



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:50 am GMT

PDB ID : 1TH3  
Title : Crystal structure of NADPH depleted bovine live catalase complexed with cyanide  
Authors : Sugadev, R.; Balasundaresan, D.; Ponnuswamy, M.N.; Kumaran, D.; Swaminathan, S.; Sekar, K.  
Deposited on : 2004-06-01  
Resolution : 2.80 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  |

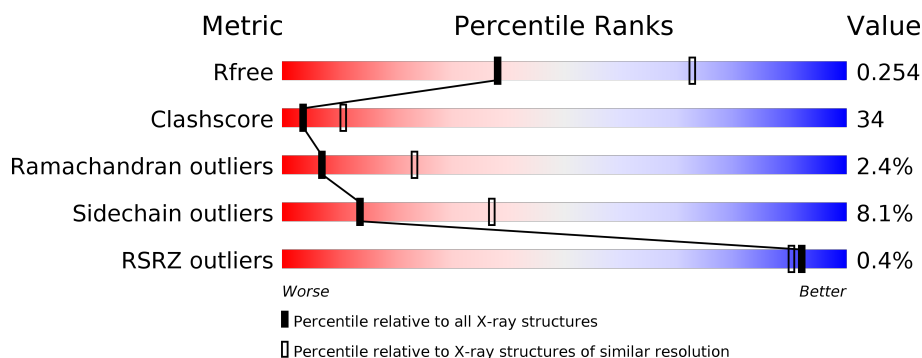
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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                      | 2583 (2.80-2.80)                                      |
| Clashscore            | 112137                      | 3033 (2.80-2.80)                                      |
| Ramachandran outliers | 110173                      | 2983 (2.80-2.80)                                      |
| Sidechain outliers    | 110143                      | 2985 (2.80-2.80)                                      |
| RSRZ outliers         | 101464                      | 2610 (2.80-2.80)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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     | 506    |                  |
| 1   | B     | 506    |                  |
| 1   | C     | 506    |                  |
| 1   | D     | 506    |                  |

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   | CYN  | A     | 3000 | -         | -        | X       | -                |
| 3   | HEM  | B     | 2001 | -         | -        | X       | X                |
| 3   | HEM  | C     | 2002 | -         | -        | X       | X                |
| 3   | HEM  | D     | 2003 | -         | -        | X       | X                |

## 2 Entry composition [i](#)

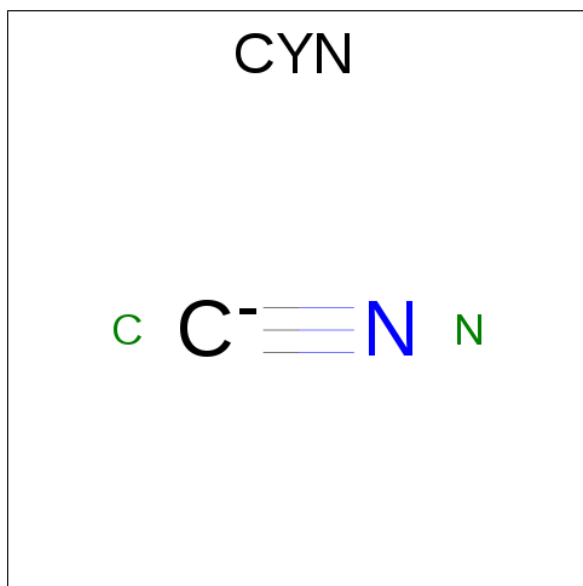
There are 4 unique types of molecules in this entry. The entry contains 16932 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Catalase.

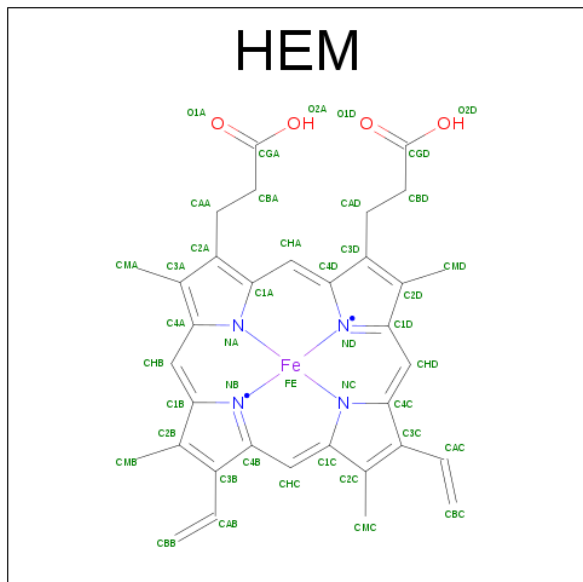
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 499      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4017  | 2548 | 715 | 740 | 14 |         |         |       |
| 1   | B     | 499      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4017  | 2548 | 715 | 740 | 14 |         |         |       |
| 1   | C     | 499      | Total | C    | N   | O   | S  | 1       | 0       | 0     |
|     |       |          | 4017  | 2548 | 715 | 740 | 14 |         |         |       |
| 1   | D     | 499      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4017  | 2548 | 715 | 740 | 14 |         |         |       |

- Molecule 2 is CYANIDE ION (three-letter code: CYN) (formula: CN).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 2   | D     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms       |         |         |        | ZeroOcc | AltConf |   |
|-----|-------|----------|-------------|---------|---------|--------|---------|---------|---|
| 3   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 3   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 3   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 3   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |

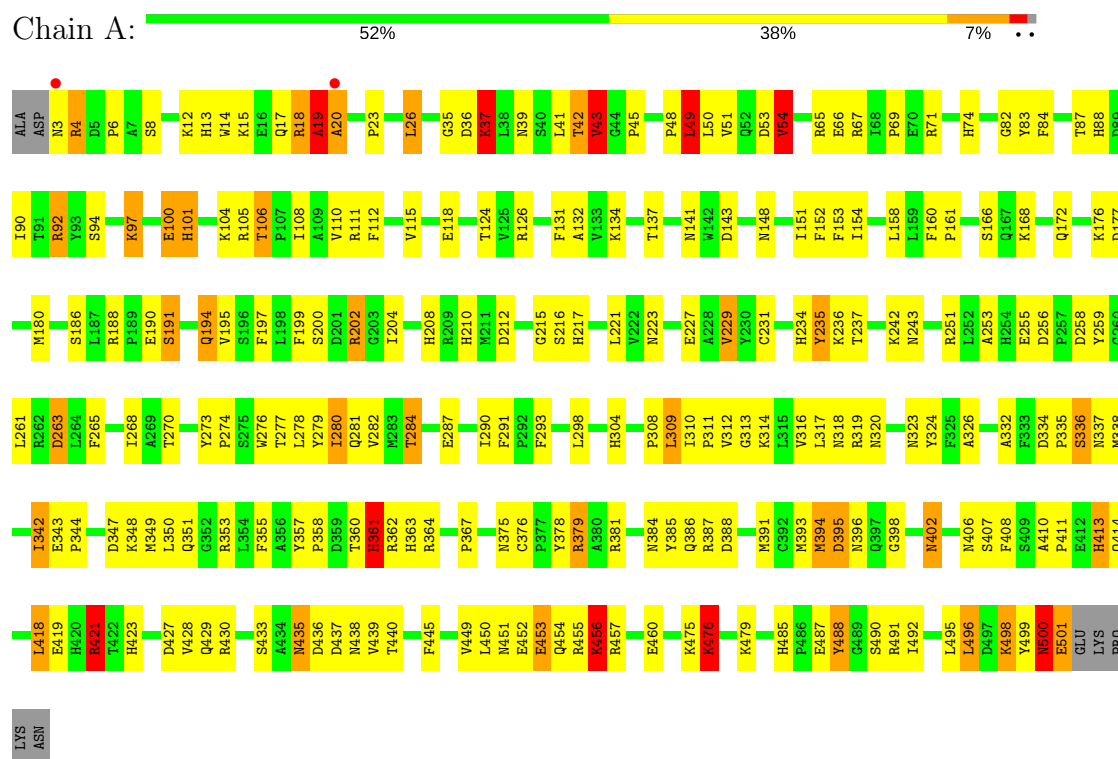
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4   | A     | 201      | Total O<br>201 201 | 0       | 0       |
| 4   | B     | 195      | Total O<br>195 195 | 0       | 0       |
| 4   | C     | 138      | Total O<br>138 138 | 0       | 0       |
| 4   | D     | 154      | Total O<br>154 154 | 0       | 0       |

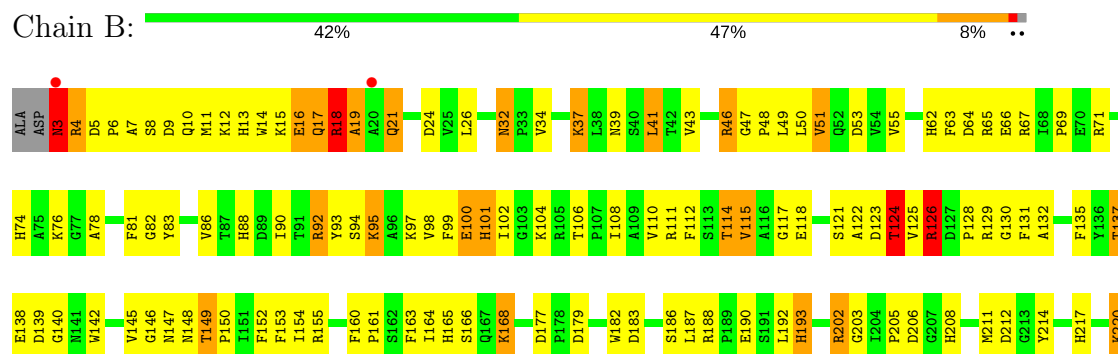
### 3 Residue-property plots

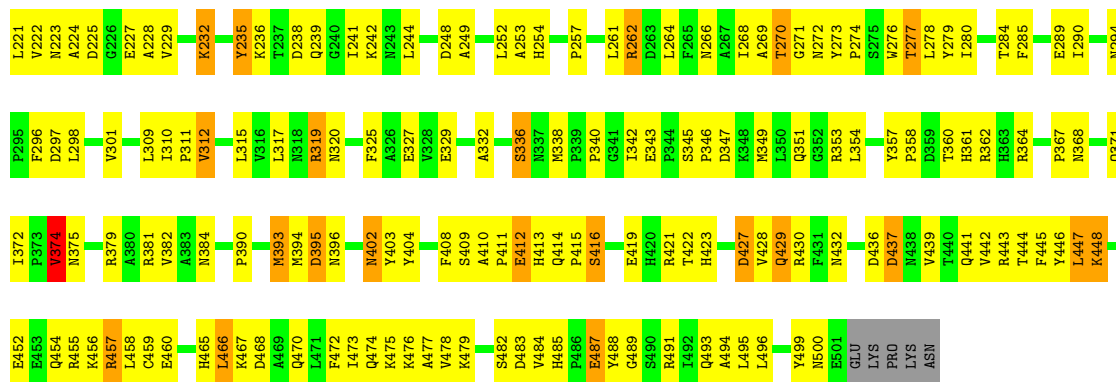
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

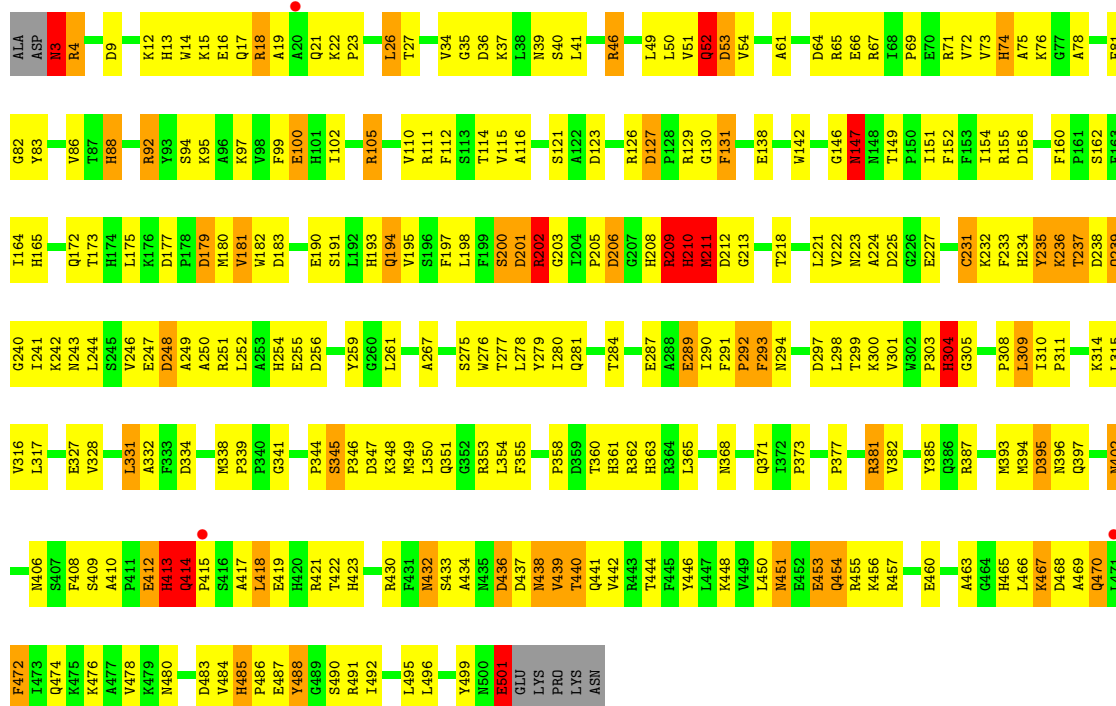
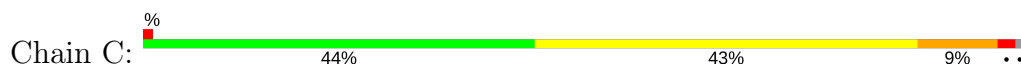


