D:213:MET:HG2  | 1:D:273:HIS:CD2  | 2.49                     | 0.47              |
| 1:D:212:LEU:HD21 | 1:D:278:ARG:HG3  | 1.95                     | 0.47              |
| 1:A:571:ASN:O    | 1:A:575:ASP:HB2  | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:52:GLU:HG3   | 1:A:59:PHE:CD1   | 2.49                     | 0.47              |
| 1:D:259:GLN:O    | 1:D:262:LEU:HB3  | 2.14                     | 0.47              |
| 1:D:370:PRO:HG2  | 1:D:371:GLU:H    | 1.79                     | 0.47              |
| 1:B:168:PRO:HG2  | 1:B:172:TYR:HB3  | 1.97                     | 0.47              |
| 1:B:96:ARG:NH2   | 1:B:315:ILE:O    | 2.46                     | 0.47              |
| 1:C:169:THR:HG22 | 7:C:736:HOH:O    | 2.13                     | 0.47              |
| 1:C:322:GLN:HG3  | 7:C:810:HOH:O    | 2.13                     | 0.47              |
| 1:C:22:ARG:NH1   | 1:C:528:PHE:HB2  | 2.29                     | 0.47              |
| 1:D:264:THR:HG23 | 1:D:392:ILE:HG23 | 1.96                     | 0.47              |
| 1:A:351:HIS:NE2  | 1:A:433:LEU:HD21 | 2.30                     | 0.47              |
| 1:B:12:LEU:HD12  | 1:B:12:LEU:HA    | 1.79                     | 0.47              |
| 1:C:230:ASN:ND2  | 1:C:232:VAL:HG22 | 2.22                     | 0.47              |
| 1:C:423:GLN:CB   | 1:C:426:HIS:CD2  | 2.97                     | 0.47              |
| 1:A:414:THR:HG22 | 7:A:721:HOH:O    | 2.15                     | 0.47              |
| 1:A:76:ARG:HH22  | 1:A:419:ASN:ND2  | 2.13                     | 0.47              |
| 1:B:30:ASN:ND2   | 1:B:36:LEU:HD12  | 2.29                     | 0.47              |
| 1:B:544:LEU:O    | 1:B:547:VAL:HG22 | 2.14                     | 0.47              |
| 1:C:221:ASP:O    | 1:C:222:HIS:C    | 2.53                     | 0.47              |
| 1:C:511:LEU:O    | 1:C:515:LEU:HG   | 2.14                     | 0.47              |
| 1:D:468:GLN:HG2  | 1:D:474:LYS:HA   | 1.96                     | 0.47              |
| 1:A:224:LEU:HB2  | 1:A:271:ARG:NH2  | 2.30                     | 0.47              |
| 1:A:363:GLU:HG2  | 7:A:816:HOH:O    | 2.15                     | 0.47              |
| 1:B:466:GLY:HA3  | 7:B:749:HOH:O    | 2.14                     | 0.47              |
| 1:C:96:ARG:CD    | 1:C:100:PHE:CD2  | 2.68                     | 0.47              |
| 1:A:302:ALA:O    | 1:A:306:ILE:HG13 | 2.14                     | 0.47              |
| 1:B:433:LEU:HD12 | 1:B:433:LEU:O    | 2.15                     | 0.47              |
| 1:C:453:ARG:HD2  | 1:C:510:LEU:HD13 | 1.96                     | 0.47              |
| 1:D:530:TRP:CE2  | 1:D:531:GLU:HG3  | 2.49                     | 0.47              |
| 1:B:138:GLU:O    | 1:B:162:ARG:HG3  | 2.14                     | 0.47              |
| 1:B:361:LEU:HB3  | 1:B:365:TYR:HA   | 1.96                     | 0.47              |
| 1:B:376:LEU:HA   | 1:B:379:LEU:HD12 | 1.97                     | 0.47              |
| 1:C:146:LYS:NZ   | 1:C:147:ASN:ND2  | 2.60                     | 0.47              |
| 1:A:343:PHE:CG   | 1:A:518:GLN:HG2  | 2.49                     | 0.46              |
| 1:A:284:ASN:ND2  | 1:A:591:ALA:HA   | 2.30                     | 0.46              |
| 5:A:609:3CJ:H7   | 6:A:610:HEM:CBD  | 2.41                     | 0.46              |
| 1:B:273:HIS:CD2  | 1:B:274:ASN:OD1  | 2.61                     | 0.46              |
| 1:A:233:LYS:HA   | 1:A:234:PRO:C    | 2.34                     | 0.46              |
| 1:A:265:VAL:O    | 1:A:269:LEU:HG   | 2.15                     | 0.46              |
| 1:A:400:LEU:HD21 | 1:A:553:ILE:CD1  | 2.46                     | 0.46              |
| 1:A:436:ILE:O    | 1:A:440:ARG:HB2  | 2.15                     | 0.46              |
| 1:B:335:VAL:HG12 | 1:B:336:ASP:N    | 2.30                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:561:LYS:O    | 1:B:562:VAL:HG13 | 2.16                     | 0.46              |
| 1:C:563:PRO:HD3  | 1:C:576:PHE:CE2  | 2.51                     | 0.46              |
| 1:D:346:ALA:C    | 1:D:348:ARG:N    | 2.68                     | 0.46              |
| 1:D:343:PHE:CG   | 1:D:518:GLN:HG2  | 2.50                     | 0.46              |
| 5:D:609:3CJ:C1   | 6:D:610:HEM:NA   | 2.78                     | 0.46              |
| 1:B:185:SER:HB3  | 1:B:339:ILE:HG12 | 1.97                     | 0.46              |
| 1:B:363:GLU:N    | 1:B:363:GLU:CD   | 2.67                     | 0.46              |
| 6:B:608:HEM:HBB2 | 6:B:608:HEM:CMB  | 2.44                     | 0.46              |
| 1:B:66:THR:HB    | 1:B:70:PHE:C     | 2.36                     | 0.46              |
| 1:C:144:PHE:CE1  | 1:C:158:MET:HG3  | 2.50                     | 0.46              |
| 1:C:30:ASN:ND2   | 1:C:333:ASN:HB2  | 2.30                     | 0.46              |
| 1:C:572:TYR:HA   | 1:C:573:PRO:HA   | 1.62                     | 0.46              |
| 1:D:113:PHE:CD1  | 1:D:255:ARG:HD3  | 2.50                     | 0.46              |
| 1:D:313:LEU:HB2  | 1:D:314:PRO:HD3  | 1.97                     | 0.46              |
| 1:A:113:PHE:CD1  | 5:A:609:3CJ:H5   | 2.50                     | 0.46              |
| 1:A:62:THR:HG21  | 1:A:65:LYS:CG    | 2.43                     | 0.46              |
| 1:B:303:PHE:HD2  | 1:B:304:ILE:HD12 | 1.80                     | 0.46              |
| 1:B:557:THR:OG1  | 1:B:559:ILE:HG12 | 2.15                     | 0.46              |
| 1:B:347:PHE:CE1  | 6:B:608:HEM:HBC1 | 2.51                     | 0.46              |
| 1:C:236:PRO:CB   | 1:C:424:PRO:HB3  | 2.45                     | 0.46              |
| 1:D:255:ARG:HD2  | 5:D:609:3CJ:C2   | 2.45                     | 0.46              |
| 1:A:348:ARG:HH11 | 1:A:437:ASN:ND2  | 2.14                     | 0.46              |
| 1:A:71:ARG:CB    | 1:A:71:ARG:NH1   | 2.79                     | 0.46              |
| 1:C:171:PRO:HD3  | 7:C:822:HOH:O    | 2.15                     | 0.46              |
| 1:D:54:GLY:HA2   | 7:D:853:HOH:O    | 2.15                     | 0.46              |
| 1:D:99:LEU:HD21  | 1:D:549:PHE:CD2  | 2.50                     | 0.46              |
| 1:A:112:ASP:HA   | 1:A:183:VAL:CG2  | 2.46                     | 0.46              |
| 1:A:522:ILE:O    | 1:A:526:ASP:HB2  | 2.16                     | 0.46              |
| 1:D:213:MET:HG2  | 1:D:273:HIS:NE2  | 2.31                     | 0.46              |
| 1:A:113:PHE:HB2  | 1:A:255:ARG:CZ   | 2.46                     | 0.46              |
| 1:A:9:PRO:O      | 1:A:10:VAL:C     | 2.52                     | 0.46              |
| 1:D:148:ASP:O    | 1:D:151:LEU:CB   | 2.64                     | 0.46              |
| 1:D:313:LEU:O    | 1:D:314:PRO:C    | 2.54                     | 0.46              |
| 1:C:129:CYS:O    | 1:C:133:CYS:HA   | 2.15                     | 0.46              |
| 1:C:213:MET:HG2  | 1:C:273:HIS:CD2  | 2.51                     | 0.46              |
| 1:C:344:THR:HB   | 6:C:610:HEM:O2D  | 2.15                     | 0.46              |
| 1:D:336:ASP:OD2  | 1:D:338:ARG:NH2  | 2.48                     | 0.46              |
| 1:A:166:VAL:C    | 1:A:167:CYS:SG   | 2.94                     | 0.46              |
| 1:A:213:MET:HB2  | 1:A:270:LEU:HD11 | 1.98                     | 0.46              |
| 1:B:17:GLU:OE2   | 1:B:31:ARG:HG2   | 2.15                     | 0.46              |
| 1:B:421:LEU:HD22 | 1:B:433:LEU:HB2  | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:93:ASP:CG    | 1:B:96:ARG:HB2   | 2.36                     | 0.46              |
| 1:C:108:ASP:HB2  | 1:C:347:PHE:CE2  | 2.50                     | 0.46              |
| 1:C:294:GLN:OE1  | 1:C:294:GLN:HA   | 2.15                     | 0.46              |
| 1:D:351:HIS:HD2  | 6:D:610:HEM:C1C  | 2.34                     | 0.46              |
| 1:D:570:ASN:HB3  | 1:D:575:ASP:HB3  | 1.98                     | 0.46              |
| 1:A:213:MET:HG2  | 1:A:273:HIS:CD2  | 2.51                     | 0.46              |
| 1:C:423:GLN:HG3  | 1:C:431:PHE:CD2  | 2.51                     | 0.46              |
| 1:C:449:TYR:OH   | 1:C:470:VAL:HG11 | 2.16                     | 0.46              |
| 5:C:609:3CJ:H5   | 6:C:610:HEM:CAA  | 2.42                     | 0.46              |
| 1:D:418:ARG:HG2  | 1:D:432:ASP:OD2  | 2.15                     | 0.46              |
| 1:D:545:GLN:OE1  | 1:D:545:GLN:HA   | 2.16                     | 0.46              |
| 1:A:260:ILE:HG23 | 1:A:261:LEU:N    | 2.31                     | 0.45              |
| 1:B:324:TRP:CZ2  | 1:B:513:CYS:HB2  | 2.51                     | 0.45              |
| 1:B:433:LEU:HA   | 1:B:436:ILE:HD12 | 1.97                     | 0.45              |
| 2:C:603:NAG:H82  | 7:C:807:HOH:O    | 2.16                     | 0.45              |
| 1:D:561:LYS:HE3  | 1:D:578:ASP:HA   | 1.98                     | 0.45              |
| 1:A:144:PHE:HE2  | 1:A:157:CYS:N    | 2.14                     | 0.45              |
| 1:A:377:HIS:CB   | 1:A:416:GLU:OE1  | 2.57                     | 0.45              |
| 1:A:419:ASN:O    | 1:A:430:GLY:HA2  | 2.17                     | 0.45              |
| 1:A:47:LEU:HD21  | 1:A:455:PHE:HD2  | 1.81                     | 0.45              |
| 1:A:82:ILE:HD13  | 1:A:480:LEU:HD23 | 1.98                     | 0.45              |
| 1:A:86:LEU:HD23  | 1:D:55:LEU:HD23  | 1.98                     | 0.45              |
| 1:B:257:SER:O    | 1:B:381:PHE:HA   | 2.16                     | 0.45              |
| 1:B:418:ARG:NH1  | 1:B:418:ARG:HG2  | 2.31                     | 0.45              |
| 1:C:244:ALA:HB1  | 1:C:246:VAL:HG23 | 1.97                     | 0.45              |