#### • Molecule 1: Catalase





• Molecule 1: Catalase



|      |      |      |      |
|------|------|------|------|
| E501 | Q239 | E329 | S407 |
| GLU  | K242 | A332 | F408 |
| LYS  | V246 | F333 | S409 |
| PRO  | E247 | D334 | A410 |
| LYS  | L261 | P335 | P411 |
| ASN  | R262 | S336 | E412 |
|      | D263 | N337 | H413 |
|      | N266 | M338 | L418 |
|      | T270 | P339 | E419 |
|      | G271 | I342 | H420 |
|      | N272 | E343 | R421 |
|      | V273 | P346 | T422 |
|      | P274 | P346 | H423 |
|      | S275 | D347 | Q429 |
|      | N276 | K348 | R430 |
|      | T277 | M349 | F431 |
|      | L278 | R353 | D437 |
|      | V279 | Y357 | N438 |
|      | I280 | P358 | V439 |
|      | Q281 | H361 | T440 |
|      | T284 | R362 | Q441 |
|      | F285 | N368 | V442 |
|      | E287 | Q371 | F445 |
|      | A288 | I372 | V449 |
|      | E289 | P373 | L450 |
|      | F291 | V374 | N451 |
|      | P292 | N375 | E452 |
|      | F293 | G376 | E453 |
|      | N294 | P377 | Q454 |
|      | P295 | Y378 | R455 |
|      | F296 | R379 | E460 |
|      | D297 | A380 | L466 |
|      | L298 | R381 | K467 |
|      | T299 | V382 | L471 |
|      | K300 | A383 | V478 |
|      | V301 | N384 | K479 |
|      | W302 | D388 | N480 |
|      | P303 | G389 | V484 |
|      | H304 | P390 | H485 |
|      | G305 | M391 | P486 |
|      | D306 | C392 | E487 |
|      | V307 | M393 | Y488 |
|      | P308 | M394 | L492 |
|      | L309 | Q397 | I492 |
|      | I310 | M402 | Q493 |
|      | P311 | Y403 | A494 |
|      | V312 | P405 | L495 |
|      | L317 | N406 | Y499 |
|      | V322 |      | N500 |
|      | N323 |      |      |



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 86.06Å 140.11Å 226.51Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)  | 39.21 – 2.80<br>42.27 – 2.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 76.4 (39.21-2.80)<br>76.5 (42.27-2.80)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.12  | Depositor        |
| $R_{sym}$   | 0.12  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.07 (at 2.81Å)   | Xtriage          |
| Refinement program  | CNS 1.1   | Depositor        |
| R, $R_{free}$   | 0.198 , 0.261<br>0.197 , 0.254                              | Depositor<br>DCC |
| $R_{free}$ test set   | 1553 reflections (3.07%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 34.6  | Xtriage          |
| Anisotropy  | 0.578   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 53.8   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.92  | EDS              |
| Total number of atoms   | 16932   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 36.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CYN

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     | 0.71         | 8/4137 (0.2%)   | 1.63        | 67/5619 (1.2%)   |
| 1   | B     | 0.98         | 5/4137 (0.1%)   | 1.47        | 29/5619 (0.5%)   |
| 1   | C     | 0.70         | 12/4137 (0.3%)  | 1.63        | 50/5619 (0.9%)   |
| 1   | D     | 0.60         | 1/4137 (0.0%)   | 0.83        | 8/5619 (0.1%)    |
| All | All   | 0.76         | 26/16548 (0.2%) | 1.43        | 154/22476 (0.7%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 2                   | 6                   |
| 1   | B     | 0                   | 4                   |
| 1   | C     | 3                   | 4                   |
| All | All   | 5                   | 14                  |

All (26) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | B     | 319 | ARG  | CD-NE | 48.75  | 2.29        | 1.46     |
| 1   | D     | 413 | HIS  | CA-CB | -20.31 | 1.09        | 1.53     |
| 1   | A     | 43  | VAL  | C-O   | 18.23  | 1.57        | 1.23     |
| 1   | C     | 202 | ARG  | NE-CZ | 16.64  | 1.54        | 1.33     |
| 1   | B     | 319 | ARG  | NE-CZ | 15.74  | 1.53        | 1.33     |
| 1   | A     | 92  | ARG  | CG-CD | 14.29  | 1.87        | 1.51     |
| 1   | A     | 20  | ALA  | CA-C  | -12.12 | 1.21        | 1.52     |
| 1   | B     | 3   | ASN  | C-N   | 11.00  | 1.59        | 1.34     |
| 1   | A     | 43  | VAL  | N-CA  | 10.14  | 1.66        | 1.46     |
| 1   | C     | 292 | PRO  | C-N   | 9.22   | 1.55        | 1.34     |
| 1   | C     | 413 | HIS  | CB-CG | 8.62   | 1.65        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 421 | ARG  | CD-NE   | -8.47 | 1.32        | 1.46     |
| 1   | C     | 292 | PRO  | CA-C    | -8.35 | 1.36        | 1.52     |
| 1   | C     | 211 | MET  | N-CA    | -7.18 | 1.31        | 1.46     |
| 1   | C     | 9   | ASP  | CB-CG   | 7.13  | 1.66        | 1.51     |
| 1   | B     | 374 | VAL  | CA-CB   | 7.10  | 1.69        | 1.54     |
| 1   | A     | 229 | VAL  | CA-CB   | -6.91 | 1.40        | 1.54     |
| 1   | B     | 319 | ARG  | CA-CB   | -6.44 | 1.39        | 1.53     |
| 1   | A     | 176 | LYS  | CD-CE   | 6.39  | 1.67        | 1.51     |
| 1   | C     | 485 | HIS  | ND1-CE1 | -6.29 | 1.19        | 1.34     |
| 1   | C     | 9   | ASP  | CA-CB   | 6.28  | 1.67        | 1.53     |
| 1   | C     | 454 | GLN  | CB-CG   | -5.66 | 1.37        | 1.52     |
| 1   | A     | 280 | ILE  | CA-CB   | 5.59  | 1.67        | 1.54     |
| 1   | C     | 210 | HIS  | CA-C    | -5.16 | 1.39        | 1.52     |
| 1   | C     | 414 | GLN  | CA-CB   | 5.03  | 1.65        | 1.53     |
| 1   | C     | 210 | HIS  | C-N     | -5.02 | 1.22        | 1.34     |

All (154) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | C     | 202 | ARG  | NE-CZ-NH2 | -52.37 | 94.12       | 120.30   |
| 1   | B     | 319 | ARG  | NE-CZ-NH1 | -46.12 | 97.24       | 120.30   |
| 1   | C     | 202 | ARG  | NE-CZ-NH1 | 43.99  | 142.29      | 120.30   |
| 1   | B     | 319 | ARG  | CG-CD-NE  | -41.07 | 25.55       | 111.80   |
| 1   | A     | 19  | ALA  | O-C-N     | -36.47 | 64.35       | 122.70   |
| 1   | B     | 395 | ASP  | N-CA-CB   | -31.42 | 54.04       | 110.60   |
| 1   | B     | 126 | ARG  | CD-NE-CZ  | 29.09  | 164.32      | 123.60   |
| 1   | A     | 304 | HIS  | CA-CB-CG  | 27.88  | 161.00      | 113.60   |
| 1   | D     | 413 | HIS  | CA-CB-CG  | 24.99  | 156.08      | 113.60   |
| 1   | C     | 483 | ASP  | N-CA-CB   | 23.74  | 153.33      | 110.60   |
| 1   | B     | 319 | ARG  | CB-CG-CD  | -23.52 | 50.45       | 111.60   |
| 1   | A     | 304 | HIS  | CB-CA-C   | 23.17  | 156.73      | 110.40   |
| 1   | A     | 54  | VAL  | CA-CB-CG2 | -22.17 | 77.64       | 110.90   |
| 1   | A     | 229 | VAL  | CA-CB-CG2 | 21.61  | 143.32      | 110.90   |
| 1   | A     | 421 | ARG  | CG-CD-NE  | 21.26  | 156.45      | 111.80   |
| 1   | C     | 453 | GLU  | CB-CG-CD  | 20.03  | 168.28      | 114.20   |
| 1   | A     | 49  | LEU  | CB-CG-CD2 | 19.96  | 144.93      | 111.00   |
| 1   | A     | 418 | LEU  | N-CA-CB   | 19.58  | 149.57      | 110.40   |
| 1   | A     | 421 | ARG  | CB-CG-CD  | 19.15  | 161.40      | 111.60   |
| 1   | C     | 414 | GLN  | CA-CB-CG  | 19.00  | 155.19      | 113.40   |
| 1   | A     | 395 | ASP  | CA-CB-CG  | 18.84  | 154.84      | 113.40   |
| 1   | C     | 501 | GLU  | CB-CA-C   | 18.65  | 147.70      | 110.40   |
| 1   | C     | 292 | PRO  | O-C-N     | -18.60 | 92.93       | 122.70   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | A     | 395 | ASP  | N-CA-CB   | 18.43  | 143.77      | 110.60   |
| 1   | B     | 487 | GLU  | CA-CB-CG  | 18.33  | 153.72      | 113.40   |
| 1   | A     | 456 | LYS  | CG-CD-CE  | 18.19  | 166.47      | 111.90   |
| 1   | B     | 487 | GLU  | CB-CG-CD  | 17.52  | 161.49      | 114.20   |
| 1   | B     | 319 | ARG  | CA-CB-CG  | 17.51  | 151.93      | 113.40   |
| 1   | D     | 453 | GLU  | CB-CG-CD  | 17.34  | 161.01      | 114.20   |
| 1   | C     | 453 | GLU  | N-CA-CB   | 17.29  | 141.72      | 110.60   |
| 1   | C     | 147 | ASN  | CB-CA-C   | 17.13  | 144.66      | 110.40   |
| 1   | A     | 43  | VAL  | O-C-N     | -16.82 | 94.61       | 123.20   |
| 1   | C     | 9   | ASP  | CA-CB-CG  | 16.74  | 150.23      | 113.40   |
| 1   | A     | 456 | LYS  | CB-CG-CD  | 16.61  | 154.78      | 111.60   |
| 1   | A     | 361 | HIS  | N-CA-CB   | -16.54 | 80.83       | 110.60   |
| 1   | A     | 43  | VAL  | CA-C-N    | 16.39  | 148.99      | 116.20   |
| 1   | C     | 453 | GLU  | CA-CB-CG  | 16.08  | 148.78      | 113.40   |
| 1   | A     | 304 | HIS  | N-CA-CB   | -16.01 | 81.79       | 110.60   |
| 1   | C     | 292 | PRO  | N-CA-C    | 15.85  | 153.31      | 112.10   |
| 1   | C     | 3   | ASN  | CB-CA-C   | 15.64  | 141.67      | 110.40   |
| 1   | C     | 52  | GLN  | CB-CG-CD  | 15.59  | 152.13      | 111.60   |
| 1   | B     | 374 | VAL  | CB-CA-C   | -15.46 | 82.03       | 111.40   |
| 1   | A     | 476 | LYS  | CD-CE-NZ  | 15.44  | 147.20      | 111.70   |
| 1   | D     | 97  | LYS  | CG-CD-CE  | 15.32  | 157.88      | 111.90   |
| 1   | B     | 429 | GLN  | CA-CB-CG  | 15.20  | 146.83      | 113.40   |
| 1   | A     | 118 | GLU  | N-CA-CB   | -15.14 | 83.35       | 110.60   |
| 1   | A     | 402 | ASN  | CA-CB-CG  | 15.13  | 146.68      | 113.40   |
| 1   | C     | 454 | GLN  | CB-CG-CD  | 14.91  | 150.36      | 111.60   |
| 1   | B     | 32  | ASN  | CB-CG-OD1 | 14.89  | 151.38      | 121.60   |
| 1   | C     | 454 | GLN  | N-CA-CB   | -14.83 | 83.90       | 110.60   |
| 1   | C     | 9   | ASP  | N-CA-CB   | -14.46 | 84.58       | 110.60   |
| 1   | A     | 501 | GLU  | CB-CA-C   | 14.38  | 139.17      | 110.40   |
| 1   | B     | 32  | ASN  | CB-CG-ND2 | -14.36 | 82.23       | 116.70   |
| 1   | B     | 412 | GLU  | CB-CG-CD  | 14.10  | 152.27      | 114.20   |
| 1   | A     | 381 | ARG  | CG-CD-NE  | 13.98  | 141.16      | 111.80   |
| 1   | A     | 19  | ALA  | CA-C-N    | 13.92  | 147.82      | 117.20   |
| 1   | A     | 435 | ASN  | CB-CA-C   | 13.69  | 137.78      | 110.40   |
| 1   | C     | 289 | GLU  | CG-CD-OE2 | -13.67 | 90.97       | 118.30   |
| 1   | A     | 97  | LYS  | CG-CD-CE  | 13.63  | 152.81      | 111.90   |
| 1   | A     | 421 | ARG  | CD-NE-CZ  | 13.58  | 142.61      | 123.60   |
| 1   | B     | 478 | VAL  | CA-CB-CG1 | -13.15 | 91.17       | 110.90   |
| 1   | D     | 453 | GLU  | CA-CB-CG  | 13.13  | 142.29      | 113.40   |
| 1   | B     | 319 | ARG  | NE-CZ-NH2 | 13.10  | 126.85      | 120.30   |
| 1   | B     | 412 | GLU  | N-CA-CB   | 13.01  | 134.02      | 110.60   |
| 1   | C     | 292 | PRO  | CA-C-O    | 12.83  | 150.99      | 120.20   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | C     | 9   | ASP  | CB-CG-OD1  | 12.44  | 129.50      | 118.30   |
| 1   | A     | 500 | ASN  | N-CA-CB    | -12.41 | 88.26       | 110.60   |
| 1   | C     | 292 | PRO  | CB-CA-C    | -12.27 | 81.33       | 112.00   |
| 1   | A     | 435 | ASN  | CA-CB-CG   | 12.24  | 140.34      | 113.40   |
| 1   | C     | 9   | ASP  | CB-CG-OD2  | -11.91 | 107.58      | 118.30   |
| 1   | B     | 3   | ASN  | O-C-N      | -11.89 | 103.68      | 122.70   |
| 1   | A     | 20  | ALA  | CB-CA-C    | -11.80 | 92.39       | 110.10   |
| 1   | C     | 210 | HIS  | O-C-N      | 11.79  | 141.57      | 122.70   |
| 1   | A     | 284 | THR  | CA-CB-CG2  | -11.79 | 95.90       | 112.40   |
| 1   | C     | 395 | ASP  | CA-CB-CG   | -11.73 | 87.58       | 113.40   |
| 1   | C     | 289 | GLU  | CB-CA-C    | 11.48  | 133.36      | 110.40   |
| 1   | C     | 147 | ASN  | CA-CB-CG   | 11.40  | 138.49      | 113.40   |
| 1   | B     | 374 | VAL  | N-CA-CB    | 11.20  | 136.13      | 111.50   |
| 1   | A     | 92  | ARG  | CG-CD-NE   | -11.02 | 88.66       | 111.80   |
| 1   | D     | 394 | MET  | CB-CG-SD   | 10.98  | 145.35      | 112.40   |
| 1   | C     | 147 | ASN  | OD1-CG-ND2 | -10.97 | 96.67       | 121.90   |
| 1   | C     | 9   | ASP  | CB-CA-C    | 10.90  | 132.21      | 110.40   |
| 1   | A     | 421 | ARG  | CA-CB-CG   | 10.86  | 137.28      | 113.40   |
| 1   | A     | 476 | LYS  | CG-CD-CE   | 10.79  | 144.28      | 111.90   |
| 1   | A     | 202 | ARG  | CD-NE-CZ   | 10.78  | 138.69      | 123.60   |
| 1   | B     | 412 | GLU  | CA-CB-CG   | 10.75  | 137.05      | 113.40   |
| 1   | C     | 483 | ASP  | CB-CA-C    | -10.73 | 88.94       | 110.40   |
| 1   | C     | 289 | GLU  | CA-CB-CG   | 10.71  | 136.97      | 113.40   |
| 1   | B     | 395 | ASP  | CA-CB-CG   | 10.62  | 136.76      | 113.40   |
| 1   | A     | 418 | LEU  | CB-CA-C    | -10.56 | 90.14       | 110.20   |
| 1   | A     | 453 | GLU  | CB-CG-CD   | 10.42  | 142.34      | 114.20   |
| 1   | A     | 456 | LYS  | CA-CB-CG   | 10.25  | 135.95      | 113.40   |
| 1   | A     | 176 | LYS  | CD-CE-NZ   | -10.19 | 88.26       | 111.70   |
| 1   | A     | 42  | THR  | C-N-CA     | 10.17  | 147.13      | 121.70   |
| 1   | A     | 490 | SER  | CA-CB-OG   | 10.12  | 138.54      | 111.20   |
| 1   | C     | 231 | CYS  | CA-CB-SG   | -10.09 | 95.84       | 114.00   |
| 1   | A     | 280 | ILE  | CB-CA-C    | -10.01 | 91.59       | 111.60   |
| 1   | B     | 478 | VAL  | CA-CB-CG2  | 9.94   | 125.80      | 110.90   |
| 1   | A     | 243 | ASN  | CB-CA-C    | -9.87  | 90.67       | 110.40   |
| 1   | C     | 3   | ASN  | CA-C-N     | -9.75  | 95.75       | 117.20   |
| 1   | C     | 210 | HIS  | N-CA-CB    | 9.71   | 128.07      | 110.60   |
| 1   | C     | 501 | GLU  | CB-CG-CD   | 9.57   | 140.04      | 114.20   |
| 1   | A     | 37  | LYS  | CG-CD-CE   | 9.56   | 140.60      | 111.90   |
| 1   | A     | 284 | THR  | CA-CB-OG1  | 9.49   | 128.93      | 109.00   |
| 1   | C     | 414 | GLN  | CB-CA-C    | 9.42   | 129.24      | 110.40   |
| 1   | B     | 416 | SER  | N-CA-CB    | -9.41  | 96.38       | 110.50   |
| 1   | B     | 478 | VAL  | CB-CA-C    | 9.40   | 129.26      | 111.40   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 277 | THR  | CB-CA-C   | 9.38  | 136.93      | 111.60   |
| 1   | C     | 501 | GLU  | N-CA-CB   | -9.27 | 93.91       | 110.60   |
| 1   | C     | 3   | ASN  | CA-C-O    | 8.88  | 138.74      | 120.10   |
| 1   | B     | 478 | VAL  | N-CA-CB   | -8.67 | 92.43       | 111.50   |
| 1   | C     | 454 | GLN  | CB-CA-C   | -8.49 | 93.41       | 110.40   |
| 1   | C     | 210 | HIS  | CA-C-N    | -8.30 | 98.94       | 117.20   |
| 1   | A     | 501 | GLU  | N-CA-CB   | -8.25 | 95.75       | 110.60   |
| 1   | D     | 147 | ASN  | CB-CA-C   | 7.82  | 126.05      | 110.40   |
| 1   | B     | 319 | ARG  | CB-CA-C   | -7.74 | 94.93       | 110.40   |
| 1   | A     | 500 | ASN  | CA-CB-CG  | 7.70  | 130.34      | 113.40   |
| 1   | C     | 309 | LEU  | CB-CG-CD1 | 7.59  | 123.90      | 111.00   |
| 1   | A     | 453 | GLU  | CA-CB-CG  | 7.57  | 130.06      | 113.40   |
| 1   | C     | 309 | LEU  | CB-CG-CD2 | -7.54 | 98.18       | 111.00   |
| 1   | B     | 374 | VAL  | CA-CB-CG1 | -7.53 | 99.60       | 110.90   |
| 1   | D     | 147 | ASN  | CA-CB-CG  | 7.52  | 129.95      | 113.40   |
| 1   | A     | 49  | LEU  | CB-CG-CD1 | -7.49 | 98.27       | 111.00   |
| 1   | A     | 92  | ARG  | CB-CG-CD  | -7.49 | 92.13       | 111.60   |
| 1   | A     | 284 | THR  | CB-CA-C   | -7.44 | 91.50       | 111.60   |
| 1   | C     | 478 | VAL  | CB-CA-C   | 7.29  | 125.25      | 111.40   |
| 1   | B     | 374 | VAL  | CA-CB-CG2 | -7.16 | 100.17      | 110.90   |
| 1   | A     | 280 | ILE  | CA-CB-CG2 | -7.11 | 96.68       | 110.90   |
| 1   | A     | 280 | ILE  | CA-CB-CG1 | 7.10  | 124.49      | 111.00   |
| 1   | A     | 435 | ASN  | N-CA-CB   | -7.06 | 97.89       | 110.60   |
| 1   | C     | 292 | PRO  | C-N-CA    | 6.64  | 138.29      | 121.70   |
| 1   | A     | 395 | ASP  | CB-CA-C   | -6.55 | 97.31       | 110.40   |
| 1   | C     | 74  | HIS  | CA-CB-CG  | 6.54  | 124.72      | 113.60   |
| 1   | C     | 147 | ASN  | CB-CG-OD1 | 6.44  | 134.47      | 121.60   |
| 1   | C     | 202 | ARG  | CD-NE-CZ  | 6.41  | 132.58      | 123.60   |
| 1   | A     | 20  | ALA  | CA-C-N    | -6.41 | 103.11      | 117.20   |
| 1   | C     | 210 | HIS  | CB-CG-ND1 | -6.32 | 107.39      | 123.20   |
| 1   | A     | 361 | HIS  | CB-CA-C   | 6.28  | 122.97      | 110.40   |
| 1   | A     | 176 | LYS  | CG-CD-CE  | 6.19  | 130.46      | 111.90   |
| 1   | A     | 342 | ILE  | CB-CA-C   | -5.94 | 99.72       | 111.60   |
| 1   | B     | 319 | ARG  | N-CA-CB   | 5.93  | 121.27      | 110.60   |
| 1   | A     | 20  | ALA  | CA-C-O    | 5.80  | 132.29      | 120.10   |
| 1   | A     | 229 | VAL  | CB-CA-C   | -5.68 | 100.61      | 111.40   |
| 1   | A     | 43  | VAL  | CA-C-O    | -5.64 | 108.26      | 120.10   |
| 1   | C     | 413 | HIS  | CB-CG-ND1 | -5.57 | 109.29      | 123.20   |
| 1   | A     | 37  | LYS  | CD-CE-NZ  | -5.56 | 98.92       | 111.70   |
| 1   | A     | 342 | ILE  | N-CA-CB   | 5.47  | 123.37      | 110.80   |
| 1   | A     | 500 | ASN  | CB-CA-C   | 5.45  | 121.30      | 110.40   |
| 1   | A     | 54  | VAL  | CB-CA-C   | 5.44  | 121.73      | 111.40   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | C     | 210 | HIS  | CA-CB-CG | 5.42  | 122.81      | 113.60   |
| 1   | D     | 20  | ALA  | N-CA-CB  | -5.39 | 102.55      | 110.10   |
| 1   | C     | 236 | LYS  | CG-CD-CE | 5.21  | 127.54      | 111.90   |
| 1   | A     | 43  | VAL  | N-CA-C   | -5.18 | 97.02       | 111.00   |
| 1   | A     | 43  | VAL  | N-CA-CB  | -5.11 | 100.27      | 111.50   |