| 1:C:31:ARG:H     | 1:C:31:ARG:HG2   | 1.59                     | 0.45              |
| 1:C:350:GLY:HA3  | 6:C:610:HEM:CBC  | 2.47                     | 0.45              |
| 1:D:239:PHE:CZ   | 1:D:427:LYS:CG   | 2.99                     | 0.45              |
| 1:B:360:ARG:O    | 1:B:368:TRP:HB3  | 2.17                     | 0.45              |
| 1:D:519:PHE:HA   | 1:D:522:ILE:HG12 | 1.97                     | 0.45              |
| 1:A:418:ARG:HG2  | 1:A:418:ARG:HH11 | 1.81                     | 0.45              |
| 1:C:15:CYS:HB3   | 1:C:17:GLU:OE2   | 2.15                     | 0.45              |
| 1:C:523:ARG:HG3  | 1:C:529:TRP:CD2  | 2.51                     | 0.45              |
| 1:C:100:PHE:HA   | 1:C:567:PHE:CD1  | 2.52                     | 0.45              |
| 1:C:99:LEU:HA    | 1:C:399:LEU:CD2  | 2.45                     | 0.45              |
| 1:D:421:LEU:O    | 1:D:431:PHE:HB2  | 2.16                     | 0.45              |
| 1:D:97:SER:O     | 1:D:100:PHE:HB3  | 2.15                     | 0.45              |
| 1:D:474:LYS:O    | 1:D:477:ALA:HB3  | 2.16                     | 0.45              |
| 1:A:353:GLU:HA   | 1:A:405:LYS:O    | 2.17                     | 0.45              |
| 1:A:95:ASN:HA    | 1:A:569:ALA:HB3  | 1.97                     | 0.45              |
| 1:B:348:ARG:NH1  | 1:B:437:ASN:ND2  | 2.64                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:454:GLY:O    | 1:B:455:PHE:C    | 2.55                     | 0.45              |
| 1:B:528:PHE:HZ   | 7:B:748:HOH:O    | 1.99                     | 0.45              |
| 1:C:344:THR:O    | 6:C:610:HEM:HAD2 | 2.16                     | 0.45              |
| 1:D:246:VAL:CG1  | 1:D:387:ILE:HD12 | 2.46                     | 0.45              |
| 1:D:484:TYR:O    | 1:D:485:LYS:HB2  | 2.17                     | 0.45              |
| 1:D:561:LYS:CE   | 1:D:578:ASP:HA   | 2.47                     | 0.45              |
| 1:A:392:ILE:HG22 | 1:A:396:VAL:CG2  | 2.47                     | 0.45              |
| 1:B:35:ALA:HB1   | 1:B:41:ARG:HE    | 1.80                     | 0.45              |
| 1:B:551:ARG:HD3  | 1:B:584:LYS:CA   | 2.37                     | 0.45              |
| 1:C:130:GLU:HB2  | 1:C:159:PRO:HB3  | 1.99                     | 0.45              |
| 1:C:552:LEU:O    | 1:C:556:ASN:ND2  | 2.46                     | 0.45              |
| 1:D:590:TRP:HE3  | 1:D:590:TRP:H    | 1.65                     | 0.45              |
| 1:A:135:GLN:HB3  | 1:A:135:GLN:HE21 | 1.49                     | 0.45              |
| 1:A:173:GLN:O    | 1:A:174:SER:HB3  | 2.17                     | 0.45              |
| 1:A:418:ARG:HG2  | 1:A:418:ARG:NH1  | 2.32                     | 0.45              |
| 1:A:442:ARG:O    | 1:A:443:ASP:C    | 2.53                     | 0.45              |
| 1:B:180:ILE:CG2  | 1:B:181:ASN:N    | 2.79                     | 0.45              |
| 1:B:221:ASP:HB2  | 1:B:226:TYR:CZ   | 2.52                     | 0.45              |
| 7:A:772:HOH:O    | 1:D:173:GLN:HB2  | 2.17                     | 0.45              |
| 1:D:229:PHE:CZ   | 1:D:387:ILE:HD13 | 2.52                     | 0.45              |
| 1:D:345:PHE:CE1  | 1:D:441:CYS:HA   | 2.52                     | 0.45              |
| 1:D:546:LYS:NZ   | 1:D:546:LYS:HB2  | 2.31                     | 0.45              |
| 1:A:59:PHE:CG    | 1:A:67:ARG:HD2   | 2.52                     | 0.45              |
| 1:A:82:ILE:HD13  | 1:A:480:LEU:CD2  | 2.46                     | 0.45              |
| 1:B:117:THR:HG21 | 1:B:138:GLU:OE1  | 2.17                     | 0.45              |
| 1:C:527:ARG:NH1  | 1:C:527:ARG:HG2  | 2.31                     | 0.45              |
| 1:D:12:LEU:C     | 1:D:13:VAL:HG23  | 2.37                     | 0.45              |
| 1:D:144:PHE:HB2  | 1:D:151:LEU:HD13 | 1.98                     | 0.45              |
| 1:D:175:LEU:HD23 | 1:D:176:ALA:H    | 1.82                     | 0.45              |
| 1:A:400:LEU:HD21 | 1:A:553:ILE:HD13 | 1.99                     | 0.45              |
| 1:C:168:PRO:HG3  | 1:C:172:TYR:CD2  | 2.49                     | 0.45              |
| 1:C:29:ASN:ND2   | 1:C:527:ARG:H    | 2.14                     | 0.45              |
| 1:D:10:VAL:HG13  | 1:D:11:PRO:HD2   | 1.98                     | 0.45              |
| 1:A:449:TYR:HB3  | 1:A:487:PRO:O    | 2.18                     | 0.44              |
| 1:B:563:PRO:HD3  | 1:B:576:PHE:CE2  | 2.51                     | 0.44              |
| 1:C:551:ARG:HD3  | 1:C:584:LYS:HA   | 1.99                     | 0.44              |
| 1:D:9:PRO:HG3    | 1:D:41:ARG:NH1   | 2.32                     | 0.44              |
| 1:A:165:PHE:CE2  | 1:A:170:PRO:O    | 2.70                     | 0.44              |
| 1:A:424:PRO:O    | 1:A:425:THR:HB   | 2.17                     | 0.44              |
| 1:A:553:ILE:O    | 1:A:557:THR:HG23 | 2.17                     | 0.44              |
| 1:B:188:ASP:N    | 1:B:188:ASP:OD1  | 2.48                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:260:ILE:HG13 | 1:B:382:ASN:O    | 2.17                     | 0.44              |
| 1:C:517:ARG:CB   | 1:C:517:ARG:HH21 | 2.30                     | 0.44              |
| 1:D:315:ILE:HD11 | 1:D:567:PHE:CD2  | 2.52                     | 0.44              |
| 1:A:213:MET:HB3  | 1:A:270:LEU:HD11 | 1.98                     | 0.44              |
| 1:B:393:ASP:OD1  | 1:B:557:THR:HB   | 2.18                     | 0.44              |
| 1:B:76:ARG:NH2   | 7:B:702:HOH:O    | 2.50                     | 0.44              |
| 1:C:124:HIS:O    | 1:C:125:SER:C    | 2.54                     | 0.44              |
| 1:C:188:ASP:OD1  | 1:C:190:SER:CB   | 2.64                     | 0.44              |
| 1:D:260:ILE:HD13 | 1:D:395:LEU:HD21 | 2.00                     | 0.44              |
| 1:D:9:PRO:HG2    | 1:D:10:VAL:H     | 1.81                     | 0.44              |
| 1:B:408:ASN:HB3  | 1:B:411:LYS:O    | 2.17                     | 0.44              |
| 1:B:588:SER:HB2  | 1:B:589:PRO:HD3  | 2.00                     | 0.44              |
| 1:B:91:VAL:HG11  | 1:B:411:LYS:HD3  | 1.99                     | 0.44              |
| 1:C:188:ASP:CG   | 1:C:190:SER:HB3  | 2.37                     | 0.44              |
| 1:C:2:TRP:CD2    | 1:C:2:TRP:N      | 2.84                     | 0.44              |
| 1:C:468:GLN:CG   | 1:C:474:LYS:HA   | 2.40                     | 0.44              |
| 1:C:29:ASN:O     | 1:C:527:ARG:HD3  | 2.18                     | 0.44              |
| 1:C:88:GLU:O     | 1:C:91:VAL:HG22  | 2.17                     | 0.44              |
| 1:A:123:GLU:HB3  | 1:A:126:LYS:HG3  | 1.99                     | 0.44              |
| 1:A:145:PRO:O    | 1:A:148:ASP:HB2  | 2.17                     | 0.44              |
| 1:A:313:LEU:HD11 | 1:A:519:PHE:CD1  | 2.53                     | 0.44              |
| 1:A:559:ILE:HD13 | 1:A:559:ILE:N    | 2.33                     | 0.44              |
| 1:C:421:LEU:HD22 | 1:C:433:LEU:HB2  | 1.98                     | 0.44              |
| 1:A:328:TYR:CD2  | 1:A:531:GLU:HB3  | 2.52                     | 0.44              |
| 1:A:462:LYS:HA   | 1:A:462:LYS:HE2  | 1.98                     | 0.44              |
| 1:C:168:PRO:HD2  | 1:C:172:TYR:HE2  | 1.83                     | 0.44              |
| 1:C:242:THR:O    | 1:C:245:HIS:CE1  | 2.71                     | 0.44              |
| 1:C:279:GLU:O    | 1:C:283:LEU:HG   | 2.17                     | 0.44              |
| 1:D:196:GLU:HG3  | 7:D:785:HOH:O    | 2.18                     | 0.44              |
| 1:A:144:PHE:CD2  | 1:A:156:LYS:C    | 2.91                     | 0.44              |
| 1:C:124:HIS:C    | 1:C:124:HIS:ND1  | 2.70                     | 0.44              |
| 1:C:265:VAL:O    | 1:C:269:LEU:HG   | 2.18                     | 0.44              |
| 1:C:402:LYS:HD3  | 4:C:607:NO3:O1   | 2.17                     | 0.44              |
| 1:D:549:PHE:O    | 1:D:552:LEU:HB3  | 2.17                     | 0.44              |
| 1:D:88:GLU:O     | 1:D:91:VAL:HG22  | 2.17                     | 0.44              |
| 1:A:117:THR:O    | 1:A:117:THR:HG23 | 2.16                     | 0.44              |
| 1:A:172:TYR:CE2  | 1:A:175:LEU:HB2  | 2.48                     | 0.44              |
| 1:A:568:GLN:HG2  | 1:A:568:GLN:O    | 2.17                     | 0.44              |
| 1:B:421:LEU:HD12 | 1:B:422:PHE:N    | 2.30                     | 0.44              |
| 1:C:231:ASN:HB2  | 7:C:775:HOH:O    | 2.17                     | 0.44              |
| 1:D:260:ILE:HG13 | 1:D:386:ILE:HD11 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:187:LEU:HD23 | 1:D:305:GLN:HA   | 2.00                     | 0.44              |
| 1:D:60:GLY:CA    | 1:D:72:VAL:HG21  | 2.48                     | 0.44              |
| 1:D:76:ARG:NH1   | 1:D:432:ASP:OD2  | 2.51                     | 0.44              |
| 1:A:203:LEU:HD22 | 7:A:775:HOH:O    | 2.17                     | 0.44              |
| 1:A:363:GLU:CG   | 7:A:816:HOH:O    | 2.65                     | 0.44              |
| 5:C:609:3CJ:C3   | 6:C:610:HEM:C2A  | 3.01                     | 0.44              |
| 1:B:10:VAL:HG21  | 1:B:41:ARG:NH1   | 2.32                     | 0.43              |
| 1:C:299:ILE:HD11 | 1:C:590:TRP:CD1  | 2.52                     | 0.43              |
| 1:B:109:HIS:NE2  | 5:B:609:3CJ:S1   | 2.91                     | 0.43              |
| 1:C:45:ARG:CZ    | 1:C:49:ALA:HB2   | 2.48                     | 0.43              |
| 1:D:85:TYR:CE2   | 1:D:91:VAL:HG11  | 2.53                     | 0.43              |
| 1:A:113:PHE:HB2  | 1:A:255:ARG:NH2  | 2.33                     | 0.43              |
| 1:A:305:GLN:NE2  | 1:A:529:TRP:CE3  | 2.86                     | 0.43              |
| 1:B:221:ASP:O    | 1:B:224:LEU:HB2  | 2.17                     | 0.43              |
| 1:B:94:GLN:O     | 1:B:569:ALA:CB   | 2.66                     | 0.43              |
| 1:C:342:VAL:HG13 | 1:C:343:PHE:N    | 2.33                     | 0.43              |
| 1:C:74:LEU:O     | 1:C:78:VAL:HG13  | 2.18                     | 0.43              |
| 1:C:91:VAL:HG23  | 1:C:92:LEU:HD23  | 2.01                     | 0.43              |
| 1:D:28:CYS:O     | 1:D:29:ASN:C     | 2.57                     | 0.43              |
| 1:A:55:LEU:HD13  | 1:A:173:GLN:HA   | 2.00                     | 0.43              |
| 1:A:382:ASN:ND2  | 1:A:385:ARG:HG3  | 2.34                     | 0.43              |
| 6:A:610:HEM:HBB2 | 6:A:610:HEM:HMB2 | 2.00                     | 0.43              |
| 1:C:385:ARG:HA   | 1:C:385:ARG:HD3  | 1.86                     | 0.43              |
| 1:C:520:GLN:O    | 1:C:524:ASP:HB2  | 2.19                     | 0.43              |
| 1:D:497:ASN:OD1  | 1:D:511:LEU:HD11 | 2.18                     | 0.43              |
| 1:D:82:ILE:HD13  | 1:D:480:LEU:CD2  | 2.49                     | 0.43              |
| 1:B:518:GLN:O    | 1:B:522:ILE:HG23 | 2.19                     | 0.43              |
| 1:C:328:TYR:CZ   | 1:C:529:TRP:CD1  | 3.07                     | 0.43              |
| 1:D:187:LEU:HG   | 1:D:187:LEU:O    | 2.17                     | 0.43              |
| 1:D:441:CYS:SG   | 1:D:492:ILE:CG2  | 3.07                     | 0.43              |
| 1:D:320:GLU:HG3  | 1:D:512:ALA:HB1  | 2.00                     | 0.43              |
| 1:B:222:HIS:HA   | 7:B:794:HOH:O    | 2.19                     | 0.43              |
| 1:B:447:PRO:HG2  | 1:B:452:TRP:CE2  | 2.54                     | 0.43              |
| 1:B:68:ASN:ND2   | 1:B:489:ASN:OD1  | 2.44                     | 0.43              |
| 1:C:353:GLU:HA   | 1:C:405:LYS:O    | 2.18                     | 0.43              |
| 1:C:366:GLN:HA   | 1:C:366:GLN:OE1  | 2.18                     | 0.43              |
| 1:C:528:PHE:O    | 1:C:529:TRP:C    | 2.57                     | 0.43              |
| 1:D:204:ARG:HG2  | 1:D:293:TYR:CE1  | 2.53                     | 0.43              |
| 1:D:312:TYR:O    | 1:D:315:ILE:HG12 | 2.17                     | 0.43              |
| 1:A:398:GLY:O    | 1:A:402:LYS:HB2  | 2.19                     | 0.43              |
| 1:D:408:ASN:O    | 1:D:410:ASN:N    | 2.51                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:585:LEU:O    | 1:D:587:LEU:N    | 2.52                     | 0.43              |
| 1:A:255:ARG:HH11 | 5:A:609:3CJ:H6   | 1.83                     | 0.43              |
| 1:A:279:GLU:HA   | 1:A:279:GLU:OE2  | 2.19                     | 0.43              |
| 1:A:519:PHE:HA   | 1:A:522:ILE:HG12 | 2.00                     | 0.43              |
| 1:B:172:TYR:OH   | 1:B:177:ARG:HA   | 2.17                     | 0.43              |
| 1:C:441:CYS:HB3  | 7:C:713:HOH:O    | 2.18                     | 0.43              |
| 1:C:81:LYS:HE2   | 7:C:821:HOH:O    | 2.19                     | 0.43              |
| 1:A:343:PHE:CE1  | 1:A:515:LEU:HD23 | 2.53                     | 0.43              |
| 1:C:37:GLY:H     | 1:C:338:ARG:CG   | 2.20                     | 0.43              |
| 1:D:119:LEU:HB3  | 7:D:773:HOH:O    | 2.19                     | 0.43              |
| 1:D:312:TYR:O    | 1:D:315:ILE:CG1  | 2.67                     | 0.43              |
| 1:D:391:GLY:O    | 1:D:394:PRO:HD2  | 2.19                     | 0.43              |
| 1:A:239:PHE:CZ   | 1:A:427:LYS:CB   | 3.02                     | 0.43              |
| 1:A:519:PHE:O    | 1:A:522:ILE:HG12 | 2.18                     | 0.43              |
| 1:B:565:HIS:HB2  | 1:B:568:GLN:HG2  | 2.00                     | 0.43              |
| 1:C:3:GLU:O      | 1:C:5:GLY:N      | 2.52                     | 0.43              |
| 1:D:167:CYS:HB3  | 1:D:168:PRO:HD2  | 2.00                     | 0.43              |
| 1:D:18:GLN:NE2   | 1:D:18:GLN:HA    | 2.33                     | 0.43              |
| 1:A:112:ASP:HA   | 1:A:183:VAL:HG22 | 2.01                     | 0.42              |
| 1:A:93:ASP:CG    | 1:A:96:ARG:HB2   | 2.39                     | 0.42              |
| 1:C:110:ASP:OD2  | 1:C:189:ALA:N    | 2.49                     | 0.42              |
| 1:C:227:PRO:HG3  | 1:C:270:LEU:CD2  | 2.48                     | 0.42              |
| 1:C:467:LEU:HA   | 1:C:467:LEU:HD12 | 1.89                     | 0.42              |
| 1:A:258:GLU:OE1  | 1:A:259:GLN:CG   | 2.66                     | 0.42              |
| 1:A:84:GLY:HA2   | 1:A:418:ARG:NE   | 2.34                     | 0.42              |
| 1:C:109:HIS:HA   | 1:C:255:ARG:HH22 | 1.81                     | 0.42              |
| 1:C:16:ASP:O     | 1:C:18:GLN:HG2   | 2.19                     | 0.42              |
| 1:A:165:PHE:CE1  | 1:A:177:ARG:CZ   | 3.01                     | 0.42              |
| 1:A:543:SER:OG   | 1:A:589:PRO:HG2  | 2.19                     | 0.42              |
| 1:B:116:GLU:HB3  | 7:B:746:HOH:O    | 2.18                     | 0.42              |
| 1:B:191:LEU:H    | 1:B:191:LEU:HD23 | 1.85                     | 0.42              |
| 1:C:108:ASP:HB2  | 1:C:347:PHE:CD2  | 2.54                     | 0.42              |
| 1:C:283:LEU:HD13 | 1:C:591:ALA:HB2  | 2.00                     | 0.42              |
| 5:C:609:3CJ:C4   | 6:C:610:HEM:C3A  | 3.02                     | 0.42              |
| 1:D:146:LYS:O    | 1:D:147:ASN:CB   | 2.65                     | 0.42              |
| 1:D:148:ASP:O    | 1:D:151:LEU:HB2  | 2.19                     | 0.42              |
| 1:B:232:VAL:O    | 1:B:232:VAL:HG23 | 2.20                     | 0.42              |
| 1:B:260:ILE:CG2  | 1:B:261:LEU:N    | 2.83                     | 0.42              |
| 1:D:12:LEU:O     | 1:D:13:VAL:HB    | 2.20                     | 0.42              |
| 1:D:474:LYS:HZ1  | 1:D:474:LYS:HB3  | 1.84                     | 0.42              |
| 1:B:335:VAL:CG1  | 1:B:336:ASP:N    | 2.82                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:168:PRO:CG   | 1:C:172:TYR:CD2  | 3.03                     | 0.42              |
| 1:C:348:ARG:NH2  | 6:C:610:HEM:HAD1 | 2.34                     | 0.42              |
| 1:D:99:LEU:O     | 1:D:100:PHE:C    | 2.57                     | 0.42              |
| 1:D:53:ASP:CG    | 1:D:57:VAL:HG23  | 2.40                     | 0.42              |
| 1:A:281:LYS:HD3  | 1:A:292:LEU:HD11 | 2.02                     | 0.42              |
| 1:A:65:LYS:HE3   | 1:A:65:LYS:HB3   | 1.61                     | 0.42              |
| 1:A:77:GLU:O     | 1:A:81:LYS:HG3   | 2.19                     | 0.42              |
| 1:B:246:VAL:HA   | 1:B:247:PRO:HD3  | 1.80                     | 0.42              |
| 1:B:64:ARG:NH2   | 7:B:704:HOH:O    | 2.53                     | 0.42              |
| 1:C:321:MET:HB3  | 1:C:322:GLN:OE1  | 2.19                     | 0.42              |
| 1:D:376:LEU:HD21 | 1:D:380:PHE:CE1  | 2.53                     | 0.42              |
| 1:A:363:GLU:OE2  | 1:A:397:ARG:NH1  | 2.52                     | 0.42              |
| 1:A:572:TYR:CG   | 1:A:573:PRO:HA   | 2.55                     | 0.42              |
| 1:A:57:VAL:HA    | 1:A:58:PRO:HD3   | 1.92                     | 0.42              |
| 1:B:248:CYS:HB3  | 1:B:257:SER:OG   | 2.19                     | 0.42              |
| 1:B:293:TYR:OH   | 1:B:297:ARG:HD2  | 2.18                     | 0.42              |
| 1:B:313:LEU:N    | 1:B:314:PRO:CD   | 2.83                     | 0.42              |
| 1:C:322:GLN:CD   | 1:C:322:GLN:H    | 2.23                     | 0.42              |
| 1:C:36:LEU:CD2   | 1:C:338:ARG:HD3  | 2.50                     | 0.42              |
| 1:D:272:GLU:O    | 1:D:276:LEU:CG   | 2.68                     | 0.42              |
| 1:D:348:ARG:HH11 | 1:D:437:ASN:HD21 | 1.60                     | 0.42              |
| 1:D:460:GLN:HA   | 1:D:461:PRO:HD2  | 1.91                     | 0.42              |
| 1:A:124:HIS:O    | 1:A:127:VAL:HB   | 2.20                     | 0.42              |
| 1:B:233:LYS:HB3  | 1:B:234:PRO:HA   | 2.01                     | 0.42              |
| 1:C:180:ILE:CG2  | 1:C:181:ASN:N    | 2.83                     | 0.42              |
| 1:C:101:MET:SD   | 1:C:354:VAL:HG22 | 2.60                     | 0.42              |
| 1:C:529:TRP:O    | 1:C:530:TRP:C    | 2.58                     | 0.42              |
| 1:C:550:SER:OG   | 1:C:563:PRO:O    | 2.26                     | 0.42              |
| 1:D:446:MET:HA   | 1:D:447:PRO:HD3  | 1.93                     | 0.42              |
| 1:A:464:LEU:HD12 | 1:A:464:LEU:C    | 2.40                     | 0.42              |
| 6:B:608:HEM:O1D  | 5:B:609:3CJ:H6   | 2.19                     | 0.42              |
| 1:C:106:ILE:HG13 | 1:C:265:VAL:HG11 | 2.02                     | 0.42              |
| 1:C:348:ARG:HB3  | 1:C:493:TRP:HE1  | 1.80                     | 0.42              |
| 1:A:24:ILE:HD13  | 1:A:24:ILE:HA    | 1.93                     | 0.42              |
| 1:B:14:THR:HG22  | 1:B:15:CYS:N     | 2.35                     | 0.42              |
| 1:B:166:VAL:CG2  | 1:B:178:ASP:HB2  | 2.50                     | 0.42              |
| 1:B:215:VAL:O    | 1:B:217:GLN:NE2  | 2.53                     | 0.42              |
| 1:B:281:LYS:HD2  | 1:B:285:PRO:HA   | 2.01                     | 0.42              |
| 1:A:217:GLN:HA   | 1:A:217:GLN:OE1  | 2.20                     | 0.41              |