All (5) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | A     | 43  | VAL  | CA   |
| 1   | A     | 395 | ASP  | CA   |
| 1   | C     | 147 | ASN  | CA   |
| 1   | C     | 453 | GLU  | CA   |
| 1   | C     | 501 | GLU  | CA   |

All (14) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | A     | 19  | ALA  | Mainchain,Peptide |
| 1   | A     | 42  | THR  | Peptide           |
| 1   | A     | 421 | ARG  | Sidechain         |
| 1   | A     | 43  | VAL  | Mainchain,Peptide |
| 1   | B     | 126 | ARG  | Sidechain         |
| 1   | B     | 3   | ASN  | Mainchain,Peptide |
| 1   | B     | 319 | ARG  | Sidechain         |
| 1   | C     | 147 | ASN  | Sidechain         |
| 1   | C     | 210 | HIS  | Sidechain         |
| 1   | C     | 289 | GLU  | Sidechain         |
| 1   | C     | 292 | PRO  | Peptide           |

## 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     | 4017  | 0        | 3837     | 240     | 0            |
| 1   | B     | 4017  | 0        | 3840     | 343     | 0            |
| 1   | C     | 4017  | 0        | 3839     | 327     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | D     | 4017  | 0        | 3839     | 270     | 0            |
| 2   | A     | 2     | 0        | 0        | 6       | 0            |
| 2   | D     | 2     | 0        | 0        | 0       | 0            |
| 3   | A     | 43    | 0        | 30       | 16      | 0            |
| 3   | B     | 43    | 0        | 30       | 25      | 0            |
| 3   | C     | 43    | 0        | 30       | 26      | 0            |
| 3   | D     | 43    | 0        | 30       | 21      | 0            |
| 4   | A     | 201   | 0        | 0        | 33      | 0            |
| 4   | B     | 195   | 0        | 0        | 33      | 0            |
| 4   | C     | 138   | 0        | 0        | 16      | 0            |
| 4   | D     | 154   | 0        | 0        | 20      | 0            |
| All | All   | 16932 | 0        | 15475    | 1083    | 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 34.