| 1:A:237:CYS:O    | 1:A:240:ILE:HG13 | 2.20                     | 0.41              |
| 1:B:113:PHE:O    | 1:B:181:ASN:HA   | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:45:ARG:NH1   | 1:B:49:ALA:HA    | 2.35                     | 0.41              |
| 1:C:240:ILE:O    | 1:C:241:ASN:HB2  | 2.20                     | 0.41              |
| 1:C:348:ARG:NH1  | 1:C:437:ASN:HD22 | 2.18                     | 0.41              |
| 1:A:354:VAL:HG21 | 6:A:610:HEM:CAB  | 2.50                     | 0.41              |
| 1:A:345:PHE:CE1  | 1:A:440:ARG:HG3  | 2.54                     | 0.41              |
| 1:C:1:SER:N      | 1:C:2:TRP:CE3    | 2.82                     | 0.41              |
| 1:D:103:TRP:O    | 1:D:104:GLY:C    | 2.58                     | 0.41              |
| 1:D:60:GLY:HA2   | 1:D:72:VAL:CG2   | 2.50                     | 0.41              |
| 1:B:31:ARG:O     | 1:B:32:ARG:C     | 2.59                     | 0.41              |
| 1:C:333:ASN:HD22 | 1:C:333:ASN:H    | 1.67                     | 0.41              |
| 1:C:494:ILE:HG23 | 1:C:495:GLY:N    | 2.36                     | 0.41              |
| 1:D:132:TYR:HB3  | 1:D:134:VAL:HG23 | 2.02                     | 0.41              |
| 1:D:532:ASN:HA   | 1:D:533:PRO:HD3  | 1.89                     | 0.41              |
| 1:A:146:LYS:HE3  | 1:A:147:ASN:OD1  | 2.20                     | 0.41              |
| 1:A:321:MET:C    | 1:A:323:LYS:H    | 2.22                     | 0.41              |
| 1:A:522:ILE:HG13 | 1:A:523:ARG:N    | 2.36                     | 0.41              |
| 1:B:117:THR:HG23 | 1:B:161:PHE:HD2  | 1.85                     | 0.41              |
| 1:B:23:THR:O     | 1:B:297:ARG:NH2  | 2.44                     | 0.41              |
| 1:B:203:LEU:HD11 | 1:B:251:ALA:O    | 2.20                     | 0.41              |
| 1:B:588:SER:N    | 1:B:589:PRO:CD   | 2.83                     | 0.41              |
| 1:C:101:MET:HB3  | 1:C:101:MET:HE2  | 1.52                     | 0.41              |
| 1:A:140:PHE:N    | 1:A:141:PRO:HD3  | 2.34                     | 0.41              |
| 1:A:335:VAL:O    | 1:A:337:PRO:HD3  | 2.20                     | 0.41              |
| 1:A:423:GLN:HA   | 1:A:424:PRO:HD3  | 1.92                     | 0.41              |
| 1:B:481:LEU:HD21 | 1:B:487:PRO:HG3  | 2.01                     | 0.41              |
| 1:C:146:LYS:CE   | 1:C:147:ASN:ND2  | 2.73                     | 0.41              |
| 1:C:17:GLU:O     | 1:C:31:ARG:NH2   | 2.54                     | 0.41              |
| 1:C:216:ASN:OD1  | 1:C:219:ALA:N    | 2.31                     | 0.41              |
| 1:D:336:ASP:OD1  | 1:D:338:ARG:HB2  | 2.21                     | 0.41              |
| 1:D:3:GLU:CG     | 1:D:4:VAL:H      | 2.31                     | 0.41              |
| 1:D:91:VAL:HG12  | 1:D:411:LYS:HD3  | 2.02                     | 0.41              |
| 1:A:471:LEU:O    | 1:A:472:LYS:HB2  | 2.21                     | 0.41              |
| 1:B:362:ASP:O    | 1:B:397:ARG:NE   | 2.53                     | 0.41              |
| 1:B:529:TRP:CD1  | 1:B:531:GLU:HB3  | 2.55                     | 0.41              |
| 1:C:82:ILE:HD12  | 1:C:480:LEU:CD2  | 2.51                     | 0.41              |
| 1:D:96:ARG:HD2   | 1:D:100:PHE:CG   | 2.55                     | 0.41              |
| 1:D:251:ALA:O    | 1:D:252:GLY:C    | 2.58                     | 0.41              |
| 1:D:347:PHE:HA   | 1:D:347:PHE:HD1  | 1.73                     | 0.41              |
| 1:D:47:LEU:HD12  | 1:D:452:TRP:CZ3  | 2.56                     | 0.41              |
| 1:D:91:VAL:HB    | 1:D:405:LYS:HG3  | 2.02                     | 0.41              |
| 1:D:9:PRO:O      | 1:D:10:VAL:CG2   | 2.69                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:572:TYR:HD2  | 1:A:576:PHE:CG   | 2.37                     | 0.41              |
| 1:B:537:THR:HG23 | 1:B:540:GLN:CD   | 2.39                     | 0.41              |
| 1:B:69:GLY:HA2   | 1:C:374:LEU:HD22 | 2.02                     | 0.41              |
| 1:D:213:MET:CG   | 1:D:273:HIS:CD2  | 3.04                     | 0.41              |
| 1:D:351:HIS:CD2  | 6:D:610:HEM:C1C  | 3.09                     | 0.41              |
| 1:D:589:PRO:HB2  | 1:D:590:TRP:CZ3  | 2.56                     | 0.41              |
| 1:A:165:PHE:HE2  | 1:A:170:PRO:O    | 2.03                     | 0.41              |
| 1:A:501:MET:SD   | 1:A:506:ARG:HA   | 2.61                     | 0.41              |
| 1:B:106:ILE:HD11 | 1:B:265:VAL:HB   | 2.03                     | 0.41              |
| 1:B:127:VAL:O    | 1:B:131:GLU:HB3  | 2.20                     | 0.41              |
| 1:B:213:MET:HG2  | 1:B:273:HIS:NE2  | 2.35                     | 0.41              |
| 1:B:493:TRP:O    | 1:B:497:ASN:ND2  | 2.53                     | 0.41              |
| 1:C:100:PHE:HA   | 1:C:567:PHE:HD1  | 1.85                     | 0.41              |
| 1:C:149:PRO:C    | 1:C:151:LEU:N    | 2.73                     | 0.41              |
| 1:C:46:TRP:CE2   | 1:C:340:SER:HB3  | 2.56                     | 0.41              |
| 1:C:3:GLU:C      | 1:C:5:GLY:H      | 2.24                     | 0.41              |
| 1:C:421:LEU:HD12 | 1:C:422:PHE:H    | 1.85                     | 0.41              |
| 1:C:481:LEU:CD2  | 1:C:487:PRO:HG3  | 2.39                     | 0.41              |
| 1:D:179:GLN:HG2  | 1:D:444:HIS:CD2  | 2.56                     | 0.41              |
| 1:A:35:ALA:HB1   | 1:A:41:ARG:CD    | 2.50                     | 0.41              |
| 1:A:424:PRO:O    | 1:A:425:THR:CB   | 2.69                     | 0.41              |
| 1:A:418:ARG:O    | 1:A:432:ASP:HA   | 2.21                     | 0.41              |
| 1:A:477:ALA:O    | 1:A:478:LYS:C    | 2.59                     | 0.41              |
| 1:B:347:PHE:HB3  | 6:B:608:HEM:CMD  | 2.51                     | 0.41              |
| 1:B:399:LEU:HA   | 1:B:399:LEU:HD23 | 1.92                     | 0.41              |
| 1:C:506:ARG:HA   | 1:C:506:ARG:HD3  | 1.89                     | 0.41              |
| 1:C:588:SER:N    | 1:C:589:PRO:CD   | 2.84                     | 0.41              |
| 1:D:272:GLU:OE2  | 1:D:276:LEU:HG   | 2.20                     | 0.41              |
| 1:D:28:CYS:HA    | 1:D:34:PRO:CB    | 2.51                     | 0.41              |
| 1:D:423:GLN:O    | 1:D:426:HIS:HB2  | 2.20                     | 0.41              |
| 1:D:51:TYR:HB3   | 1:D:57:VAL:O     | 2.20                     | 0.41              |
| 1:D:523:ARG:HG3  | 1:D:529:TRP:CE2  | 2.56                     | 0.41              |
| 1:A:121:SER:C    | 1:A:123:GLU:N    | 2.75                     | 0.41              |
| 1:A:288:ASP:OD2  | 1:A:290:GLU:HB3  | 2.20                     | 0.41              |
| 1:A:407:MET:SD   | 1:A:408:ASN:N    | 2.94                     | 0.41              |
| 6:B:608:HEM:CHA  | 5:B:609:3CJ:H9   | 2.34                     | 0.41              |
| 1:C:1:SER:N      | 1:C:2:TRP:CZ3    | 2.68                     | 0.41              |
| 1:C:419:ASN:HD22 | 1:C:419:ASN:HA   | 1.70                     | 0.41              |
| 6:C:610:HEM:HBC2 | 6:C:610:HEM:HMC2 | 2.02                     | 0.41              |
| 1:D:366:GLN:HB3  | 1:D:367:PRO:CD   | 2.51                     | 0.41              |
| 1:B:362:ASP:OD1  | 1:B:366:GLN:HB2  | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:124:HIS:HD1  | 1:C:125:SER:CA   | 2.34                     | 0.40              |
| 1:C:424:PRO:O    | 1:C:425:THR:CB   | 2.69                     | 0.40              |
| 1:C:460:GLN:HA   | 1:C:461:PRO:HD2  | 1.90                     | 0.40              |
| 1:C:85:TYR:CD2   | 1:C:411:LYS:HA   | 2.57                     | 0.40              |
| 1:D:165:PHE:CD1  | 1:D:165:PHE:N    | 2.89                     | 0.40              |
| 1:A:221:ASP:HB3  | 1:A:224:LEU:HB2  | 2.03                     | 0.40              |
| 1:A:517:ARG:NH2  | 1:A:521:GLN:OE1  | 2.54                     | 0.40              |
| 1:B:24:ILE:HD13  | 1:B:24:ILE:HA    | 1.93                     | 0.40              |
| 1:B:332:ASN:OD1  | 1:B:334:SER:N    | 2.45                     | 0.40              |
| 1:B:468:GLN:HG2  | 1:B:474:LYS:HA   | 2.03                     | 0.40              |
| 1:C:103:TRP:O    | 1:C:104:GLY:C    | 2.58                     | 0.40              |
| 1:C:274:ASN:O    | 1:C:278:ARG:HG3  | 2.21                     | 0.40              |
| 1:C:363:GLU:CD   | 1:C:363:GLU:N    | 2.75                     | 0.40              |
| 1:C:382:ASN:OD1  | 1:C:385:ARG:HB2  | 2.21                     | 0.40              |
| 1:C:497:ASN:HA   | 1:C:511:LEU:HD11 | 2.03                     | 0.40              |
| 1:D:70:PHE:CD1   | 1:D:70:PHE:N     | 2.89                     | 0.40              |
| 1:A:309:PHE:CZ   | 1:A:522:ILE:HD11 | 2.55                     | 0.40              |
| 1:A:549:PHE:O    | 1:A:552:LEU:HB3  | 2.21                     | 0.40              |
| 1:B:308:THR:HA   | 1:B:312:TYR:HB3  | 2.03                     | 0.40              |
| 6:B:608:HEM:HBA2 | 6:B:608:HEM:HHA  | 2.02                     | 0.40              |
| 1:C:471:LEU:HD23 | 1:C:499:GLU:HA   | 2.02                     | 0.40              |
| 1:D:61:TRP:CE2   | 1:D:135:GLN:NE2  | 2.89                     | 0.40              |
| 1:D:324:TRP:O    | 1:D:520:GLN:HB2  | 2.21                     | 0.40              |
| 1:D:537:THR:OG1  | 1:D:540:GLN:HG3  | 2.21                     | 0.40              |
| 1:D:572:TYR:HA   | 1:D:573:PRO:HA   | 1.75                     | 0.40              |
| 1:A:367:PRO:HB2  | 1:D:64:ARG:HE    | 1.86                     | 0.40              |
| 1:A:233:LYS:NZ   | 1:B:322:GLN:HE21 | 2.19                     | 0.40              |
| 1:A:260:ILE:CG2  | 1:A:261:LEU:N    | 2.84                     | 0.40              |
| 1:A:588:SER:N    | 1:A:589:PRO:CD   | 2.84                     | 0.40              |
| 1:B:45:ARG:NH2   | 1:B:177:ARG:O    | 2.53                     | 0.40              |
| 1:C:514:LEU:O    | 1:C:515:LEU:C    | 2.60                     | 0.40              |
| 1:C:93:ASP:HB2   | 1:C:406:LEU:HB2  | 2.03                     | 0.40              |
| 1:D:78:VAL:O     | 1:D:82:ILE:HB    | 2.21                     | 0.40              |
| 1:A:203:LEU:HD23 | 1:A:203:LEU:HA   | 1.86                     | 0.40              |
| 1:A:518:GLN:O    | 1:A:522:ILE:HG23 | 2.21                     | 0.40              |
| 1:A:568:GLN:O    | 1:A:570:ASN:ND2  | 2.54                     | 0.40              |
| 1:A:77:GLU:CG    | 1:A:81:LYS:HD2   | 2.51                     | 0.40              |
| 1:B:213:MET:CB   | 1:B:270:LEU:HD11 | 2.52                     | 0.40              |
| 1:B:320:GLU:O    | 1:B:323:LYS:HB3  | 2.21                     | 0.40              |
| 1:B:418:ARG:O    | 1:B:432:ASP:HB2  | 2.21                     | 0.40              |
| 1:C:124:HIS:O    | 1:C:126:LYS:N    | 2.54                     | 0.40              |

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| Atom-1         | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 1:D:2:TRP:CD1  | 1:D:175:LEU:CD2  | 3.04                     | 0.40              |
| 1:D:296:ALA:HA | 1:D:299:ILE:HD12 | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed         | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|------------------|------------|-----------|----------|-------------|----|
| 1   | A     | 593/595 (100%)   | 520 (88%)  | 68 (12%)  | 5 (1%)   | 22          | 39 |
| 1   | B     | 593/595 (100%)   | 524 (88%)  | 63 (11%)  | 6 (1%)   | 18          | 32 |
| 1   | C     | 593/595 (100%)   | 523 (88%)  | 61 (10%)  | 9 (2%)   | 12          | 21 |
| 1   | D     | 593/595 (100%)   | 515 (87%)  | 67 (11%)  | 11 (2%)  | 9           | 15 |
| All | All   | 2372/2380 (100%) | 2082 (88%) | 259 (11%) | 31 (1%)  | 14          | 25 |

All (31) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 8   | ALA  |
| 1   | A     | 167 | CYS  |
| 1   | B     | 167 | CYS  |
| 1   | C     | 8   | ALA  |
| 1   | C     | 12  | LEU  |
| 1   | C     | 167 | CYS  |
| 1   | C     | 174 | SER  |
| 1   | D     | 13  | VAL  |
| 1   | D     | 167 | CYS  |
| 1   | D     | 174 | SER  |
| 1   | D     | 3   | GLU  |
| 1   | A     | 327 | PRO  |
| 1   | B     | 27  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 128 | GLN  |
| 1   | C     | 352 | MET  |
| 1   | D     | 9   | PRO  |
| 1   | D     | 347 | PHE  |
| 1   | D     | 587 | LEU  |
| 1   | B     | 14  | THR  |
| 1   | B     | 370 | PRO  |
| 1   | C     | 13  | VAL  |
| 1   | D     | 367 | PRO  |
| 1   | D     | 589 | PRO  |
| 1   | C     | 4   | VAL  |
| 1   | C     | 492 | ILE  |
| 1   | A     | 9   | PRO  |
| 1   | A     | 285 | PRO  |
| 1   | B     | 492 | ILE  |
| 1   | D     | 170 | PRO  |
| 1   | D     | 516 | GLY  |
| 1   | B     | 573 | 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   | A     | 517/517 (100%)   | 471 (91%)  | 46 (9%)  | 11          | 22 |
| 1   | B     | 517/517 (100%)   | 472 (91%)  | 45 (9%)  | 12          | 23 |
| 1   | C     | 517/517 (100%)   | 475 (92%)  | 42 (8%)  | 14          | 26 |
| 1   | D     | 517/517 (100%)   | 463 (90%)  | 54 (10%) | 8           | 15 |
| All | All   | 2068/2068 (100%) | 1881 (91%) | 187 (9%) | 11          | 21 |

All (187) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | CYS  |
| 1   | A     | 9   | PRO  |
| 1   | A     | 12  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 23  | THR  |
| 1   | A     | 24  | ILE  |
| 1   | A     | 32  | ARG  |
| 1   | A     | 40  | ASN  |
| 1   | A     | 64  | ARG  |
| 1   | A     | 65  | LYS  |
| 1   | A     | 71  | ARG  |
| 1   | A     | 78  | VAL  |
| 1   | A     | 116 | GLU  |
| 1   | A     | 118 | GLU  |
| 1   | A     | 119 | LEU  |
| 1   | A     | 139 | CYS  |
| 1   | A     | 154 | GLN  |
| 1   | A     | 157 | CYS  |
| 1   | A     | 167 | CYS  |
| 1   | A     | 177 | ARG  |
| 1   | A     | 201 | SER  |
| 1   | A     | 202 | ARG  |
| 1   | A     | 218 | GLU  |
| 1   | A     | 232 | VAL  |
| 1   | A     | 240 | ILE  |
| 1   | A     | 257 | SER  |
| 1   | A     | 258 | GLU  |
| 1   | A     | 266 | HIS  |
| 1   | A     | 311 | ASP  |
| 1   | A     | 322 | GLN  |
| 1   | A     | 327 | PRO  |
| 1   | A     | 344 | THR  |
| 1   | A     | 347 | PHE  |
| 1   | A     | 348 | ARG  |
| 1   | A     | 364 | ASN  |
| 1   | A     | 366 | GLN  |
| 1   | A     | 408 | ASN  |
| 1   | A     | 464 | LEU  |
| 1   | A     | 481 | LEU  |
| 1   | A     | 517 | ARG  |
| 1   | A     | 538 | GLU  |
| 1   | A     | 542 | ASP  |
| 1   | A     | 551 | ARG  |
| 1   | A     | 564 | LEU  |
| 1   | A     | 568 | GLN  |
| 1   | A     | 580 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 593 | ARG  |
| 1   | B     | 3   | GLU  |
| 1   | B     | 6   | CYS  |
| 1   | B     | 22  | ARG  |
| 1   | B     | 53  | ASP  |
| 1   | B     | 63  | GLN  |
| 1   | B     | 66  | THR  |
| 1   | B     | 78  | VAL  |
| 1   | B     | 86  | LEU  |
| 1   | B     | 95  | ASN  |
| 1   | B     | 118 | GLU  |
| 1   | B     | 119 | LEU  |
| 1   | B     | 125 | SER  |
| 1   | B     | 128 | GLN  |
| 1   | B     | 151 | LEU  |
| 1   | B     | 156 | LYS  |
| 1   | B     | 167 | CYS  |
| 1   | B     | 175 | LEU  |
| 1   | B     | 196 | GLU  |
| 1   | B     | 198 | SER  |
| 1   | B     | 202 | ARG  |
| 1   | B     | 231 | ASN  |
| 1   | B     | 242 | THR  |
| 1   | B     | 266 | HIS  |
| 1   | B     | 321 | MET  |
| 1   | B     | 322 | GLN  |
| 1   | B     | 337 | PRO  |
| 1   | B     | 347 | PHE  |
| 1   | B     | 356 | SER  |
| 1   | B     | 359 | SER  |
| 1   | B     | 360 | ARG  |
| 1   | B     | 371 | GLU  |
| 1   | B     | 383 | THR  |
| 1   | B     | 423 | GLN  |
| 1   | B     | 439 | GLN  |
| 1   | B     | 472 | LYS  |
| 1   | B     | 481 | LEU  |
| 1   | B     | 486 | THR  |
| 1   | B     | 513 | CYS  |
| 1   | B     | 522 | ILE  |
| 1   | B     | 542 | ASP  |
| 1   | B     | 551 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 573 | PRO  |
| 1   | B     | 574 | HIS  |
| 1   | B     | 592 | SER  |
| 1   | B     | 593 | ARG  |
| 1   | C     | 2   | TRP  |
| 1   | C     | 3   | GLU  |
| 1   | C     | 4   | VAL  |
| 1   | C     | 6   | CYS  |
| 1   | C     | 19  | SER  |
| 1   | C     | 31  | ARG  |
| 1   | C     | 32  | ARG  |
| 1   | C     | 89  | GLU  |
| 1   | C     | 102 | GLN  |
| 1   | C     | 118 | GLU  |
| 1   | C     | 119 | LEU  |
| 1   | C     | 124 | HIS  |
| 1   | C     | 139 | CYS  |
| 1   | C     | 146 | LYS  |
| 1   | C     | 153 | THR  |
| 1   | C     | 156 | LYS  |
| 1   | C     | 157 | CYS  |
| 1   | C     | 173 | GLN  |
| 1   | C     | 177 | ARG  |
| 1   | C     | 207 | SER  |
| 1   | C     | 242 | THR  |
| 1   | C     | 254 | SER  |
| 1   | C     | 266 | HIS  |
| 1   | C     | 284 | ASN  |
| 1   | C     | 293 | TYR  |
| 1   | C     | 323 | LYS  |
| 1   | C     | 333 | ASN  |
| 1   | C     | 344 | THR  |
| 1   | C     | 360 | ARG  |
| 1   | C     | 364 | ASN  |
| 1   | C     | 376 | LEU  |
| 1   | C     | 404 | SER  |
| 1   | C     | 429 | HIS  |
| 1   | C     | 474 | LYS  |
| 1   | C     | 520 | GLN  |
| 1   | C     | 524 | ASP  |
| 1   | C     | 564 | LEU  |
| 1   | C     | 578 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 580 | SER  |
| 1   | C     | 593 | ARG  |
| 1   | C     | 594 | GLU  |
| 1   | C     | 595 | ASN  |
| 1   | D     | 12  | LEU  |
| 1   | D     | 23  | THR  |
| 1   | D     | 32  | ARG  |
| 1   | D     | 36  | LEU  |
| 1   | D     | 40  | ASN  |
| 1   | D     | 64  | ARG  |
| 1   | D     | 65  | LYS  |
| 1   | D     | 66  | THR  |
| 1   | D     | 70  | PHE  |
| 1   | D     | 86  | LEU  |
| 1   | D     | 118 | GLU  |
| 1   | D     | 119 | LEU  |
| 1   | D     | 124 | HIS  |
| 1   | D     | 127 | VAL  |
| 1   | D     | 129 | CYS  |
| 1   | D     | 168 | PRO  |
| 1   | D     | 169 | THR  |
| 1   | D     | 175 | LEU  |
| 1   | D     | 177 | ARG  |
| 1   | D     | 185 | SER  |
| 1   | D     | 198 | SER  |
| 1   | D     | 202 | ARG  |
| 1   | D     | 230 | ASN  |
| 1   | D     | 240 | ILE  |
| 1   | D     | 266 | HIS  |
| 1   | D     | 286 | HIS  |
| 1   | D     | 315 | ILE  |
| 1   | D     | 322 | GLN  |
| 1   | D     | 323 | LYS  |
| 1   | D     | 329 | GLN  |
| 1   | D     | 333 | ASN  |
| 1   | D     | 334 | SER  |
| 1   | D     | 337 | PRO  |
| 1   | D     | 347 | PHE  |
| 1   | D     | 356 | SER  |
| 1   | D     | 360 | ARG  |
| 1   | D     | 371 | GLU  |
| 1   | D     | 376 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 414 | THR  |
| 1   | D     | 428 | VAL  |
| 1   | D     | 446 | MET  |
| 1   | D     | 462 | LYS  |
| 1   | D     | 474 | LYS  |
| 1   | D     | 475 | VAL  |
| 1   | D     | 501 | MET  |
| 1   | D     | 503 | GLU  |
| 1   | D     | 513 | CYS  |
| 1   | D     | 538 | GLU  |
| 1   | D     | 568 | GLN  |
| 1   | D     | 573 | PRO  |
| 1   | D     | 583 | ASP  |
| 1   | D     | 586 | ASP  |
| 1   | D     | 592 | SER  |
| 1   | D     | 595 | ASN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 128 | GLN  |
| 1   | A     | 135 | GLN  |
| 1   | A     | 230 | ASN  |
| 1   | A     | 250 | GLN  |
| 1   | A     | 322 | GLN  |
| 1   | A     | 366 | GLN  |
| 1   | A     | 419 | ASN  |
| 1   | A     | 437 | ASN  |
| 1   | A     | 468 | GLN  |
| 1   | A     | 565 | HIS  |
| 1   | B     | 217 | GLN  |