All (1083) 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:A:92:ARG:CD    | 1:A:92:ARG:CG     | 1.87                     | 1.49              |
| 1:C:147:ASN:CG   | 3:C:2002:HEM:HAC  | 1.16                     | 1.45              |
| 1:C:147:ASN:OD1  | 3:C:2002:HEM:CAC  | 1.63                     | 1.42              |
| 1:C:147:ASN:ND2  | 3:C:2002:HEM:HAC  | 1.26                     | 1.40              |
| 1:B:111:ARG:CD   | 3:B:2001:HEM:O1D  | 1.70                     | 1.38              |
| 1:D:111:ARG:CD   | 3:D:2003:HEM:O2D  | 1.69                     | 1.37              |
| 1:C:209:ARG:NH1  | 1:C:267:ALA:HB1   | 1.43                     | 1.34              |
| 1:C:147:ASN:OD1  | 3:C:2002:HEM:C3C  | 1.81                     | 1.33              |
| 1:A:351:GLN:HE22 | 1:C:52:GLN:NE2    | 1.34                     | 1.25              |
| 1:B:384:ASN:HB2  | 4:B:2078:HOH:O    | 1.27                     | 1.23              |
| 1:C:209:ARG:NH1  | 1:C:267:ALA:CB    | 1.99                     | 1.23              |
| 1:D:52:GLN:HB2   | 4:D:3005:HOH:O    | 1.40                     | 1.21              |
| 1:A:351:GLN:NE2  | 1:C:52:GLN:HE21   | 1.39                     | 1.19              |
| 1:C:147:ASN:CG   | 3:C:2002:HEM:CAC  | 2.02                     | 1.18              |
| 1:D:147:ASN:OD1  | 3:D:2003:HEM:CAC  | 1.90                     | 1.18              |
| 1:A:298:LEU:HD21 | 3:A:2000:HEM:HBC1 | 1.19                     | 1.16              |
| 1:C:147:ASN:OD1  | 3:C:2002:HEM:HAC  | 1.27                     | 1.14              |
| 1:B:111:ARG:HD2  | 3:B:2001:HEM:O1D  | 1.40                     | 1.14              |
| 1:B:39:ASN:OD1   | 4:B:2053:HOH:O    | 1.62                     | 1.14              |
| 1:B:111:ARG:HD3  | 3:B:2001:HEM:O1D  | 1.33                     | 1.12              |
| 1:B:3:ASN:O      | 1:B:4:ARG:O       | 1.70                     | 1.09              |
| 1:D:111:ARG:HD3  | 3:D:2003:HEM:O2D  | 1.46                     | 1.08              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:A:3000:CYN:C   | 3:A:2000:HEM:NC   | 2.17                     | 1.08              |
| 1:C:147:ASN:ND2  | 3:C:2002:HEM:CAC  | 2.14                     | 1.07              |
| 1:B:396:ASN:ND2  | 4:B:2120:HOH:O    | 1.86                     | 1.06              |
| 1:D:406:ASN:HD21 | 1:D:410:ALA:HB3   | 1.12                     | 1.05              |
| 1:B:413:HIS:NE2  | 4:B:2134:HOH:O    | 1.86                     | 1.05              |
| 1:A:298:LEU:CD2  | 3:A:2000:HEM:HBC1 | 1.87                     | 1.03              |
| 1:C:209:ARG:CZ   | 1:C:267:ALA:HB2   | 1.87                     | 1.03              |
| 1:B:413:HIS:CD2  | 4:B:2134:HOH:O    | 2.07                     | 1.03              |
| 1:D:111:ARG:HD2  | 3:D:2003:HEM:O2D  | 1.55                     | 1.01              |
| 1:C:190:GLU:HA   | 1:C:438:ASN:HB3   | 1.38                     | 1.01              |
| 1:D:39:ASN:OD1   | 4:D:3021:HOH:O    | 1.78                     | 1.01              |
| 1:C:394:MET:HE2  | 4:C:2137:HOH:O    | 1.62                     | 1.00              |
| 1:A:413:HIS:ND1  | 4:A:3145:HOH:O    | 1.94                     | 1.00              |
| 1:B:19:ALA:HB3   | 1:B:21:GLN:HE21   | 1.25                     | 0.99              |
| 1:D:174:HIS:ND1  | 4:D:3042:HOH:O    | 1.92                     | 0.99              |
| 1:B:78:ALA:HB2   | 1:B:261:LEU:HD12  | 1.41                     | 0.98              |
| 1:A:298:LEU:HD21 | 3:A:2000:HEM:CBC  | 1.94                     | 0.98              |
| 1:B:100:GLU:HB3  | 1:B:104:LYS:HG3   | 1.46                     | 0.97              |
| 1:B:242:LYS:NZ   | 4:B:2095:HOH:O    | 1.89                     | 0.95              |
| 1:B:112:PHE:HA   | 1:B:130:GLY:O     | 1.67                     | 0.93              |
| 1:C:402:ASN:HD22 | 1:C:402:ASN:H     | 1.05                     | 0.93              |
| 1:D:147:ASN:OD1  | 3:D:2003:HEM:HAC  | 1.66                     | 0.93              |
| 1:A:92:ARG:CB    | 1:A:92:ARG:CD     | 2.45                     | 0.93              |
| 1:C:208:HIS:O    | 1:C:209:ARG:HG2   | 1.69                     | 0.92              |
| 1:A:223:ASN:HD21 | 1:A:227:GLU:HB2   | 1.34                     | 0.92              |
| 1:D:223:ASN:HD21 | 1:D:227:GLU:HB3   | 1.36                     | 0.90              |
| 1:A:92:ARG:NE    | 1:A:92:ARG:CG     | 2.35                     | 0.89              |
| 1:A:324:TYR:OH   | 4:A:3179:HOH:O    | 1.89                     | 0.89              |
| 1:A:429:GLN:NE2  | 1:B:421:ARG:HD2   | 1.87                     | 0.88              |
| 1:D:90:ILE:HG21  | 1:D:312:VAL:HG22  | 1.56                     | 0.88              |
| 1:D:406:ASN:ND2  | 1:D:410:ALA:HB3   | 1.87                     | 0.88              |
| 1:A:351:GLN:NE2  | 1:C:52:GLN:NE2    | 2.09                     | 0.88              |
| 1:B:71:ARG:HH11  | 1:B:71:ARG:HG3    | 1.39                     | 0.88              |
| 1:C:209:ARG:NH1  | 1:C:267:ALA:HB2   | 1.85                     | 0.87              |
| 1:C:394:MET:CE   | 4:C:2137:HOH:O    | 2.21                     | 0.87              |
| 1:A:451:ASN:H    | 1:A:454:GLN:HE21  | 1.16                     | 0.87              |
| 1:C:205:PRO:HG2  | 1:C:211:MET:HE2   | 1.57                     | 0.87              |
| 1:D:291:PHE:HE1  | 1:D:293:PHE:HB2   | 1.39                     | 0.86              |
| 1:B:129:ARG:HB2  | 1:B:211:MET:HE1   | 1.57                     | 0.86              |
| 1:C:406:ASN:HD21 | 1:C:410:ALA:HB3   | 1.39                     | 0.85              |
| 1:B:15:LYS:HD2   | 1:D:408:PHE:HA    | 1.57                     | 0.85              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:395:ASP:HB3   | 4:C:2106:HOH:O   | 1.75                     | 0.85              |
| 2:A:3000:CYN:C    | 3:A:2000:HEM:NB  | 2.40                     | 0.84              |
| 1:C:74:HIS:CE1    | 3:C:2002:HEM:C1D | 2.65                     | 0.84              |
| 1:D:190:GLU:HA    | 1:D:438:ASN:HB3  | 1.58                     | 0.84              |
| 1:C:209:ARG:HH11  | 1:C:267:ALA:HB1  | 1.42                     | 0.83              |
| 1:C:151:ILE:HG13  | 1:C:194:GLN:HG2  | 1.60                     | 0.83              |
| 3:B:2001:HEM:HBD2 | 4:B:2179:HOH:O   | 1.78                     | 0.83              |
| 1:B:92:ARG:HD2    | 4:B:2163:HOH:O   | 1.78                     | 0.83              |
| 1:C:129:ARG:CB    | 1:C:211:MET:HE1  | 2.09                     | 0.83              |
| 1:A:223:ASN:ND2   | 1:A:227:GLU:HB2  | 1.92                     | 0.83              |
| 1:C:212:ASP:OD1   | 1:C:236:LYS:HA   | 1.79                     | 0.83              |
| 1:D:170:ASN:ND2   | 1:D:172:GLN:H    | 1.74                     | 0.83              |
| 1:C:413:HIS:CD2   | 4:C:2037:HOH:O   | 2.31                     | 0.82              |
| 1:B:92:ARG:CG     | 4:B:2163:HOH:O   | 2.26                     | 0.82              |
| 1:A:36:ASP:OD2    | 1:A:39:ASN:HB2   | 1.80                     | 0.81              |
| 2:A:3000:CYN:C    | 3:A:2000:HEM:FE  | 1.62                     | 0.81              |
| 1:C:402:ASN:HD22  | 1:C:402:ASN:N    | 1.75                     | 0.81              |
| 1:C:488:TYR:O     | 1:C:492:ILE:HG12 | 1.80                     | 0.81              |
| 2:A:3000:CYN:C    | 3:A:2000:HEM:ND  | 2.43                     | 0.81              |
| 1:C:177:ASP:O     | 1:C:181:VAL:HG23 | 1.80                     | 0.81              |
| 1:C:209:ARG:CZ    | 1:C:267:ALA:CB   | 2.54                     | 0.81              |
| 1:C:146:GLY:O     | 1:C:147:ASN:HB3  | 1.81                     | 0.81              |
| 1:C:334:ASP:OD2   | 4:C:2085:HOH:O   | 1.99                     | 0.80              |
| 1:A:451:ASN:H     | 1:A:454:GLN:NE2  | 1.79                     | 0.80              |
| 1:B:124:THR:HG22  | 1:B:249:ALA:HA   | 1.63                     | 0.80              |
| 1:B:202:ARG:HH21  | 1:B:241:ILE:HD13 | 1.46                     | 0.80              |
| 1:A:391:MET:HE3   | 1:A:393:MET:HE1  | 1.64                     | 0.80              |
| 1:B:444:THR:O     | 1:B:448:LYS:HB3  | 1.80                     | 0.80              |
| 1:C:50:LEU:HD22   | 1:D:48:PRO:HB2   | 1.63                     | 0.79              |
| 1:C:402:ASN:HD21  | 1:D:180:MET:HE1  | 1.46                     | 0.79              |
| 1:B:361:HIS:CD2   | 3:B:2001:HEM:O1A | 2.35                     | 0.79              |
| 1:B:223:ASN:HD21  | 1:B:227:GLU:HB2  | 1.45                     | 0.79              |
| 1:D:333:PHE:CE1   | 3:D:2003:HEM:O1D | 2.35                     | 0.79              |
| 2:A:3000:CYN:C    | 3:A:2000:HEM:NA  | 2.46                     | 0.79              |
| 4:A:3093:HOH:O    | 1:C:22:LYS:HE2   | 1.83                     | 0.79              |
| 1:A:357:TYR:O     | 1:A:361:HIS:HB2  | 1.84                     | 0.78              |
| 1:D:136:TYR:O     | 1:D:379:ARG:HG3  | 1.84                     | 0.78              |
| 1:B:100:GLU:CB    | 1:B:104:LYS:HG3  | 2.14                     | 0.78              |
| 1:B:285:PHE:HD1   | 4:B:2172:HOH:O   | 1.67                     | 0.78              |
| 1:B:372:ILE:HB    | 1:B:375:ASN:HD22 | 1.48                     | 0.78              |
| 1:A:100:GLU:O     | 1:A:101:HIS:HB3  | 1.84                     | 0.78              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:475:LYS:HG2  | 4:A:3100:HOH:O    | 1.83                     | 0.78              |
| 1:D:111:ARG:NE   | 3:D:2003:HEM:O2D  | 2.16                     | 0.78              |
| 1:C:209:ARG:HH12 | 1:C:267:ALA:HB1   | 1.48                     | 0.77              |
| 1:D:111:ARG:CD   | 3:D:2003:HEM:CGD  | 2.61                     | 0.77              |
| 1:C:147:ASN:OD1  | 3:C:2002:HEM:C4C  | 2.38                     | 0.77              |
| 1:B:101:HIS:O    | 1:B:104:LYS:HB2   | 1.85                     | 0.77              |
| 1:B:443:ARG:HD3  | 4:B:2184:HOH:O    | 1.83                     | 0.77              |
| 1:C:147:ASN:HD21 | 3:C:2002:HEM:HAC  | 1.45                     | 0.77              |
| 1:D:111:ARG:HD2  | 3:D:2003:HEM:CGD  | 2.15                     | 0.77              |
| 1:A:12:LYS:NZ    | 4:A:3157:HOH:O    | 2.17                     | 0.76              |
| 1:D:170:ASN:HD22 | 1:D:172:GLN:H     | 1.32                     | 0.76              |
| 1:C:147:ASN:CB   | 3:C:2002:HEM:HAC  | 2.16                     | 0.76              |
| 1:C:123:ASP:OD1  | 4:C:2021:HOH:O    | 2.04                     | 0.76              |
| 1:B:485:HIS:CE1  | 1:B:487:GLU:HG3   | 2.20                     | 0.76              |
| 1:D:223:ASN:ND2  | 1:D:227:GLU:HB3   | 2.00                     | 0.76              |
| 1:B:294:ASN:ND2  | 1:C:46:ARG:HD2    | 2.01                     | 0.76              |
| 1:D:418:LEU:HD23 | 1:D:419:GLU:H     | 1.48                     | 0.75              |
| 1:C:486:PRO:HD3  | 4:C:2140:HOH:O    | 1.86                     | 0.75              |
| 1:A:177:ASP:HB3  | 1:A:180:MET:HB2   | 1.69                     | 0.75              |
| 1:C:402:ASN:H    | 1:C:402:ASN:ND2   | 1.83                     | 0.75              |
| 1:B:393:MET:CE   | 1:D:372:ILE:HA    | 2.15                     | 0.75              |
| 1:B:129:ARG:CB   | 1:B:211:MET:HE1   | 2.17                     | 0.75              |
| 1:A:284:THR:OG1  | 1:A:287:GLU:HG3   | 1.87                     | 0.74              |
| 1:A:485:HIS:HD2  | 1:A:487:GLU:HB3   | 1.51                     | 0.74              |
| 1:B:208:HIS:O    | 1:B:211:MET:HG2   | 1.86                     | 0.74              |
| 1:B:447:LEU:HD21 | 1:B:485:HIS:HD2   | 1.52                     | 0.74              |
| 1:C:450:LEU:HA   | 1:C:454:GLN:HE21  | 1.50                     | 0.74              |
| 1:B:95:LYS:HB3   | 1:B:224:ALA:N     | 2.01                     | 0.74              |
| 1:A:391:MET:CE   | 1:A:393:MET:HE1   | 2.18                     | 0.74              |
| 1:C:402:ASN:HD21 | 1:D:180:MET:CE    | 2.00                     | 0.74              |
| 1:C:147:ASN:N    | 3:C:2002:HEM:HBC1 | 2.02                     | 0.74              |
| 1:B:268:ILE:HB   | 1:B:320:ASN:ND2   | 2.02                     | 0.74              |
| 1:B:217:HIS:NE2  | 3:B:2001:HEM:CBC  | 2.51                     | 0.73              |