| 1   | B     | 231 | ASN  |
| 1   | B     | 273 | HIS  |
| 1   | B     | 305 | GLN  |
| 1   | B     | 322 | GLN  |
| 1   | B     | 409 | GLN  |
| 1   | B     | 410 | ASN  |
| 1   | B     | 429 | HIS  |
| 1   | B     | 437 | ASN  |
| 1   | B     | 468 | GLN  |
| 1   | B     | 545 | GLN  |
| 1   | B     | 574 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 18  | GLN  |
| 1   | C     | 94  | GLN  |
| 1   | C     | 135 | GLN  |
| 1   | C     | 147 | ASN  |
| 1   | C     | 154 | GLN  |
| 1   | C     | 217 | GLN  |
| 1   | C     | 222 | HIS  |
| 1   | C     | 230 | ASN  |
| 1   | C     | 250 | GLN  |
| 1   | C     | 286 | HIS  |
| 1   | C     | 333 | ASN  |
| 1   | C     | 403 | ASN  |
| 1   | C     | 419 | ASN  |
| 1   | C     | 426 | HIS  |
| 1   | C     | 437 | ASN  |
| 1   | C     | 521 | GLN  |
| 1   | C     | 558 | HIS  |
| 1   | C     | 595 | ASN  |
| 1   | D     | 18  | GLN  |
| 1   | D     | 29  | ASN  |
| 1   | D     | 40  | ASN  |
| 1   | D     | 128 | GLN  |
| 1   | D     | 135 | GLN  |
| 1   | D     | 154 | GLN  |
| 1   | D     | 245 | HIS  |
| 1   | D     | 322 | GLN  |
| 1   | D     | 329 | GLN  |
| 1   | D     | 333 | ASN  |
| 1   | D     | 403 | ASN  |
| 1   | D     | 437 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 4 are monoatomic - leaving 35 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 |
| 2   | NAG  | A     | 601 | 1    | 14,14,15     | 0.99 | 0        | 15,19,21    | 2.38 | 7 (46%)  |
| 2   | NAG  | A     | 602 | 1    | 14,14,15     | 0.28 | 0        | 15,19,21    | 0.57 | 0        |
| 2   | NAG  | A     | 603 | 1,2  | 14,14,15     | 1.29 | 2 (14%)  | 15,19,21    | 1.55 | 1 (6%)   |
| 2   | NAG  | A     | 604 | 2    | 14,14,15     | 0.90 | 1 (7%)   | 15,19,21    | 3.00 | 6 (40%)  |
| 4   | NO3  | A     | 606 | -    | 1,3,3        | 1.50 | 0        | 0,3,3       | 0.00 | -        |
| 4   | NO3  | A     | 607 | -    | 1,3,3        | 4.43 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 4   | NO3  | A     | 608 | -    | 1,3,3        | 0.36 | 0        | 0,3,3       | 0.00 | -        |
| 5   | 3CJ  | A     | 609 | 6    | 8,11,11      | 1.95 | 2 (25%)  | 9,14,14     | 2.81 | 6 (66%)  |
| 6   | HEM  | A     | 610 | 1,5  | 28,50,50     | 1.47 | 3 (10%)  | 17,82,82    | 2.26 | 5 (29%)  |
| 2   | NAG  | B     | 601 | 1    | 14,14,15     | 1.16 | 1 (7%)   | 15,19,21    | 1.93 | 6 (40%)  |
| 2   | NAG  | B     | 602 | 1,2  | 14,14,15     | 1.44 | 2 (14%)  | 15,19,21    | 2.12 | 5 (33%)  |
| 2   | NAG  | B     | 603 | 2    | 14,14,15     | 0.98 | 1 (7%)   | 15,19,21    | 2.04 | 5 (33%)  |
| 4   | NO3  | B     | 605 | -    | 1,3,3        | 0.37 | 0        | 0,3,3       | 0.00 | -        |
| 4   | NO3  | B     | 606 | -    | 1,3,3        | 4.45 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 4   | NO3  | B     | 607 | -    | 1,3,3        | 0.50 | 0        | 0,3,3       | 0.00 | -        |
| 6   | HEM  | B     | 608 | 1    | 28,50,50     | 1.35 | 3 (10%)  | 17,82,82    | 1.89 | 6 (35%)  |
| 5   | 3CJ  | B     | 609 | -    | 8,11,11      | 2.53 | 3 (37%)  | 9,14,14     | 3.33 | 5 (55%)  |
| 2   | NAG  | C     | 601 | 1    | 14,14,15     | 0.30 | 0        | 15,19,21    | 0.57 | 0        |
| 2   | NAG  | C     | 602 | 2    | 14,14,15     | 0.28 | 0        | 15,19,21    | 0.57 | 0        |
| 2   | NAG  | C     | 603 | 1,2  | 14,14,15     | 0.26 | 0        | 15,19,21    | 0.54 | 0        |
| 2   | NAG  | C     | 604 | 1    | 14,14,15     | 0.28 | 0        | 15,19,21    | 0.57 | 0        |
| 4   | NO3  | C     | 606 | -    | 1,3,3        | 0.36 | 0        | 0,3,3       | 0.00 | -        |
| 4   | NO3  | C     | 607 | -    | 1,3,3        | 4.31 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 4   | NO3  | C     | 608 | -    | 1,3,3        | 0.33 | 0        | 0,3,3       | 0.00 | -        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | 3CJ  | C     | 609 | -    | 8,11,11      | 2.20 | 2 (25%)  | 9,14,14     | 2.99 | 5 (55%)  |
| 6   | HEM  | C     | 610 | 1    | 28,50,50     | 1.05 | 2 (7%)   | 17,82,82    | 2.07 | 8 (47%)  |
| 2   | NAG  | D     | 601 | 1    | 14,14,15     | 0.79 | 0        | 15,19,21    | 2.18 | 5 (33%)  |
| 2   | NAG  | D     | 602 | 1    | 14,14,15     | 0.28 | 0        | 15,19,21    | 0.60 | 0        |
| 2   | NAG  | D     | 603 | 1,2  | 14,14,15     | 0.82 | 0        | 15,19,21    | 1.59 | 3 (20%)  |
| 2   | NAG  | D     | 604 | 2    | 14,14,15     | 0.71 | 0        | 15,19,21    | 1.74 | 3 (20%)  |
| 4   | NO3  | D     | 606 | -    | 1,3,3        | 0.36 | 0        | 0,3,3       | 0.00 | -        |
| 4   | NO3  | D     | 607 | -    | 1,3,3        | 4.44 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 4   | NO3  | D     | 608 | -    | 1,3,3        | 0.37 | 0        | 0,3,3       | 0.00 | -        |
| 5   | 3CJ  | D     | 609 | -    | 8,11,11      | 2.95 | 4 (50%)  | 9,14,14     | 4.52 | 6 (66%)  |
| 6   | HEM  | D     | 610 | 1    | 28,50,50     | 1.51 | 5 (17%)  | 17,82,82    | 2.16 | 5 (29%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | NAG  | A     | 601 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | A     | 602 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | A     | 603 | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | A     | 604 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NO3  | A     | 606 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | NO3  | A     | 607 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | NO3  | A     | 608 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 5   | 3CJ  | A     | 609 | 6    | -       | 0/3/3/3   | 0/1/1/1 |
| 6   | HEM  | A     | 610 | 1,5  | -       | 0/6/54/54 | 0/0/8/8 |
| 2   | NAG  | B     | 601 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | B     | 602 | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | B     | 603 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NO3  | B     | 605 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | NO3  | B     | 606 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | NO3  | B     | 607 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 6   | HEM  | B     | 608 | 1    | -       | 0/6/54/54 | 0/0/8/8 |
| 5   | 3CJ  | B     | 609 | -    | -       | 0/3/3/3   | 0/1/1/1 |
| 2   | NAG  | C     | 601 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | C     | 602 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | C     | 603 | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | C     | 604 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NO3  | C     | 606 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | NO3  | C     | 607 | -    | -       | 0/0/0/0   | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4   | NO3  | C     | 608 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 5   | 3CJ  | C     | 609 | -    | -       | 0/3/3/3   | 0/1/1/1 |
| 6   | HEM  | C     | 610 | 1    | -       | 0/6/54/54 | 0/0/8/8 |
| 2   | NAG  | D     | 601 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | D     | 602 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | D     | 603 | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | D     | 604 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NO3  | D     | 606 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | NO3  | D     | 607 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | NO3  | D     | 608 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 5   | 3CJ  | D     | 609 | -    | -       | 0/3/3/3   | 0/1/1/1 |
| 6   | HEM  | D     | 610 | 1    | -       | 0/6/54/54 | 0/0/8/8 |

All (35) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | A     | 610 | HEM  | C4D-ND  | -4.15 | 1.31        | 1.36     |
| 6   | A     | 610 | HEM  | C1B-NB  | -4.10 | 1.31        | 1.36     |
| 6   | D     | 610 | HEM  | C1B-NB  | -4.01 | 1.32        | 1.36     |
| 6   | B     | 608 | HEM  | C1B-NB  | -3.49 | 1.32        | 1.36     |
| 6   | D     | 610 | HEM  | C3B-C2B | -2.83 | 1.36        | 1.40     |
| 6   | C     | 610 | HEM  | C1B-NB  | -2.83 | 1.33        | 1.36     |
| 6   | B     | 608 | HEM  | C4D-ND  | -2.74 | 1.33        | 1.36     |
| 6   | B     | 608 | HEM  | C3B-C2B | -2.73 | 1.36        | 1.40     |
| 6   | D     | 610 | HEM  | C4C-NC  | -2.72 | 1.33        | 1.36     |
| 2   | A     | 603 | NAG  | C2-N2   | -2.71 | 1.41        | 1.46     |
| 2   | A     | 603 | NAG  | O5-C1   | -2.63 | 1.39        | 1.43     |
| 6   | C     | 610 | HEM  | C4D-ND  | -2.53 | 1.33        | 1.36     |
| 2   | A     | 604 | NAG  | C2-N2   | -2.42 | 1.42        | 1.46     |
| 6   | A     | 610 | HEM  | C1A-CHA | -2.31 | 1.34        | 1.40     |
| 2   | B     | 601 | NAG  | C4-C5   | -2.30 | 1.48        | 1.53     |
| 6   | D     | 610 | HEM  | C1C-NC  | -2.12 | 1.34        | 1.36     |
| 6   | D     | 610 | HEM  | CAA-C2A | -2.05 | 1.48        | 1.52     |
| 2   | B     | 602 | NAG  | O5-C1   | -2.02 | 1.40        | 1.43     |
| 5   | D     | 609 | 3CJ  | C4-N2   | 2.05  | 1.36        | 1.33     |
| 2   | B     | 603 | NAG  | C1-C2   | 2.06  | 1.55        | 1.52     |
| 5   | A     | 609 | 3CJ  | C1-S1   | 2.30  | 1.71        | 1.66     |
| 5   | B     | 609 | 3CJ  | C4-N2   | 2.67  | 1.37        | 1.33     |
| 5   | C     | 609 | 3CJ  | C1-S1   | 2.73  | 1.72        | 1.66     |
| 2   | B     | 602 | NAG  | C1-C2   | 2.98  | 1.56        | 1.52     |
| 5   | D     | 609 | 3CJ  | C2-N1   | 3.49  | 1.40        | 1.34     |
| 5   | B     | 609 | 3CJ  | C1-S1   | 3.76  | 1.74        | 1.66     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4   | C     | 607 | NO3  | O1-N  | 4.31 | 1.40        | 1.23     |