| 1:B:205:PRO:HG3  | 1:B:211:MET:HE3   | 1.69                     | 0.73              |
| 1:C:432:ASN:HD22 | 1:C:433:SER:N     | 1.85                     | 0.73              |
| 1:A:186:SER:HB2  | 1:A:476:LYS:HG2   | 1.69                     | 0.73              |
| 1:D:111:ARG:HH11 | 1:D:111:ARG:HG3   | 1.54                     | 0.73              |
| 1:B:92:ARG:CD    | 4:B:2163:HOH:O    | 2.36                     | 0.72              |
| 1:A:51:VAL:HG21  | 1:B:49:LEU:HD23   | 1.71                     | 0.72              |
| 1:D:115:VAL:HB   | 1:D:127:ASP:OD2   | 1.88                     | 0.72              |
| 1:B:479:LYS:O    | 1:B:482:SER:HB2   | 1.89                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:66:GLU:HB3   | 1:D:388:ASP:HB2  | 1.70                     | 0.72              |
| 1:D:97:LYS:HA    | 1:D:100:GLU:HG3  | 1.70                     | 0.72              |
| 1:D:183:ASP:O    | 1:D:187:LEU:HG   | 1.88                     | 0.72              |
| 1:B:428:VAL:O    | 1:B:428:VAL:HG23 | 1.89                     | 0.72              |
| 1:C:78:ALA:HB2   | 1:C:261:LEU:HD22 | 1.70                     | 0.72              |
| 1:B:183:ASP:O    | 1:B:187:LEU:HG   | 1.90                     | 0.71              |
| 1:D:220:LYS:HD2  | 1:D:343:GLU:HB2  | 1.73                     | 0.71              |
| 1:C:209:ARG:O    | 1:C:210:HIS:CG   | 2.44                     | 0.71              |
| 1:C:88:HIS:CD2   | 1:C:311:PRO:HB2  | 2.25                     | 0.71              |
| 1:B:360:THR:OG1  | 1:C:64:ASP:HB3   | 1.91                     | 0.71              |
| 1:C:421:ARG:HD3  | 4:D:3049:HOH:O   | 1.89                     | 0.71              |
| 1:A:188:ARG:O    | 1:A:191:SER:OG   | 2.09                     | 0.71              |
| 1:B:95:LYS:HG3   | 1:B:222:VAL:O    | 1.91                     | 0.70              |
| 1:B:124:THR:CG2  | 1:B:249:ALA:HA   | 2.21                     | 0.70              |
| 1:B:268:ILE:HB   | 1:B:320:ASN:HD21 | 1.57                     | 0.70              |
| 1:C:74:HIS:O     | 1:C:111:ARG:NH2  | 2.25                     | 0.70              |
| 1:C:239:GLN:HE22 | 1:C:275:SER:H    | 1.38                     | 0.70              |
| 1:C:492:ILE:HG22 | 1:C:496:LEU:HD23 | 1.73                     | 0.70              |
| 1:A:487:GLU:O    | 1:A:491:ARG:HG3  | 1.91                     | 0.70              |
| 1:C:197:PHE:O    | 1:C:200:SER:HB3  | 1.91                     | 0.70              |
| 1:C:487:GLU:HA   | 1:C:490:SER:HB3  | 1.73                     | 0.69              |
| 1:D:362:ARG:NH1  | 4:D:3111:HOH:O   | 2.25                     | 0.69              |
| 1:B:320:ASN:OD1  | 4:B:2055:HOH:O   | 2.10                     | 0.69              |
| 1:B:26:LEU:HD12  | 1:D:384:ASN:HA   | 1.73                     | 0.69              |
| 1:B:34:VAL:HG11  | 1:B:37:LYS:HB3   | 1.72                     | 0.69              |
| 1:B:476:LYS:NZ   | 4:B:2168:HOH:O   | 2.20                     | 0.69              |
| 1:B:447:LEU:HD21 | 1:B:485:HIS:CD2  | 2.28                     | 0.68              |
| 1:D:286:SER:O    | 1:D:289:GLU:HB3  | 1.93                     | 0.68              |
| 1:C:205:PRO:HG2  | 1:C:211:MET:CE   | 2.22                     | 0.68              |
| 1:B:254:HIS:HB3  | 1:C:254:HIS:HB3  | 1.75                     | 0.68              |
| 1:A:453:GLU:HG2  | 1:A:457:ARG:HH12 | 1.59                     | 0.68              |
| 1:C:308:PRO:O    | 1:C:310:ILE:HD12 | 1.94                     | 0.68              |
| 1:D:147:ASN:OD1  | 3:D:2003:HEM:C3C | 2.47                     | 0.68              |
| 1:C:129:ARG:HB2  | 1:C:211:MET:HE1  | 1.75                     | 0.68              |
| 1:A:74:HIS:NE2   | 1:A:115:VAL:HG22 | 2.09                     | 0.68              |
| 1:D:291:PHE:HD1  | 1:D:293:PHE:H    | 1.39                     | 0.68              |
| 1:C:154:ILE:HG13 | 1:C:349:MET:HE1  | 1.75                     | 0.68              |
| 1:D:148:ASN:HD22 | 1:D:148:ASN:H    | 1.40                     | 0.68              |
| 1:D:333:PHE:CD1  | 3:D:2003:HEM:O1D | 2.47                     | 0.68              |
| 1:B:368:ASN:O    | 1:B:371:GLN:HB2  | 1.94                     | 0.67              |
| 1:A:376:CYS:SG   | 4:A:3184:HOH:O   | 2.50                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:82:GLY:HA3   | 1:C:316:VAL:O    | 1.93                     | 0.67              |
| 1:C:92:ARG:HD3   | 1:C:92:ARG:H     | 1.59                     | 0.67              |
| 1:A:485:HIS:CD2  | 1:A:487:GLU:HB3  | 2.29                     | 0.67              |
| 1:B:182:TRP:NE1  | 1:B:465:HIS:ND1  | 2.40                     | 0.67              |
| 1:C:248:ASP:HA   | 1:C:251:ARG:NH1  | 2.09                     | 0.67              |
| 1:A:215:GLY:O    | 1:A:216:SER:HB2  | 1.94                     | 0.67              |
| 1:B:413:HIS:ND1  | 1:B:413:HIS:O    | 2.28                     | 0.67              |
| 1:B:496:LEU:O    | 1:B:500:ASN:HB2  | 1.95                     | 0.67              |
| 1:A:71:ARG:HG3   | 1:A:71:ARG:HH11  | 1.60                     | 0.67              |
| 1:B:217:HIS:CD2  | 3:B:2001:HEM:CBC | 2.78                     | 0.67              |
| 1:D:71:ARG:HG3   | 1:D:71:ARG:HH11  | 1.58                     | 0.67              |
| 1:D:12:LYS:O     | 1:D:16:GLU:HG3   | 1.94                     | 0.67              |
| 1:C:191:SER:O    | 1:C:195:VAL:HG23 | 1.95                     | 0.66              |
| 1:B:393:MET:HE2  | 1:D:373:PRO:HD3  | 1.77                     | 0.66              |
| 1:C:162:SER:HB3  | 1:D:404:TYR:H    | 1.60                     | 0.66              |
| 1:A:332:ALA:HB1  | 1:A:361:HIS:CE1  | 2.30                     | 0.66              |
| 1:C:460:GLU:HA   | 1:C:495:LEU:HD13 | 1.76                     | 0.66              |
| 1:A:43:VAL:HG12  | 1:A:50:LEU:HD21  | 1.77                     | 0.66              |
| 1:B:422:THR:HG22 | 1:B:423:HIS:H    | 1.59                     | 0.66              |
| 1:C:115:VAL:HG12 | 1:C:116:ALA:N    | 2.10                     | 0.66              |
| 1:D:291:PHE:CE1  | 1:D:293:PHE:HB2  | 2.26                     | 0.66              |
| 1:B:69:PRO:HD3   | 1:C:69:PRO:HG3   | 1.77                     | 0.66              |
| 1:B:97:LYS:HD3   | 1:B:138:GLU:HB2  | 1.77                     | 0.66              |
| 1:C:210:HIS:CD2  | 1:C:242:LYS:HB3  | 2.31                     | 0.66              |
| 3:B:2001:HEM:CBD | 4:B:2179:HOH:O   | 2.41                     | 0.66              |
| 1:C:74:HIS:CE1   | 3:C:2002:HEM:C2D | 2.84                     | 0.66              |
| 1:C:160:PHE:CE1  | 1:C:164:ILE:HD11 | 2.31                     | 0.66              |
| 1:D:418:LEU:HD23 | 1:D:419:GLU:N    | 2.11                     | 0.66              |
| 1:B:106:THR:HG23 | 1:B:379:ARG:NH2  | 2.10                     | 0.65              |
| 1:B:5:ASP:OD2    | 1:B:7:ALA:HB3    | 1.95                     | 0.65              |
| 1:C:208:HIS:O    | 1:C:209:ARG:CG   | 2.44                     | 0.65              |
| 1:A:49:LEU:HD13  | 1:B:51:VAL:HG11  | 1.79                     | 0.65              |
| 1:B:466:LEU:HD22 | 1:B:474:GLN:HG2  | 1.78                     | 0.65              |
| 1:C:193:HIS:HA   | 1:C:442:VAL:HG22 | 1.79                     | 0.65              |
| 1:D:6:PRO:HD2    | 1:D:266:ASN:OD1  | 1.96                     | 0.65              |
| 3:A:2000:HEM:O2D | 4:A:3016:HOH:O   | 2.15                     | 0.65              |
| 1:B:457:ARG:HH11 | 1:B:457:ARG:HB2  | 1.61                     | 0.65              |
| 1:C:287:GLU:HA   | 1:C:290:ILE:HG12 | 1.77                     | 0.65              |
| 1:D:333:PHE:HE1  | 3:D:2003:HEM:O1D | 1.79                     | 0.65              |
| 1:A:210:HIS:HB3  | 1:A:242:LYS:H    | 1.62                     | 0.65              |
| 1:B:338:MET:HE2  | 1:B:342:ILE:HG22 | 1.78                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:304:HIS:CD2  | 1:C:309:LEU:HD13 | 2.32                     | 0.65              |
| 1:C:450:LEU:HG   | 1:C:454:GLN:HB3  | 1.79                     | 0.65              |
| 1:C:231:CYS:HA   | 1:C:281:GLN:O    | 1.97                     | 0.65              |
| 1:B:135:PHE:HB2  | 1:B:142:TRP:HB3  | 1.79                     | 0.64              |
| 1:D:111:ARG:HD3  | 3:D:2003:HEM:CGD | 2.27                     | 0.64              |
| 1:A:108:ILE:HA   | 1:A:134:LYS:O    | 1.97                     | 0.64              |
| 1:B:124:THR:HG21 | 1:B:252:LEU:HB2  | 1.79                     | 0.64              |
| 1:B:217:HIS:CD2  | 1:B:353:ARG:HH11 | 2.16                     | 0.64              |
| 1:B:5:ASP:HB2    | 1:B:6:PRO:HD2    | 1.79                     | 0.64              |
| 1:D:148:ASN:N    | 1:D:148:ASN:HD22 | 1.95                     | 0.64              |
| 1:B:19:ALA:CB    | 1:B:21:GLN:HE21  | 2.06                     | 0.64              |
| 1:B:457:ARG:NH1  | 1:B:457:ARG:HB2  | 2.11                     | 0.64              |
| 1:C:200:SER:OG   | 1:C:201:ASP:N    | 2.30                     | 0.64              |
| 1:D:294:ASN:HB3  | 1:D:297:ASP:HB2  | 1.80                     | 0.64              |
| 1:D:26:LEU:O     | 1:D:34:VAL:HG22  | 1.97                     | 0.64              |
| 1:A:217:HIS:NE2  | 3:A:2000:HEM:CBC | 2.61                     | 0.64              |
| 1:B:238:ASP:OD1  | 1:B:277:THR:HG22 | 1.98                     | 0.64              |
| 1:A:309:LEU:N    | 1:A:309:LEU:HD22 | 2.13                     | 0.63              |
| 1:A:358:PRO:O    | 1:A:362:ARG:HG3  | 1.98                     | 0.63              |
| 1:D:232:LYS:O    | 1:D:280:ILE:HA   | 1.98                     | 0.63              |
| 1:C:238:ASP:OD2  | 1:C:314:LYS:HE3  | 1.98                     | 0.63              |
| 1:C:492:ILE:HG22 | 1:C:496:LEU:CD2  | 2.27                     | 0.63              |
| 1:A:353:ARG:NH2  | 1:A:357:TYR:OH   | 2.32                     | 0.63              |
| 1:B:261:LEU:HD23 | 1:C:175:LEU:HD23 | 1.81                     | 0.63              |
| 1:C:129:ARG:HG2  | 1:C:211:MET:HE3  | 1.80                     | 0.63              |
| 1:C:436:ASP:O    | 1:C:437:ASP:HB3  | 1.97                     | 0.63              |
| 1:C:209:ARG:HH12 | 1:C:267:ALA:CB   | 2.06                     | 0.63              |
| 1:C:453:GLU:HB3  | 1:C:457:ARG:HH12 | 1.63                     | 0.63              |
| 1:D:310:ILE:HD12 | 1:D:310:ILE:N    | 2.14                     | 0.63              |
| 1:A:309:LEU:H    | 1:A:309:LEU:HD22 | 1.63                     | 0.63              |
| 1:A:3:ASN:N      | 4:A:3165:HOH:O   | 2.32                     | 0.62              |
| 1:D:235:TYR:HA   | 1:D:277:THR:O    | 1.99                     | 0.62              |
| 1:A:406:ASN:HD21 | 1:A:410:ALA:HB3  | 1.64                     | 0.62              |
| 1:A:455:ARG:CZ   | 4:A:3196:HOH:O   | 2.46                     | 0.62              |
| 1:D:189:PRO:HG3  | 1:D:480:ASN:ND2  | 2.14                     | 0.62              |
| 1:D:154:ILE:HG13 | 1:D:349:MET:CE   | 2.29                     | 0.62              |
| 1:A:74:HIS:O     | 1:A:111:ARG:NH2  | 2.33                     | 0.62              |
| 1:C:112:PHE:HA   | 1:C:130:GLY:O    | 2.00                     | 0.62              |
| 1:D:246:VAL:HG22 | 4:D:3141:HOH:O   | 1.98                     | 0.62              |
| 1:B:206:ASP:OD1  | 1:B:244:LEU:HD21 | 1.99                     | 0.62              |
| 1:C:179:ASP:O    | 1:C:183:ASP:HB2  | 2.00                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:97:LYS:HB2   | 4:B:2040:HOH:O   | 1.98                     | 0.62              |
| 1:A:456:LYS:HD3  | 1:A:460:GLU:OE2  | 2.00                     | 0.61              |
| 1:D:148:ASN:ND2  | 1:D:148:ASN:H    | 1.98                     | 0.61              |
| 1:D:239:GLN:HE22 | 1:D:275:SER:H    | 1.47                     | 0.61              |
| 1:A:26:LEU:HD22  | 1:C:385:TYR:HE2  | 1.65                     | 0.61              |
| 1:B:419:GLU:HB2  | 4:B:2022:HOH:O   | 1.99                     | 0.61              |
| 1:C:487:GLU:CG   | 1:C:491:ARG:HD2  | 2.31                     | 0.61              |
| 1:D:135:PHE:HB2  | 1:D:142:TRP:HB3  | 1.81                     | 0.61              |
| 1:A:172:GLN:HE21 | 1:D:322:VAL:HA   | 1.65                     | 0.61              |