| 4   | A     | 607 | NO3  | O1-N  | 4.43 | 1.40        | 1.23     |
| 4   | D     | 607 | NO3  | O1-N  | 4.44 | 1.40        | 1.23     |
| 4   | B     | 606 | NO3  | O1-N  | 4.45 | 1.40        | 1.23     |
| 5   | A     | 609 | 3CJ  | O1-C4 | 4.53 | 1.35        | 1.24     |
| 5   | D     | 609 | 3CJ  | C1-S1 | 4.89 | 1.76        | 1.66     |
| 5   | B     | 609 | 3CJ  | O1-C4 | 5.02 | 1.37        | 1.24     |
| 5   | D     | 609 | 3CJ  | O1-C4 | 5.21 | 1.37        | 1.24     |
| 5   | C     | 609 | 3CJ  | O1-C4 | 5.23 | 1.37        | 1.24     |

All (87) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | B     | 609 | 3CJ  | C3-C2-N1    | -6.11 | 116.28      | 122.91   |
| 6   | A     | 610 | HEM  | CBD-CAD-C3D | -5.83 | 101.34      | 112.47   |
| 2   | D     | 601 | NAG  | O5-C1-C2    | -5.44 | 103.90      | 111.47   |
| 6   | D     | 610 | HEM  | CBD-CAD-C3D | -5.26 | 102.43      | 112.47   |
| 6   | A     | 610 | HEM  | C1D-C2D-C3D | -4.97 | 103.54      | 107.00   |
| 2   | B     | 603 | NAG  | C4-C3-C2    | -4.75 | 104.06      | 111.02   |
| 5   | A     | 609 | 3CJ  | C3-C2-N1    | -4.66 | 117.86      | 122.91   |
| 5   | D     | 609 | 3CJ  | C3-C2-N1    | -4.58 | 117.94      | 122.91   |
| 2   | A     | 603 | NAG  | C2-N2-C7    | -4.28 | 116.70      | 122.94   |
| 2   | A     | 601 | NAG  | C4-C3-C2    | -4.26 | 104.78      | 111.02   |
| 6   | B     | 608 | HEM  | CBD-CAD-C3D | -4.21 | 104.44      | 112.47   |
| 2   | D     | 604 | NAG  | C3-C4-C5    | -4.11 | 102.98      | 110.22   |
| 5   | C     | 609 | 3CJ  | C3-C2-N1    | -4.09 | 118.47      | 122.91   |
| 5   | D     | 609 | 3CJ  | C5-C2-C3    | -3.86 | 115.99      | 121.19   |
| 5   | C     | 609 | 3CJ  | C3-C4-N2    | -3.86 | 119.50      | 124.06   |
| 2   | A     | 604 | NAG  | O4-C4-C3    | -3.82 | 102.04      | 110.36   |
| 2   | D     | 603 | NAG  | O5-C1-C2    | -3.81 | 106.17      | 111.47   |
| 2   | B     | 601 | NAG  | O5-C1-C2    | -3.72 | 106.30      | 111.47   |
| 2   | D     | 601 | NAG  | C2-N2-C7    | -3.55 | 117.76      | 122.94   |
| 6   | C     | 610 | HEM  | CBD-CAD-C3D | -3.39 | 105.99      | 112.47   |
| 2   | B     | 602 | NAG  | O4-C4-C3    | -3.37 | 103.02      | 110.36   |
| 2   | D     | 603 | NAG  | C2-N2-C7    | -3.34 | 118.07      | 122.94   |
| 2   | A     | 601 | NAG  | C2-N2-C7    | -3.27 | 118.18      | 122.94   |
| 2   | A     | 604 | NAG  | O5-C1-C2    | -3.23 | 106.98      | 111.47   |
| 2   | A     | 601 | NAG  | C3-C4-C5    | -3.11 | 104.73      | 110.22   |
| 6   | B     | 608 | HEM  | CAA-C2A-C3A | -2.92 | 120.66      | 129.00   |
| 5   | D     | 609 | 3CJ  | C3-C4-N2    | -2.88 | 120.66      | 124.06   |
| 6   | B     | 608 | HEM  | C1D-C2D-C3D | -2.78 | 105.06      | 107.00   |
| 2   | B     | 601 | NAG  | C2-N2-C7    | -2.75 | 118.94      | 122.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 602 | NAG  | C6-C5-C4    | -2.74 | 106.58      | 113.00   |
| 2   | A     | 604 | NAG  | O3-C3-C4    | -2.68 | 104.53      | 110.36   |
| 2   | B     | 601 | NAG  | O6-C6-C5    | -2.65 | 102.42      | 111.34   |
| 6   | D     | 610 | HEM  | CBA-CAA-C2A | -2.61 | 107.50      | 112.48   |
| 2   | D     | 603 | NAG  | C6-C5-C4    | -2.57 | 106.99      | 113.00   |
| 6   | C     | 610 | HEM  | C1D-C2D-C3D | -2.48 | 105.27      | 107.00   |
| 2   | D     | 604 | NAG  | O5-C1-C2    | -2.47 | 108.04      | 111.47   |
| 6   | D     | 610 | HEM  | C4C-C3C-C2C | -2.46 | 105.18      | 106.90   |
| 2   | B     | 602 | NAG  | O4-C4-C5    | -2.46 | 103.09      | 109.28   |
| 6   | B     | 608 | HEM  | C4C-C3C-C2C | -2.43 | 105.20      | 106.90   |
| 6   | C     | 610 | HEM  | CAA-C2A-C3A | -2.43 | 122.07      | 129.00   |
| 5   | A     | 609 | 3CJ  | C3-C4-N2    | -2.39 | 121.23      | 124.06   |
| 2   | B     | 601 | NAG  | O3-C3-C4    | -2.38 | 105.17      | 110.36   |
| 6   | A     | 610 | HEM  | C4C-C3C-C2C | -2.38 | 105.24      | 106.90   |
| 2   | B     | 601 | NAG  | C6-C5-C4    | -2.37 | 107.45      | 113.00   |
| 2   | D     | 601 | NAG  | O3-C3-C4    | -2.32 | 105.32      | 110.36   |
| 5   | B     | 609 | 3CJ  | C3-C4-N2    | -2.30 | 121.35      | 124.06   |
| 2   | D     | 601 | NAG  | C8-C7-N2    | -2.27 | 112.00      | 116.11   |
| 6   | C     | 610 | HEM  | CAA-CBA-CGA | -2.26 | 108.79      | 112.66   |
| 2   | A     | 604 | NAG  | C2-N2-C7    | -2.19 | 119.75      | 122.94   |
| 2   | A     | 601 | NAG  | O4-C4-C3    | -2.17 | 105.64      | 110.36   |
| 6   | C     | 610 | HEM  | C3B-C4B-NB  | -2.06 | 106.55      | 109.21   |
| 2   | B     | 603 | NAG  | O4-C4-C3    | 2.01  | 114.74      | 110.36   |
| 6   | A     | 610 | HEM  | CMB-C2B-C3B | 2.02  | 128.64      | 124.89   |
| 2   | B     | 603 | NAG  | C2-N2-C7    | 2.03  | 125.91      | 122.94   |
| 6   | B     | 608 | HEM  | CMD-C2D-C3D | 2.04  | 128.78      | 124.94   |
| 2   | D     | 601 | NAG  | C4-C3-C2    | 2.05  | 114.03      | 111.02   |
| 5   | A     | 609 | 3CJ  | C6-C5-C2    | 2.11  | 122.94      | 115.43   |
| 5   | C     | 609 | 3CJ  | C1-N1-C2    | 2.13  | 120.41      | 115.10   |
| 6   | B     | 608 | HEM  | CMB-C2B-C3B | 2.19  | 128.95      | 124.89   |
| 6   | C     | 610 | HEM  | CMC-C2C-C3C | 2.48  | 129.50      | 124.89   |
| 6   | D     | 610 | HEM  | CMB-C2B-C3B | 2.52  | 129.56      | 124.89   |
| 2   | D     | 604 | NAG  | C1-O5-C5    | 2.62  | 115.77      | 112.17   |
| 5   | A     | 609 | 3CJ  | C1-N1-C2    | 2.81  | 122.08      | 115.10   |
| 2   | B     | 603 | NAG  | C1-O5-C5    | 2.99  | 116.29      | 112.17   |
| 2   | B     | 601 | NAG  | C1-O5-C5    | 3.02  | 116.32      | 112.17   |
| 6   | A     | 610 | HEM  | CMD-C2D-C3D | 3.06  | 130.71      | 124.94   |
| 5   | D     | 609 | 3CJ  | C1-N1-C2    | 3.09  | 122.78      | 115.10   |
| 2   | B     | 602 | NAG  | C3-C4-C5    | 3.13  | 115.72      | 110.22   |
| 2   | A     | 601 | NAG  | O4-C4-C5    | 3.36  | 117.75      | 109.28   |
| 2   | A     | 601 | NAG  | C1-C2-N2    | 3.38  | 116.26      | 110.49   |
| 5   | A     | 609 | 3CJ  | C5-C2-C3    | 3.41  | 125.80      | 121.19   |

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| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2   | A     | 601 | NAG  | C1-O5-C5    | 3.43 | 116.89      | 112.17   |
| 6   | C     | 610 | HEM  | CAD-CBD-CGD | 3.55 | 118.72      | 112.66   |
| 6   | C     | 610 | HEM  | CMB-C2B-C3B | 3.66 | 131.69      | 124.89   |
| 5   | B     | 609 | 3CJ  | C5-C2-N1    | 3.67 | 121.09      | 115.78   |
| 5   | B     | 609 | 3CJ  | C1-N1-C2    | 3.85 | 124.67      | 115.10   |
| 2   | B     | 603 | NAG  | O3-C3-C2    | 3.97 | 117.90      | 109.39   |
| 5   | C     | 609 | 3CJ  | C5-C2-N1    | 4.02 | 121.60      | 115.78   |
| 2   | A     | 604 | NAG  | C4-C3-C2    | 4.17 | 117.14      | 111.02   |
| 6   | D     | 610 | HEM  | CMC-C2C-C3C | 4.26 | 132.79      | 124.89   |
| 5   | A     | 609 | 3CJ  | C4-N2-C1    | 4.40 | 118.94      | 114.74   |
| 2   | B     | 602 | NAG  | O3-C3-C2    | 4.61 | 119.27      | 109.39   |
| 5   | B     | 609 | 3CJ  | C4-N2-C1    | 5.03 | 119.54      | 114.74   |
| 5   | C     | 609 | 3CJ  | C4-N2-C1    | 5.11 | 119.62      | 114.74   |
| 5   | D     | 609 | 3CJ  | C5-C2-N1    | 7.03 | 125.94      | 115.78   |
| 2   | A     | 604 | NAG  | C1-O5-C5    | 8.44 | 123.80      | 112.17   |
| 5   | D     | 609 | 3CJ  | C4-N2-C1    | 8.78 | 123.11      | 114.74   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 94 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | A     | 604 | NAG  | 1       | 0            |
| 4   | A     | 607 | NO3  | 1       | 0            |
| 5   | A     | 609 | 3CJ  | 11      | 0            |
| 6   | A     | 610 | HEM  | 12      | 0            |
| 2   | B     | 602 | NAG  | 2       | 0            |
| 2   | B     | 603 | NAG  | 2       | 0            |
| 4   | B     | 605 | NO3  | 1       | 0            |
| 6   | B     | 608 | HEM  | 14      | 0            |
| 5   | B     | 609 | 3CJ  | 12      | 0            |
| 2   | C     | 603 | NAG  | 1       | 0            |
| 4   | C     | 606 | NO3  | 1       | 0            |
| 4   | C     | 607 | NO3  | 1       | 0            |
| 4   | C     | 608 | NO3  | 2       | 0            |
| 5   | C     | 609 | 3CJ  | 9       | 0            |
| 6   | C     | 610 | HEM  | 17      | 0            |
| 2   | D     | 602 | NAG  | 1       | 0            |
| 4   | D     | 606 | NO3  | 2       | 0            |
| 4   | D     | 607 | NO3  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | D     | 608 | NO3  | 4       | 0            |
| 5   | D     | 609 | 3CJ  | 11      | 0            |
| 6   | D     | 610 | HEM  | 15      | 0            |

## 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 [i](#)

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

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

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2  |       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|----------|-------|-----------------------|-------|
| 1   | A     | 595/595 (100%)   | 0.24   | 31 (5%)  | 28 29 | 16, 42, 78, 117       | 0     |
| 1   | B     | 595/595 (100%)   | 0.27   | 34 (5%)  | 24 25 | 20, 43, 76, 100       | 0     |
| 1   | C     | 595/595 (100%)   | 0.43   | 53 (8%)  | 10 10 | 20, 43, 83, 100       | 0     |
| 1   | D     | 595/595 (100%)   | 0.34   | 40 (6%)  | 19 19 | 14, 41, 79, 100       | 0     |
| All | All   | 2380/2380 (100%) | 0.32   | 158 (6%) | 19 19 | 14, 42, 79, 117       | 0     |

All (158) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 4   | VAL  | 19.3 |
| 1   | C     | 6   | CYS  | 13.6 |
| 1   | D     | 2   | TRP  | 12.4 |