| 1:B:97:LYS:HD2   | 1:B:139:ASP:CG   | 2.20                     | 0.61              |
| 1:D:338:MET:HE2  | 1:D:342:ILE:HG22 | 1.82                     | 0.61              |
| 1:D:460:GLU:HA   | 1:D:495:LEU:HD13 | 1.83                     | 0.61              |
| 1:A:92:ARG:CD    | 1:A:92:ARG:HB3   | 2.29                     | 0.61              |
| 1:C:298:LEU:CD2  | 1:C:349:MET:HG2  | 2.31                     | 0.61              |
| 1:D:142:TRP:HA   | 1:D:337:ASN:O    | 2.01                     | 0.61              |
| 1:A:332:ALA:HB1  | 1:A:361:HIS:NE2  | 2.15                     | 0.61              |
| 1:A:50:LEU:HD12  | 1:B:48:PRO:HB2   | 1.83                     | 0.61              |
| 1:C:328:VAL:O    | 1:C:331:LEU:HB2  | 2.01                     | 0.61              |
| 1:C:154:ILE:CG1  | 1:C:349:MET:HE1  | 2.31                     | 0.61              |
| 1:A:496:LEU:O    | 1:A:500:ASN:HB2  | 2.01                     | 0.61              |
| 1:C:129:ARG:HG2  | 1:C:211:MET:CE   | 2.31                     | 0.61              |
| 1:A:336:SER:OG   | 4:A:3181:HOH:O   | 2.16                     | 0.60              |
| 1:B:160:PHE:N    | 1:B:161:PRO:HD2  | 2.16                     | 0.60              |
| 1:C:154:ILE:HG13 | 1:C:349:MET:CE   | 2.30                     | 0.60              |
| 1:C:205:PRO:CG   | 1:C:211:MET:HE2  | 2.30                     | 0.60              |
| 1:B:222:VAL:HG22 | 1:B:228:ALA:HB2  | 1.83                     | 0.60              |
| 1:B:223:ASN:ND2  | 1:B:227:GLU:HB2  | 2.14                     | 0.60              |
| 1:C:193:HIS:CA   | 1:C:442:VAL:HG22 | 2.31                     | 0.60              |
| 1:D:52:GLN:N     | 4:D:3005:HOH:O   | 2.23                     | 0.60              |
| 1:D:90:ILE:HD11  | 1:D:99:PHE:CG    | 2.36                     | 0.60              |
| 1:B:76:LYS:HE3   | 1:B:121:SER:O    | 2.01                     | 0.60              |
| 1:C:350:LEU:O    | 1:C:353:ARG:N    | 2.34                     | 0.60              |
| 1:D:231:CYS:HA   | 1:D:281:GLN:O    | 2.01                     | 0.60              |
| 1:B:94:SER:HB2   | 1:B:221:LEU:HD22 | 1.82                     | 0.60              |
| 1:B:393:MET:HE2  | 1:D:372:ILE:HA   | 1.83                     | 0.60              |
| 1:A:421:ARG:CG   | 1:B:429:GLN:HG2  | 2.32                     | 0.60              |
| 1:B:485:HIS:HE1  | 1:B:487:GLU:HG3  | 1.64                     | 0.60              |
| 1:C:18:ARG:O     | 1:C:21:GLN:HB2   | 2.01                     | 0.60              |
| 1:B:152:PHE:HB3  | 1:B:298:LEU:HD23 | 1.82                     | 0.60              |
| 1:B:454:GLN:HA   | 1:B:457:ARG:NH1  | 2.17                     | 0.60              |
| 4:B:2002:HOH:O   | 1:D:29:GLY:HA3   | 2.02                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:74:HIS:CE1   | 1:A:115:VAL:HG22  | 2.37                     | 0.59              |
| 1:B:145:VAL:HG23 | 4:B:2061:HOH:O    | 2.01                     | 0.59              |
| 1:B:63:PHE:O     | 1:B:66:GLU:HG3    | 2.02                     | 0.59              |
| 1:D:221:LEU:O    | 1:D:228:ALA:HA    | 2.02                     | 0.59              |
| 1:B:90:ILE:O     | 1:B:93:TYR:HB2    | 2.02                     | 0.59              |
| 1:C:251:ARG:HG3  | 1:C:252:LEU:N     | 2.17                     | 0.59              |
| 1:D:145:VAL:HG12 | 3:D:2003:HEM:CMD  | 2.32                     | 0.59              |
| 1:B:12:LYS:O     | 1:B:16:GLU:HG3    | 2.01                     | 0.59              |
| 1:B:447:LEU:CD2  | 1:B:485:HIS:CD2   | 2.85                     | 0.59              |
| 1:D:94:SER:HB2   | 1:D:221:LEU:HD22  | 1.84                     | 0.59              |
| 1:D:338:MET:CE   | 1:D:342:ILE:HG22  | 2.32                     | 0.59              |
| 1:D:293:PHE:HZ   | 1:D:440:THR:HG21  | 1.68                     | 0.59              |
| 1:B:97:LYS:HD2   | 1:B:139:ASP:OD2   | 2.00                     | 0.59              |
| 1:B:217:HIS:NE2  | 3:B:2001:HEM:HBC1 | 2.16                     | 0.59              |
| 1:B:88:HIS:CE1   | 1:B:311:PRO:HB2   | 2.37                     | 0.59              |
| 1:B:4:ARG:HD2    | 1:B:8:SER:HB3     | 1.82                     | 0.59              |
| 1:C:351:GLN:O    | 1:C:354:LEU:HB2   | 2.02                     | 0.59              |
| 1:B:111:ARG:CD   | 3:B:2001:HEM:CGD  | 2.74                     | 0.59              |
| 1:B:393:MET:HE1  | 1:D:372:ILE:HA    | 1.82                     | 0.59              |
| 1:C:298:LEU:HD22 | 1:C:349:MET:HG2   | 1.84                     | 0.59              |
| 1:B:294:ASN:HA   | 1:C:46:ARG:HH12   | 1.66                     | 0.59              |
| 1:B:50:LEU:N     | 1:B:50:LEU:HD22   | 2.18                     | 0.59              |
| 1:C:3:ASN:C      | 1:C:4:ARG:HG3     | 2.23                     | 0.59              |
| 1:D:151:ILE:HD13 | 1:D:193:HIS:CD2   | 2.37                     | 0.59              |
| 1:B:64:ASP:HB3   | 1:C:360:THR:HB    | 1.83                     | 0.59              |
| 1:B:147:ASN:OD1  | 3:B:2001:HEM:C3C  | 2.56                     | 0.59              |
| 1:C:438:ASN:ND2  | 1:C:438:ASN:N     | 2.49                     | 0.59              |
| 1:A:4:ARG:HH22   | 1:D:179:ASP:CG    | 2.06                     | 0.59              |
| 1:B:110:VAL:HA   | 1:B:132:ALA:O     | 2.03                     | 0.59              |
| 1:B:248:ASP:O    | 1:B:252:LEU:HD13  | 2.02                     | 0.59              |
| 1:B:147:ASN:OD1  | 3:B:2001:HEM:CMC  | 2.51                     | 0.58              |
| 1:C:486:PRO:O    | 1:C:490:SER:HB2   | 2.03                     | 0.58              |
| 1:A:17:GLN:HA    | 4:A:3158:HOH:O    | 2.02                     | 0.58              |
| 1:C:173:THR:O    | 1:C:175:LEU:HG    | 2.04                     | 0.58              |
| 1:A:94:SER:HB2   | 1:A:221:LEU:HD22  | 1.86                     | 0.58              |
| 1:B:273:TYR:HB3  | 1:B:317:LEU:O     | 2.04                     | 0.58              |
| 1:C:414:GLN:HE22 | 1:C:417:ALA:HB2   | 1.67                     | 0.58              |
| 1:D:106:THR:HG21 | 1:D:137:THR:HG22  | 1.85                     | 0.58              |
| 1:A:67:ARG:HH21  | 1:D:168:LYS:HE3   | 1.67                     | 0.58              |
| 1:B:422:THR:HG22 | 1:B:423:HIS:N     | 2.18                     | 0.58              |
| 1:B:294:ASN:HB3  | 1:B:297:ASP:HB2   | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:86:VAL:HG12  | 1:B:102:ILE:HD13 | 1.85                     | 0.58              |
| 1:C:130:GLY:HA2  | 1:C:147:ASN:HB2  | 1.85                     | 0.58              |
| 1:C:94:SER:HB2   | 1:C:221:LEU:HD22 | 1.85                     | 0.58              |
| 1:A:357:TYR:HB2  | 1:A:358:PRO:HD3  | 1.85                     | 0.58              |
| 1:B:413:HIS:O    | 1:B:415:PRO:HD3  | 2.04                     | 0.58              |
| 1:C:76:LYS:HE3   | 1:C:121:SER:O    | 2.02                     | 0.58              |
| 1:D:111:ARG:HG3  | 1:D:111:ARG:NH1  | 2.18                     | 0.58              |
| 1:B:456:LYS:O    | 1:B:460:GLU:HG3  | 2.03                     | 0.58              |
| 1:B:64:ASP:HB3   | 1:C:360:THR:CB   | 2.33                     | 0.58              |
| 1:C:74:HIS:NE2   | 3:C:2002:HEM:C1D | 2.72                     | 0.58              |
| 1:C:234:HIS:HB2  | 1:C:279:TYR:HB2  | 1.85                     | 0.58              |
| 1:C:432:ASN:ND2  | 1:C:434:ALA:H    | 2.02                     | 0.58              |
| 1:D:112:PHE:HA   | 1:D:130:GLY:O    | 2.04                     | 0.57              |
| 1:A:18:ARG:NE    | 4:A:3200:HOH:O   | 2.37                     | 0.57              |
| 1:A:358:PRO:HD3  | 4:A:3181:HOH:O   | 2.05                     | 0.57              |
| 1:B:338:MET:CE   | 1:B:342:ILE:HG22 | 2.33                     | 0.57              |
| 1:D:160:PHE:CZ   | 1:D:164:ILE:HD11 | 2.39                     | 0.57              |
| 1:B:358:PRO:HB2  | 1:B:362:ARG:NH1  | 2.19                     | 0.57              |
| 1:C:418:LEU:HD11 | 4:D:3037:HOH:O   | 2.04                     | 0.57              |
| 1:A:253:ALA:HA   | 4:A:3021:HOH:O   | 2.04                     | 0.57              |
| 1:C:415:PRO:O    | 1:C:418:LEU:HB2  | 2.05                     | 0.57              |
| 1:C:492:ILE:O    | 1:C:496:LEU:HD23 | 2.04                     | 0.57              |
| 1:A:84:PHE:O     | 1:A:105:ARG:HA   | 2.05                     | 0.57              |
| 1:C:75:ALA:N     | 4:C:2022:HOH:O   | 2.37                     | 0.57              |
| 1:B:140:GLY:HA3  | 1:D:32:ASN:HD22  | 1.68                     | 0.57              |
| 1:B:358:PRO:HB2  | 1:B:362:ARG:HH12 | 1.70                     | 0.57              |
| 1:A:51:VAL:HG12  | 1:B:51:VAL:HA    | 1.86                     | 0.57              |
| 1:C:110:VAL:HG21 | 1:C:317:LEU:HD11 | 1.85                     | 0.57              |
| 1:D:145:VAL:HB   | 1:D:353:ARG:HH22 | 1.69                     | 0.57              |
| 1:B:336:SER:HB3  | 1:D:54:VAL:HG11  | 1.85                     | 0.57              |
| 1:B:361:HIS:HD2  | 3:B:2001:HEM:O1A | 1.86                     | 0.57              |
| 1:B:393:MET:SD   | 1:D:393:MET:HG3  | 2.45                     | 0.57              |
| 1:C:347:ASP:HB3  | 1:C:350:LEU:CB   | 2.35                     | 0.57              |
| 1:A:319:ARG:NH2  | 4:A:3028:HOH:O   | 2.36                     | 0.57              |
| 1:B:382:VAL:O    | 1:B:382:VAL:HG13 | 2.05                     | 0.57              |
| 1:C:126:ARG:HE   | 1:C:203:GLY:HA3  | 1.70                     | 0.57              |
| 1:A:151:ILE:HG13 | 1:A:194:GLN:HG2  | 1.87                     | 0.57              |
| 1:A:53:ASP:CG    | 1:D:430:ARG:HH22 | 2.08                     | 0.57              |
| 1:B:479:LYS:HE2  | 1:B:483:ASP:OD2  | 2.05                     | 0.57              |
| 1:D:78:ALA:HB2   | 1:D:261:LEU:HG   | 1.86                     | 0.57              |
| 1:A:309:LEU:CD2  | 1:A:309:LEU:H    | 2.17                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:146:GLY:C    | 3:C:2002:HEM:HBC1 | 2.26                     | 0.56              |
| 1:C:485:HIS:CE1  | 1:C:487:GLU:H     | 2.23                     | 0.56              |
| 1:C:190:GLU:HA   | 1:C:438:ASN:CB    | 2.24                     | 0.56              |
| 1:A:217:HIS:CE1  | 3:A:2000:HEM:CBC  | 2.88                     | 0.56              |
| 1:B:186:SER:OG   | 1:B:476:LYS:HG2   | 2.06                     | 0.56              |
| 1:C:251:ARG:O    | 1:C:255:GLU:HG3   | 2.05                     | 0.56              |
| 1:C:347:ASP:HB3  | 1:C:350:LEU:HB3   | 1.87                     | 0.56              |
| 1:D:108:ILE:HA   | 1:D:134:LYS:O     | 2.05                     | 0.56              |
| 1:B:111:ARG:HD2  | 3:B:2001:HEM:CGD  | 2.29                     | 0.56              |
| 1:B:106:THR:HG23 | 1:B:379:ARG:HH21  | 1.67                     | 0.56              |
| 1:C:146:GLY:C    | 3:C:2002:HEM:CBC  | 2.73                     | 0.56              |
| 1:C:437:ASP:C    | 1:C:438:ASN:HD22  | 2.09                     | 0.56              |
| 1:B:62:HIS:HE1   | 1:D:368:ASN:ND2   | 2.02                     | 0.56              |
| 1:B:278:LEU:O    | 1:B:312:VAL:HG13  | 2.05                     | 0.56              |
| 1:B:17:GLN:C     | 1:B:19:ALA:H      | 2.09                     | 0.56              |
| 1:C:147:ASN:HD21 | 3:C:2002:HEM:CAC  | 2.05                     | 0.56              |
| 1:B:62:HIS:HE1   | 1:D:368:ASN:HD21  | 1.54                     | 0.56              |
| 1:A:394:MET:HG3  | 4:A:3187:HOH:O    | 2.05                     | 0.56              |
| 1:C:438:ASN:N    | 1:C:438:ASN:HD22  | 2.03                     | 0.56              |
| 1:A:124:THR:HA   | 4:A:3171:HOH:O    | 2.04                     | 0.56              |
| 1:B:202:ARG:HH21 | 1:B:241:ILE:CD1   | 2.16                     | 0.56              |
| 1:C:234:HIS:O    | 1:C:279:TYR:N     | 2.32                     | 0.56              |
| 1:A:277:THR:OG1  | 1:A:314:LYS:NZ    | 2.39                     | 0.56              |
| 1:A:298:LEU:CD2  | 3:A:2000:HEM:CBC  | 2.67                     | 0.56              |
| 1:B:6:PRO:HG2    | 1:B:266:ASN:OD1   | 2.06                     | 0.56              |