| 1   | A     | 171 | PRO  | 11.2 |
| 1   | D     | 7   | GLY  | 11.2 |
| 1   | D     | 13  | VAL  | 10.2 |
| 1   | B     | 121 | SER  | 9.8  |
| 1   | D     | 1   | SER  | 9.7  |
| 1   | B     | 1   | SER  | 9.7  |
| 1   | A     | 2   | TRP  | 9.4  |
| 1   | A     | 5   | GLY  | 9.1  |
| 1   | B     | 2   | TRP  | 8.9  |
| 1   | D     | 3   | GLU  | 8.9  |
| 1   | A     | 1   | SER  | 8.9  |
| 1   | C     | 5   | GLY  | 8.5  |
| 1   | A     | 4   | VAL  | 8.4  |
| 1   | B     | 6   | CYS  | 8.4  |
| 1   | C     | 4   | VAL  | 7.7  |
| 1   | C     | 9   | PRO  | 7.7  |
| 1   | A     | 172 | TYR  | 7.1  |
| 1   | B     | 4   | VAL  | 6.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 5   | GLY  | 6.7  |
| 1   | C     | 7   | GLY  | 6.7  |
| 1   | C     | 1   | SER  | 6.4  |
| 1   | B     | 122 | SER  | 6.3  |
| 1   | D     | 11  | PRO  | 6.3  |
| 1   | C     | 121 | SER  | 6.2  |
| 1   | C     | 8   | ALA  | 6.2  |
| 1   | C     | 2   | TRP  | 5.9  |
| 1   | C     | 129 | CYS  | 5.9  |
| 1   | A     | 170 | PRO  | 5.8  |
| 1   | A     | 119 | LEU  | 5.7  |
| 1   | C     | 3   | GLU  | 5.6  |
| 1   | D     | 170 | PRO  | 5.3  |
| 1   | A     | 3   | GLU  | 5.3  |
| 1   | A     | 12  | LEU  | 5.2  |
| 1   | C     | 96  | ARG  | 5.1  |
| 1   | D     | 592 | SER  | 5.1  |
| 1   | C     | 132 | TYR  | 5.0  |
| 1   | A     | 6   | CYS  | 5.0  |
| 1   | B     | 3   | GLU  | 4.9  |
| 1   | B     | 120 | GLY  | 4.8  |
| 1   | D     | 120 | GLY  | 4.8  |
| 1   | A     | 121 | SER  | 4.8  |
| 1   | A     | 585 | LEU  | 4.7  |
| 1   | B     | 582 | VAL  | 4.7  |
| 1   | C     | 172 | TYR  | 4.7  |
| 1   | B     | 170 | PRO  | 4.6  |
| 1   | D     | 12  | LEU  | 4.6  |
| 1   | C     | 13  | VAL  | 4.6  |
| 1   | C     | 119 | LEU  | 4.5  |
| 1   | A     | 13  | VAL  | 4.5  |
| 1   | D     | 5   | GLY  | 4.5  |
| 1   | D     | 595 | ASN  | 4.4  |
| 1   | A     | 173 | GLN  | 4.3  |
| 1   | D     | 172 | TYR  | 4.2  |
| 1   | C     | 591 | ALA  | 4.2  |
| 1   | D     | 207 | SER  | 4.2  |
| 1   | D     | 169 | THR  | 4.2  |
| 1   | B     | 189 | ALA  | 4.2  |
| 1   | B     | 595 | ASN  | 4.2  |
| 1   | B     | 11  | PRO  | 4.0  |
| 1   | B     | 171 | PRO  | 3.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 8   | ALA  | 3.9  |
| 1   | D     | 10  | VAL  | 3.8  |
| 1   | A     | 169 | THR  | 3.8  |
| 1   | D     | 6   | CYS  | 3.7  |
| 1   | C     | 249 | PHE  | 3.7  |
| 1   | C     | 161 | PHE  | 3.7  |
| 1   | A     | 9   | PRO  | 3.6  |
| 1   | B     | 8   | ALA  | 3.6  |
| 1   | A     | 223 | GLY  | 3.5  |
| 1   | A     | 136 | GLY  | 3.5  |
| 1   | C     | 11  | PRO  | 3.5  |
| 1   | A     | 122 | SER  | 3.5  |
| 1   | C     | 153 | THR  | 3.5  |
| 1   | C     | 10  | VAL  | 3.4  |
| 1   | C     | 580 | SER  | 3.4  |
| 1   | B     | 581 | ALA  | 3.4  |
| 1   | C     | 595 | ASN  | 3.4  |
| 1   | B     | 173 | GLN  | 3.4  |
| 1   | A     | 7   | GLY  | 3.3  |
| 1   | C     | 117 | THR  | 3.3  |
| 1   | B     | 172 | TYR  | 3.3  |
| 1   | C     | 138 | GLU  | 3.3  |
| 1   | B     | 530 | TRP  | 3.2  |
| 1   | B     | 369 | GLY  | 3.2  |
| 1   | B     | 262 | LEU  | 3.1  |
| 1   | D     | 209 | PRO  | 3.0  |
| 1   | D     | 132 | TYR  | 3.0  |
| 1   | B     | 137 | ASP  | 3.0  |
| 1   | B     | 583 | ASP  | 3.0  |
| 1   | B     | 9   | PRO  | 3.0  |
| 1   | C     | 209 | PRO  | 2.9  |
| 1   | D     | 190 | SER  | 2.9  |
| 1   | B     | 425 | THR  | 2.9  |
| 1   | C     | 106 | ILE  | 2.9  |
| 1   | B     | 282 | ARG  | 2.8  |
| 1   | C     | 169 | THR  | 2.8  |
| 1   | C     | 127 | VAL  | 2.8  |
| 1   | A     | 582 | VAL  | 2.7  |
| 1   | B     | 7   | GLY  | 2.7  |
| 1   | D     | 173 | GLN  | 2.7  |
| 1   | C     | 215 | VAL  | 2.7  |
| 1   | B     | 545 | GLN  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 175 | LEU  | 2.7  |
| 1   | C     | 351 | HIS  | 2.6  |
| 1   | D     | 574 | HIS  | 2.6  |
| 1   | D     | 171 | PRO  | 2.6  |
| 1   | C     | 464 | LEU  | 2.6  |
| 1   | A     | 174 | SER  | 2.6  |
| 1   | D     | 351 | HIS  | 2.6  |
| 1   | A     | 56  | ALA  | 2.5  |
| 1   | C     | 120 | GLY  | 2.5  |
| 1   | C     | 173 | GLN  | 2.5  |
| 1   | D     | 243 | THR  | 2.5  |
| 1   | B     | 593 | ARG  | 2.4  |
| 1   | C     | 175 | LEU  | 2.4  |
| 1   | D     | 585 | LEU  | 2.4  |
| 1   | C     | 542 | ASP  | 2.4  |
| 1   | C     | 118 | GLU  | 2.4  |
| 1   | A     | 137 | ASP  | 2.4  |
| 1   | D     | 107 | VAL  | 2.4  |
| 1   | D     | 134 | VAL  | 2.4  |
| 1   | A     | 425 | THR  | 2.3  |
| 1   | C     | 243 | THR  | 2.3  |
| 1   | D     | 17  | GLU  | 2.3  |
| 1   | C     | 130 | GLU  | 2.3  |
| 1   | C     | 14  | THR  | 2.3  |
| 1   | A     | 11  | PRO  | 2.3  |
| 1   | B     | 586 | ASP  | 2.3  |
| 1   | C     | 12  | LEU  | 2.3  |
| 1   | A     | 10  | VAL  | 2.2  |
| 1   | D     | 567 | PHE  | 2.2  |
| 1   | C     | 170 | PRO  | 2.2  |
| 1   | B     | 588 | SER  | 2.2  |
| 1   | D     | 223 | GLY  | 2.2  |
| 1   | A     | 21  | TYR  | 2.1  |
| 1   | C     | 581 | ALA  | 2.1  |
| 1   | C     | 494 | ILE  | 2.1  |
| 1   | C     | 592 | SER  | 2.1  |
| 1   | D     | 208 | SER  | 2.1  |
| 1   | A     | 485 | LYS  | 2.1  |
| 1   | C     | 582 | VAL  | 2.1  |
| 1   | D     | 582 | VAL  | 2.1  |
| 1   | C     | 355 | PRO  | 2.1  |
| 1   | D     | 303 | PHE  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 351 | HIS  | 2.1  |
| 1   | B     | 10  | VAL  | 2.1  |
| 1   | C     | 108 | ASP  | 2.0  |
| 1   | D     | 168 | PRO  | 2.0  |
| 1   | C     | 164 | GLY  | 2.0  |
| 1   | D     | 15  | CYS  | 2.0  |
| 1   | C     | 159 | PRO  | 2.0  |
| 1   | C     | 546 | LYS  | 2.0  |
| 1   | C     | 276 | LEU  | 2.0  |
| 1   | D     | 331 | TYR  | 2.0  |
| 1   | D     | 206 | LEU  | 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 4   | NO3  | C     | 606 | 4/4   | 0.92 | 0.59 | 10.60 | 24,27,29,31                | 0     |
| 4   | NO3  | D     | 608 | 4/4   | 0.94 | 0.46 | 10.37 | 23,23,26,30                | 0     |
| 4   | NO3  | B     | 607 | 4/4   | 0.91 | 0.66 | 7.83  | 24,24,24,28                | 0     |
| 4   | NO3  | A     | 608 | 4/4   | 0.96 | 0.42 | 6.79  | 23,24,26,27                | 0     |
| 4   | NO3  | C     | 608 | 4/4   | 0.87 | 0.25 | 4.44  | 24,28,29,30                | 0     |
| 4   | NO3  | A     | 606 | 4/4   | 0.96 | 0.30 | 3.77  | 23,23,24,26                | 0     |
| 2   | NAG  | A     | 601 | 14/15 | 0.74 | 0.20 | 3.27  | 64,79,81,81                | 0     |
| 5   | 3CJ  | D     | 609 | 11/11 | 0.83 | 0.41 | 3.15  | 39,48,58,58                | 0     |
| 5   | 3CJ  | C     | 609 | 11/11 | 0.74 | 0.36 | 2.31  | 69,79,84,85                | 0     |
| 4   | NO3  | B     | 605 | 4/4   | 0.89 | 0.20 | 1.76  | 22,25,27,28                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 4   | NO3  | D     | 606 | 4/4   | 0.95 | 0.22 | 1.67  | 21,24,24,26                | 0     |
| 6   | HEM  | A     | 610 | 43/43 | 0.95 | 0.23 | 1.41  | 31,39,44,49                | 0     |
| 2   | NAG  | C     | 603 | 14/15 | 0.86 | 0.24 | 1.25  | 20,20,20,20                | 0     |
| 2   | NAG  | B     | 601 | 14/15 | 0.91 | 0.15 | 1.09  | 55,63,73,75                | 0     |
| 6   | HEM  | B     | 608 | 43/43 | 0.94 | 0.23 | 1.02  | 33,42,54,62                | 0     |
| 5   | 3CJ  | B     | 609 | 11/11 | 0.84 | 0.24 | 1.01  | 48,52,58,61                | 0     |
| 3   | CA   | C     | 605 | 1/1   | 0.94 | 0.23 | 0.66  | 46,46,46,46                | 0     |
| 3   | CA   | A     | 605 | 1/1   | 0.91 | 0.18 | 0.53  | 43,43,43,43                | 0     |
| 2   | NAG  | C     | 604 | 14/15 | 0.89 | 0.20 | 0.48  | 48,55,60,61                | 0     |
| 3   | CA   | D     | 605 | 1/1   | 0.97 | 0.24 | 0.21  | 36,36,36,36                | 0     |
| 2   | NAG  | B     | 602 | 14/15 | 0.85 | 0.19 | 0.15  | 36,50,59,66                | 0     |
| 2   | NAG  | C     | 601 | 14/15 | 0.64 | 0.39 | -0.11 | 78,86,89,90                | 0     |
| 6   | HEM  | C     | 610 | 43/43 | 0.94 | 0.19 | -0.16 | 35,45,51,53                | 0     |
| 6   | HEM  | D     | 610 | 43/43 | 0.95 | 0.19 | -0.17 | 19,25,39,45                | 0     |
| 2   | NAG  | A     | 602 | 14/15 | 0.94 | 0.12 | -0.38 | 38,46,51,54                | 0     |
| 5   | 3CJ  | A     | 609 | 11/11 | 0.92 | 0.19 | -0.38 | 47,50,55,56                | 0     |
| 2   | NAG  | A     | 603 | 14/15 | 0.93 | 0.14 | -0.55 | 33,41,52,54                | 0     |
| 3   | CA   | B     | 604 | 1/1   | 0.93 | 0.14 | -0.71 | 44,44,44,44                | 0     |
| 2   | NAG  | D     | 601 | 14/15 | 0.84 | 0.20 | -0.72 | 52,60,65,66                | 0     |
| 2   | NAG  | D     | 602 | 14/15 | 0.82 | 0.17 | -0.82 | 46,54,59,60                | 0     |
| 2   | NAG  | D     | 603 | 14/15 | 0.94 | 0.11 | -0.96 | 70,79,82,85                | 0     |
| 2   | NAG  | B     | 603 | 14/15 | 0.81 | 0.27 | -     | 45,53,55,58                | 14    |
| 2   | NAG  | A     | 604 | 14/15 | 0.88 | 0.20 | -     | 43,50,51,52                | 14    |
| 2   | NAG  | C     | 602 | 14/15 | 0.83 | 0.21 | -     | 49,56,63,63                | 14    |
| 4   | NO3  | C     | 607 | 4/4   | 0.86 | 0.43 | -     | 24,24,27,31                | 0     |
| 4   | NO3  | B     | 606 | 4/4   | 0.90 | 0.40 | -     | 26,26,27,29                | 0     |
| 2   | NAG  | D     | 604 | 14/15 | 0.84 | 0.20 | -     | 61,67,70,70                | 14    |
| 4   | NO3  | D     | 607 | 4/4   | 0.90 | 0.38 | -     | 25,26,27,28                | 0     |
| 4   | NO3  | A     | 607 | 4/4   | 0.97 | 0.17 | -     | 24,26,28,32                | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.