| 1:A:355:PHE:CZ   | 1:D:57:THR:HG23   | 2.41                     | 0.55              |
| 1:B:349:MET:SD   | 3:B:2001:HEM:HBB1 | 2.46                     | 0.55              |
| 1:A:430:ARG:NE   | 1:B:419:GLU:OE1   | 2.39                     | 0.55              |
| 1:C:14:TRP:O     | 1:C:18:ARG:HB2    | 2.06                     | 0.55              |
| 1:D:95:LYS:HG2   | 1:D:222:VAL:O     | 2.06                     | 0.55              |
| 1:B:332:ALA:HB1  | 1:B:361:HIS:CE1   | 2.41                     | 0.55              |
| 1:B:269:ALA:C    | 1:B:271:GLY:H     | 2.09                     | 0.55              |
| 1:D:187:LEU:O    | 1:D:188:ARG:HD2   | 2.06                     | 0.55              |
| 1:C:74:HIS:CE1   | 3:C:2002:HEM:CHD  | 2.90                     | 0.55              |
| 1:C:377:PRO:HG2  | 1:C:382:VAL:CG2   | 2.36                     | 0.55              |
| 1:C:74:HIS:CD2   | 3:C:2002:HEM:C4D  | 2.95                     | 0.55              |
| 1:A:13:HIS:O     | 1:A:17:GLN:HB2    | 2.07                     | 0.55              |
| 1:C:61:ALA:O     | 1:C:65:ARG:HG3    | 2.07                     | 0.55              |
| 1:D:43:VAL:CG1   | 1:D:48:PRO:HD2    | 2.37                     | 0.55              |
| 1:C:451:ASN:O    | 1:C:454:GLN:HB2   | 2.06                     | 0.55              |
| 1:D:110:VAL:HG21 | 1:D:317:LEU:HD21  | 1.89                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:298:LEU:CD2  | 1:D:349:MET:HG3   | 2.37                     | 0.55              |
| 1:D:140:GLY:H    | 1:D:380:ALA:HB2   | 1.71                     | 0.55              |
| 1:D:499:TYR:C    | 1:D:501:GLU:H     | 2.09                     | 0.55              |
| 1:A:166:SER:HA   | 1:A:180:MET:HE2   | 1.89                     | 0.55              |
| 1:B:220:LYS:HD3  | 1:B:228:ALA:HB1   | 1.89                     | 0.55              |
| 1:D:145:VAL:HG12 | 3:D:2003:HEM:C2D  | 2.42                     | 0.55              |
| 1:A:451:ASN:N    | 1:A:454:GLN:HE21  | 1.96                     | 0.55              |
| 1:B:235:TYR:CD1  | 1:B:235:TYR:N     | 2.74                     | 0.55              |
| 1:C:485:HIS:ND1  | 1:C:485:HIS:C     | 2.60                     | 0.55              |
| 1:A:323:ASN:HD21 | 1:C:396:ASN:HD22  | 1.53                     | 0.55              |
| 1:C:112:PHE:CG   | 1:C:208:HIS:HB3   | 2.42                     | 0.55              |
| 1:C:247:GLU:HG3  | 1:C:248:ASP:N     | 2.22                     | 0.55              |
| 1:C:413:HIS:C    | 1:C:413:HIS:ND1   | 2.60                     | 0.55              |
| 1:B:221:LEU:O    | 1:B:228:ALA:HA    | 2.07                     | 0.54              |
| 1:B:277:THR:HG21 | 4:B:2026:HOH:O    | 2.07                     | 0.54              |
| 1:A:408:PHE:HA   | 1:C:15:LYS:HD2    | 1.89                     | 0.54              |
| 1:D:332:ALA:HB1  | 1:D:361:HIS:CE1   | 2.41                     | 0.54              |
| 1:B:26:LEU:CD1   | 1:D:384:ASN:HA    | 2.37                     | 0.54              |
| 1:A:71:ARG:HG3   | 4:A:3007:HOH:O    | 2.06                     | 0.54              |
| 1:B:24:ASP:O     | 1:D:411:PRO:HA    | 2.07                     | 0.54              |
| 1:B:232:LYS:O    | 1:B:280:ILE:HA    | 2.07                     | 0.54              |
| 1:A:251:ARG:O    | 1:A:255:GLU:HG3   | 2.07                     | 0.54              |
| 1:A:67:ARG:CZ    | 1:D:72:VAL:HG23   | 2.38                     | 0.54              |
| 1:B:353:ARG:NH1  | 3:B:2001:HEM:HBC2 | 2.22                     | 0.54              |
| 1:A:190:GLU:HA   | 1:A:438:ASN:HB3   | 1.88                     | 0.54              |
| 1:B:168:LYS:NZ   | 1:C:67:ARG:HH21   | 2.04                     | 0.54              |
| 1:B:367:PRO:HG2  | 1:B:390:PRO:CG    | 2.38                     | 0.54              |
| 1:A:387:ARG:O    | 1:C:66:GLU:HG2    | 2.07                     | 0.54              |
| 1:D:18:ARG:O     | 1:D:19:ALA:HB3    | 2.08                     | 0.54              |
| 1:A:106:THR:HG23 | 1:A:379:ARG:NH2   | 2.22                     | 0.54              |
| 1:A:414:GLN:O    | 1:C:35:GLY:HA2    | 2.07                     | 0.54              |
| 1:A:4:ARG:HB2    | 1:A:8:SER:HB2     | 1.89                     | 0.54              |
| 1:D:381:ARG:HG2  | 1:D:381:ARG:HH11  | 1.73                     | 0.54              |
| 1:B:279:TYR:HB3  | 1:B:309:LEU:HB3   | 1.89                     | 0.54              |
| 1:B:37:LYS:O     | 1:B:37:LYS:HG3    | 2.08                     | 0.54              |
| 1:A:367:PRO:HG3  | 1:C:65:ARG:HD3    | 1.90                     | 0.53              |
| 1:B:202:ARG:NH2  | 1:B:241:ILE:HD13  | 2.19                     | 0.53              |
| 1:A:23:PRO:HB2   | 1:C:412:GLU:CG    | 2.38                     | 0.53              |
| 1:B:442:VAL:HG12 | 1:B:484:VAL:HG11  | 1.89                     | 0.53              |
| 1:B:71:ARG:HG3   | 1:B:71:ARG:NH1    | 2.16                     | 0.53              |
| 1:C:126:ARG:HD2  | 1:C:198:LEU:HG    | 1.89                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:52:GLN:O     | 1:C:54:VAL:HG13   | 2.08                     | 0.53              |
| 1:B:148:ASN:HB3  | 1:B:211:MET:HE2   | 1.89                     | 0.53              |
| 1:A:499:TYR:O    | 1:A:501:GLU:N     | 2.35                     | 0.53              |
| 1:C:328:VAL:HA   | 1:C:331:LEU:HD12  | 1.90                     | 0.53              |
| 1:A:65:ARG:HG3   | 1:A:65:ARG:HH11   | 1.74                     | 0.53              |
| 1:B:261:LEU:HD23 | 1:C:175:LEU:CD2   | 2.37                     | 0.53              |
| 1:A:353:ARG:HG3  | 3:A:2000:HEM:HBB2 | 1.90                     | 0.53              |
| 1:B:452:GLU:N    | 1:B:455:ARG:NH2   | 2.57                     | 0.53              |
| 1:C:160:PHE:CZ   | 1:C:164:ILE:HD11  | 2.44                     | 0.53              |
| 1:A:39:ASN:C     | 1:D:158:LEU:HD12  | 2.29                     | 0.53              |
| 1:B:154:ILE:O    | 1:B:349:MET:HE2   | 2.08                     | 0.53              |
| 1:B:41:LEU:HB2   | 1:B:53:ASP:HB2    | 1.91                     | 0.53              |
| 1:C:252:LEU:HA   | 1:C:255:GLU:HB2   | 1.90                     | 0.53              |
| 1:C:297:ASP:OD1  | 1:C:299:THR:N     | 2.41                     | 0.53              |
| 1:D:191:SER:O    | 1:D:195:VAL:HG23  | 2.08                     | 0.53              |
| 1:A:166:SER:HA   | 1:A:180:MET:CE    | 2.38                     | 0.53              |
| 1:A:479:LYS:O    | 1:A:479:LYS:HD2   | 2.08                     | 0.53              |
| 1:B:345:SER:HB2  | 1:B:346:PRO:HD2   | 1.91                     | 0.53              |
| 1:D:298:LEU:HD23 | 1:D:349:MET:HG3   | 1.91                     | 0.53              |
| 1:A:101:HIS:CE1  | 1:A:104:LYS:HB2   | 2.44                     | 0.53              |
| 1:A:450:LEU:HA   | 1:A:454:GLN:NE2   | 2.23                     | 0.53              |
| 1:B:69:PRO:O     | 1:B:364:ARG:HG3   | 2.08                     | 0.53              |
| 1:C:147:ASN:CB   | 3:C:2002:HEM:CAC  | 2.80                     | 0.53              |
| 1:A:195:VAL:O    | 1:A:199:PHE:HD1   | 1.92                     | 0.53              |
| 1:A:353:ARG:CG   | 3:A:2000:HEM:HBB2 | 2.39                     | 0.53              |
| 1:B:206:ASP:OD2  | 1:B:242:LYS:HD2   | 2.10                     | 0.53              |
| 1:C:13:HIS:O     | 1:C:17:GLN:HG2    | 2.09                     | 0.53              |
| 1:C:235:TYR:HA   | 1:C:277:THR:O     | 2.09                     | 0.53              |
| 1:D:378:TYR:CE1  | 1:D:379:ARG:HG2   | 2.45                     | 0.53              |
| 1:B:439:VAL:O    | 1:B:442:VAL:HB    | 2.08                     | 0.52              |
| 1:C:246:VAL:O    | 1:C:250:ALA:HB2   | 2.09                     | 0.52              |
| 1:C:279:TYR:HA   | 1:C:310:ILE:O     | 2.08                     | 0.52              |
| 1:D:33:PRO:HG3   | 4:D:3045:HOH:O    | 2.08                     | 0.52              |
| 1:B:65:ARG:HA    | 1:C:363:HIS:CD2   | 2.45                     | 0.52              |
| 1:D:378:TYR:CD1  | 1:D:379:ARG:HG2   | 2.44                     | 0.52              |
| 1:B:360:THR:HG21 | 4:B:2003:HOH:O    | 2.09                     | 0.52              |
| 1:A:308:PRO:HD2  | 4:A:3013:HOH:O    | 2.09                     | 0.52              |
| 1:B:83:TYR:CA    | 1:B:108:ILE:HG12  | 2.38                     | 0.52              |
| 1:C:177:ASP:OD1  | 1:C:179:ASP:HB2   | 2.09                     | 0.52              |
| 1:D:293:PHE:O    | 1:D:295:PRO:HD3   | 2.10                     | 0.52              |
| 1:C:421:ARG:HD2  | 1:D:429:GLN:CB    | 2.40                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:280:ILE:CD1  | 1:D:310:ILE:HB   | 2.40                     | 0.52              |
| 1:C:332:ALA:HB1  | 1:C:361:HIS:CE1  | 2.45                     | 0.52              |
| 1:C:413:HIS:CE1  | 4:C:2018:HOH:O   | 2.62                     | 0.52              |
| 1:C:442:VAL:HG12 | 1:C:484:VAL:HG11 | 1.91                     | 0.52              |
| 1:D:309:LEU:HD12 | 1:D:309:LEU:N    | 2.24                     | 0.52              |
| 1:A:343:GLU:HB3  | 1:A:344:PRO:HD2  | 1.91                     | 0.52              |
| 1:B:26:LEU:HD21  | 1:B:37:LYS:CD    | 2.40                     | 0.52              |
| 1:C:160:PHE:CD1  | 3:C:2002:HEM:HAB | 2.45                     | 0.52              |
| 1:C:213:GLY:HA3  | 1:C:235:TYR:CE2  | 2.45                     | 0.52              |
| 1:C:131:PHE:CD1  | 1:C:235:TYR:HE2  | 2.27                     | 0.52              |
| 1:D:154:ILE:HG13 | 1:D:349:MET:HE1  | 1.90                     | 0.52              |
| 1:A:393:MET:SD   | 1:C:393:MET:HG3  | 2.50                     | 0.52              |
| 1:B:115:VAL:HG21 | 1:B:128:PRO:HD2  | 1.91                     | 0.52              |
| 1:C:381:ARG:HG3  | 1:C:381:ARG:O    | 2.09                     | 0.52              |
| 1:D:193:HIS:HE1  | 4:D:3028:HOH:O   | 1.93                     | 0.52              |
| 1:A:235:TYR:HA   | 1:A:277:THR:O    | 2.10                     | 0.52              |
| 1:A:487:GLU:CD   | 1:A:491:ARG:HD2  | 2.29                     | 0.52              |
| 1:B:491:ARG:O    | 1:B:495:LEU:HD23 | 2.10                     | 0.52              |
| 1:C:303:PRO:C    | 1:C:305:GLY:N    | 2.62                     | 0.52              |
| 1:D:22:LYS:HE3   | 1:D:22:LYS:HA    | 1.90                     | 0.52              |
| 1:D:67:ARG:N     | 4:D:3004:HOH:O   | 2.21                     | 0.52              |
| 1:D:155:ARG:NH1  | 1:D:299:THR:OG1  | 2.42                     | 0.52              |
| 1:A:343:GLU:HB3  | 1:A:344:PRO:CD   | 2.40                     | 0.51              |
| 1:B:81:PHE:CD1   | 1:B:81:PHE:N     | 2.77                     | 0.51              |
| 1:B:205:PRO:HG3  | 1:B:211:MET:CE   | 2.39                     | 0.51              |
| 1:B:252:LEU:N    | 1:B:252:LEU:HD12 | 2.25                     | 0.51              |
| 1:D:290:ILE:O    | 1:D:291:PHE:C    | 2.48                     | 0.51              |
| 1:B:78:ALA:HB2   | 1:B:261:LEU:CD1  | 2.29                     | 0.51              |
| 1:D:223:ASN:HD21 | 1:D:227:GLU:CB   | 2.16                     | 0.51              |
| 1:D:437:ASP:OD2  | 1:D:440:THR:HB   | 2.10                     | 0.51              |
| 1:A:168:LYS:HD3  | 4:A:3162:HOH:O   | 2.09                     | 0.51              |
| 1:A:358:PRO:HB2  | 1:A:362:ARG:NH1  | 2.25                     | 0.51              |
| 1:A:492:ILE:O    | 1:A:496:LEU:HD13 | 2.11                     | 0.51              |
| 1:B:43:VAL:O     | 1:B:47:GLY:HA3   | 2.11                     | 0.51              |
| 1:C:218:THR:O    | 1:C:345:SER:HB3  | 2.10                     | 0.51              |
| 1:C:303:PRO:C    | 1:C:305:GLY:H    | 2.14                     | 0.51              |
| 1:D:335:PRO:CD   | 1:D:357:TYR:CG   | 2.93                     | 0.51              |
| 1:B:34:VAL:HG13  | 1:B:55:VAL:HG11  | 1.92                     | 0.51              |
| 1:A:323:ASN:ND2  | 1:C:396:ASN:HD22 | 2.09                     | 0.51              |
| 1:A:23:PRO:HB2   | 1:C:412:GLU:HG2  | 1.91                     | 0.51              |
| 1:A:290:ILE:C    | 1:A:290:ILE:HD12 | 2.31                     | 0.51              |

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| Atom-1          | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 1:A:501:GLU:OE1 | 1:A:501:GLU:CA    | 2.59                     | 0.51              |
| 1:A:50:LEU:HD13 | 1:B:50:LEU:HD13   | 1.92                     | 0.51              |
| 1:B:88:HIS:HB2  | 1:B:312:VAL:HA    | 1.93                     | 0.51              |
| 1:B:428:VAL:O   | 1:B:428:VAL:CG2   | 2.57                     | 0.51              |
| 1:B:92:ARG:HG3  | 4:B:2163:HOH:O    | 2.04                     | 0.51              |
| 1:C:234:HIS:O   | 1:C:278:LEU:HD12  | 2.11                     | 0.51              |
| 1:C:395:ASP:CB  | 4:C:2106:HOH:O    | 2.47                     | 0.51              |
| 1:A:347:ASP:HB3 | 1:A:350:LEU:HB3   | 1.92                     | 0.51              |
| 1:B:148:ASN:CB  | 1:B:211:MET:HE2   | 2.41                     | 0.51              |
| 1:B:217:HIS:CD2 | 3:B:2001:HEM:HBC2 | 2.45                     | 0.51              |
| 1:C:22:LYS:HD3  | 1:C:23:PRO:CD     | 2.41                     | 0.51              |
| 1:D:221:LEU:HB2 | 1:D:229:VAL:CG2   | 2.41                     | 0.51              |
| 1:D:301:VAL:O   | 1:D:303:PRO:HD3   | 2.11                     | 0.51              |
| 1:A:4:ARG:HD3   | 1:A:8:SER:HB3     | 1.93                     | 0.51              |
| 1:B:43:VAL:CG1  | 1:B:48:PRO:HD2    | 2.41                     | 0.51              |
| 1:C:97:LYS:HD2  | 1:C:138:GLU:HB2   | 1.92                     | 0.51              |
| 1:D:445:PHE:HA  | 1:D:449:VAL:CG2   | 2.41                     | 0.51              |
| 1:A:498:LYS:O   | 1:A:499:TYR:C     | 2.49                     | 0.50              |
| 1:D:206:ASP:OD2 | 1:D:242:LYS:HE3   | 2.11                     | 0.50              |
| 1:A:45:PRO:HD3  | 1:D:431:PHE:CZ    | 2.46                     | 0.50              |
| 1:A:326:ALA:HB2 | 1:C:396:ASN:HB2   | 1.93                     | 0.50              |
| 1:A:485:HIS:HB3 | 1:A:488:TYR:HB2   | 1.94                     | 0.50              |
| 1:B:74:HIS:ND1  | 1:B:114:THR:O     | 2.44                     | 0.50              |
| 1:B:395:ASP:HA  | 4:B:2080:HOH:O    | 2.10                     | 0.50              |
| 1:A:48:PRO:HB2  | 1:B:50:LEU:HD12   | 1.93                     | 0.50              |
| 1:A:143:ASP:HB2 | 1:A:334:ASP:O     | 2.12                     | 0.50              |
| 1:C:182:TRP:O   | 1:C:183:ASP:C     | 2.49                     | 0.50              |
| 1:D:71:ARG:HG3  | 1:D:71:ARG:NH1    | 2.24                     | 0.50              |
| 1:B:83:TYR:HA   | 1:B:108:ILE:HG12  | 1.93                     | 0.50              |
| 1:B:81:PHE:HZ   | 1:B:327:GLU:HB3   | 1.75                     | 0.50              |
| 1:D:19:ALA:O    | 4:D:3145:HOH:O    | 2.19                     | 0.50              |
| 1:A:71:ARG:NH1  | 4:A:3007:HOH:O    | 2.32                     | 0.50              |
| 1:D:234:HIS:O   | 1:D:278:LEU:HD12  | 2.11                     | 0.50              |
| 1:D:71:ARG:NH2  | 1:D:329:GLU:O     | 2.43                     | 0.50              |
| 1:A:160:PHE:HB3 | 1:A:161:PRO:HD3   | 1.92                     | 0.50              |
| 1:A:433:SER:HB3 | 4:A:3030:HOH:O    | 2.10                     | 0.50              |
| 1:B:360:THR:OG1 | 1:C:64:ASP:CB     | 2.60                     | 0.50              |
| 1:B:98:VAL:HG13 | 1:B:99:PHE:CD1    | 2.46                     | 0.50              |
| 1:B:4:ARG:NH2   | 1:C:470:GLN:HG3   | 2.26                     | 0.50              |
| 1:C:472:PHE:C   | 1:C:472:PHE:CD1   | 2.85                     | 0.50              |
| 1:B:374:VAL:CG2 | 4:B:2178:HOH:O    | 2.58                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:35:GLY:HA2   | 1:C:414:GLN:O     | 2.11                     | 0.50              |
| 1:A:423:HIS:HA   | 1:B:427:ASP:HA    | 1.93                     | 0.50              |
| 1:B:135:PHE:O    | 1:B:137:THR:HG23  | 2.11                     | 0.50              |
| 1:C:338:MET:HE3  | 1:C:344:PRO:HD3   | 1.94                     | 0.50              |
| 1:C:418:LEU:HD23 | 1:C:419:GLU:H     | 1.76                     | 0.50              |
| 1:D:193:HIS:CE1  | 4:D:3028:HOH:O    | 2.64                     | 0.50              |
| 1:A:355:PHE:CE2  | 1:D:57:THR:HG23   | 2.46                     | 0.50              |
| 1:B:160:PHE:CE1  | 1:B:164:ILE:HD11  | 2.47                     | 0.50              |
| 1:A:87:THR:HG23  | 1:A:313:GLY:HA2   | 1.93                     | 0.49              |
| 1:A:82:GLY:HA3   | 1:A:316:VAL:O     | 2.12                     | 0.49              |
| 1:C:126:ARG:O    | 1:C:127:ASP:HB2   | 2.12                     | 0.49              |
| 1:C:165:HIS:HB3  | 1:D:402:ASN:OD1   | 2.13                     | 0.49              |
| 1:C:223:ASN:C    | 1:C:225:ASP:H     | 2.15                     | 0.49              |
| 1:A:258:ASP:HB3  | 1:A:261:LEU:HD12  | 1.92                     | 0.49              |
| 1:C:353:ARG:HG3  | 3:C:2002:HEM:HBB2 | 1.94                     | 0.49              |
| 1:C:303:PRO:O    | 1:C:305:GLY:N     | 2.45                     | 0.49              |
| 1:C:451:ASN:ND2  | 1:C:453:GLU:H     | 2.10                     | 0.49              |
| 1:D:170:ASN:HD22 | 1:D:173:THR:H     | 1.58                     | 0.49              |
| 1:D:270:THR:O    | 1:D:272:ASN:N     | 2.45                     | 0.49              |
| 1:D:285:PHE:HD1  | 1:D:285:PHE:H     | 1.58                     | 0.49              |
| 1:A:384:ASN:HA   | 1:C:26:LEU:HD13   | 1.94                     | 0.49              |
| 1:B:360:THR:CG2  | 4:B:2003:HOH:O    | 2.61                     | 0.49              |
| 1:C:290:ILE:O    | 1:C:291:PHE:C     | 2.49                     | 0.49              |
| 1:A:66:GLU:HG2   | 1:C:387:ARG:O     | 2.13                     | 0.49              |
| 1:D:129:ARG:O    | 1:D:147:ASN:HB3   | 2.12                     | 0.49              |
| 1:D:142:TRP:CZ2  | 1:D:342:ILE:HD13  | 2.48                     | 0.49              |
| 1:D:189:PRO:HG3  | 1:D:480:ASN:HD21  | 1.77                     | 0.49              |
| 1:B:367:PRO:HD2  | 4:B:2005:HOH:O    | 2.13                     | 0.49              |
| 1:D:372:ILE:HB   | 1:D:375:ASN:HD22  | 1.76                     | 0.49              |
| 1:A:291:PHE:HD2  | 1:A:293:PHE:O     | 1.96                     | 0.49              |
| 1:B:90:ILE:O     | 1:B:93:TYR:N      | 2.41                     | 0.49              |
| 1:B:11:MET:CE    | 1:C:180:MET:HG2   | 2.43                     | 0.49              |
| 1:B:294:ASN:HA   | 1:C:46:ARG:NH1    | 2.27                     | 0.49              |
| 1:C:83:TYR:CD1   | 1:C:105:ARG:HD3   | 2.47                     | 0.49              |
| 1:B:163:PHE:O    | 1:B:166:SER:HB3   | 2.13                     | 0.49              |
| 1:D:222:VAL:HG22 | 1:D:228:ALA:HB2   | 1.95                     | 0.49              |
| 1:D:281:GLN:O    | 1:D:302:TRP:HZ3   | 1.95                     | 0.49              |
| 1:A:212:ASP:OD1  | 1:A:236:LYS:HA    | 2.13                     | 0.49              |
| 1:A:460:GLU:HA   | 1:A:495:LEU:HD13  | 1.95                     | 0.49              |
| 1:C:338:MET:CE   | 1:C:344:PRO:HD3   | 2.43                     | 0.49              |
| 1:C:474:GLN:NE2  | 1:C:496:LEU:HD12  | 2.27                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:116:ALA:O    | 1:D:168:LYS:NZ   | 2.45                     | 0.49              |
| 1:A:14:TRP:CZ3   | 1:A:18:ARG:HD2   | 2.48                     | 0.49              |
| 1:A:231:CYS:HB2  | 1:A:281:GLN:O    | 2.12                     | 0.49              |
| 1:B:71:ARG:HH11  | 1:B:71:ARG:CG    | 2.15                     | 0.49              |
| 1:B:168:LYS:HZ1  | 1:C:67:ARG:HH21  | 1.61                     | 0.49              |
| 1:D:148:ASN:N    | 1:D:148:ASN:ND2  | 2.60                     | 0.49              |
| 1:A:395:ASP:OD1  | 1:C:327:GLU:OE2  | 2.31                     | 0.49              |
| 1:B:125:VAL:HG22 | 1:B:126:ARG:N    | 2.27                     | 0.49              |
| 1:B:327:GLU:OE2  | 4:B:2082:HOH:O   | 2.20                     | 0.49              |
| 1:C:86:VAL:HG12  | 1:C:102:ILE:HA   | 1.94                     | 0.49              |
| 1:C:142:TRP:HB2  | 1:C:339:PRO:CD   | 2.43                     | 0.49              |
| 1:C:439:VAL:O    | 1:C:440:THR:C    | 2.50                     | 0.49              |
| 1:D:193:HIS:HA   | 1:D:442:VAL:HG22 | 1.95                     | 0.49              |
| 1:A:67:ARG:NH2   | 1:D:72:VAL:HG23  | 2.28                     | 0.49              |
| 1:B:117:GLY:O    | 4:B:2160:HOH:O   | 2.20                     | 0.48              |
| 1:C:22:LYS:HD3   | 1:C:23:PRO:HD2   | 1.94                     | 0.48              |
| 1:C:74:HIS:HA    | 1:C:114:THR:O    | 2.13                     | 0.48              |
| 1:D:72:VAL:O     | 1:D:168:LYS:HE3  | 2.13                     | 0.48              |
| 1:C:78:ALA:HB2   | 1:C:261:LEU:CD2  | 2.40                     | 0.48              |
| 1:D:306:ASP:O    | 1:D:308:PRO:HD3  | 2.13                     | 0.48              |
| 1:B:10:GLN:HE21  | 1:C:172:GLN:NE2  | 2.12                     | 0.48              |
| 1:A:126:ARG:HA   | 1:A:204:ILE:HG12 | 1.93                     | 0.48              |
| 1:B:53:ASP:OD2   | 1:C:430:ARG:NH1  | 2.41                     | 0.48              |
| 1:C:350:LEU:O    | 1:C:351:GLN:C    | 2.51                     | 0.48              |
| 1:D:239:GLN:NE2  | 1:D:275:SER:H    | 2.10                     | 0.48              |
| 1:D:142:TRP:CE2  | 1:D:342:ILE:HD13 | 2.48                     | 0.48              |
| 1:D:471:LEU:HG   | 4:D:3023:HOH:O   | 2.14                     | 0.48              |
| 1:A:335:PRO:HD2  | 4:A:3181:HOH:O   | 2.13                     | 0.48              |
| 1:A:348:LYS:NZ   | 4:D:3021:HOH:O   | 2.47                     | 0.48              |
| 1:A:349:MET:O    | 1:A:353:ARG:HG3  | 2.12                     | 0.48              |
| 1:A:43:VAL:CG1   | 1:A:50:LEU:HD21  | 2.43                     | 0.48              |
| 1:B:155:ARG:HD3  | 1:B:297:ASP:OD1  | 2.13                     | 0.48              |
| 1:C:485:HIS:CE1  | 1:C:487:GLU:HB3  | 2.49                     | 0.48              |
| 1:D:74:HIS:CE1   | 1:D:115:VAL:HG22 | 2.49                     | 0.48              |
| 1:A:256:ASP:OD2  | 1:A:259:TYR:HA   | 2.14                     | 0.48              |
| 1:B:14:TRP:CH2   | 1:B:18:ARG:HD2   | 2.49                     | 0.48              |
| 1:B:266:ASN:O    | 1:B:270:THR:HG23 | 2.13                     | 0.48              |
| 1:B:4:ARG:HH21   | 1:C:470:GLN:H    | 1.61                     | 0.48              |
| 1:D:88:HIS:CD2   | 1:D:311:PRO:HG2  | 2.48                     | 0.48              |
| 1:A:501:GLU:HA   | 1:A:501:GLU:OE1  | 2.14                     | 0.48              |
| 1:C:18:ARG:HH12  | 1:C:23:PRO:HA    | 1.79                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:290:ILE:HG13 | 1:C:291:PHE:N    | 2.29                     | 0.48              |
| 1:D:43:VAL:HG13  | 1:D:48:PRO:HD2   | 1.95                     | 0.48              |
| 1:C:18:ARG:NH1   | 1:C:23:PRO:HA    | 2.28                     | 0.48              |
| 1:D:378:TYR:CD1  | 1:D:378:TYR:C    | 2.88                     | 0.48              |
| 1:A:45:PRO:HD3   | 1:D:431:PHE:CE2  | 2.49                     | 0.48              |
| 1:D:155:ARG:NH2  | 1:D:438:ASN:OD1  | 2.47                     | 0.48              |
| 1:D:89:ASP:OD1   | 1:D:91:THR:OG1   | 2.32                     | 0.48              |
| 1:A:263:ASP:C    | 1:A:263:ASP:OD1  | 2.52                     | 0.48              |
| 1:A:54:VAL:HG22  | 1:A:54:VAL:H     | 1.62                     | 0.48              |
| 1:A:71:ARG:HG3   | 1:A:71:ARG:NH1   | 2.25                     | 0.48              |
| 1:B:154:ILE:HG13 | 1:B:349:MET:HE1  | 1.96                     | 0.48              |
| 1:C:111:ARG:HB3  | 3:C:2002:HEM:O1D | 2.12                     | 0.48              |
| 1:C:365:LEU:HD22 | 4:C:2125:HOH:O   | 2.14                     | 0.48              |
| 1:C:41:LEU:HB3   | 1:C:53:ASP:HB2   | 1.96                     | 0.48              |
| 1:C:51:VAL:HG21  | 1:D:49:LEU:HD23  | 1.95                     | 0.48              |
| 1:B:118:GLU:OE1  | 1:B:118:GLU:N    | 2.47                     | 0.47              |
| 1:C:26:LEU:HD12  | 1:C:27:THR:N     | 2.30                     | 0.47              |
| 1:C:377:PRO:HG2  | 1:C:382:VAL:HG23 | 1.95                     | 0.47              |
| 1:D:97:LYS:CA    | 1:D:100:GLU:HG3  | 2.42                     | 0.47              |
| 1:D:177:ASP:O    | 1:D:181:VAL:HG23 | 2.14                     | 0.47              |
| 1:D:219:PHE:O    | 1:D:230:TYR:HA   | 2.13                     | 0.47              |
| 1:D:110:VAL:CG2  | 1:D:317:LEU:HD21 | 2.44                     | 0.47              |
| 1:D:357:TYR:CE2  | 3:D:2003:HEM:CHA | 2.97                     | 0.47              |
| 1:A:279:TYR:HA   | 1:A:310:ILE:O    | 2.13                     | 0.47              |
| 1:B:146:GLY:HA3  | 1:B:214:TYR:O    | 2.14                     | 0.47              |
| 1:C:223:ASN:HD21 | 1:C:227:GLU:HB2  | 1.80                     | 0.47              |
| 1:D:488:TYR:CE1  | 1:D:492:ILE:HD11 | 2.49                     | 0.47              |
| 1:A:112:PHE:CG   | 1:A:208:HIS:HB3  | 2.49                     | 0.47              |
| 1:A:53:ASP:OD2   | 1:D:430:ARG:NH1  | 2.44                     | 0.47              |
| 1:A:97:LYS:O     | 1:A:100:GLU:HB2  | 2.14                     | 0.47              |
| 1:D:99:PHE:O     | 1:D:100:GLU:C    | 2.53                     | 0.47              |
| 1:D:381:ARG:HG2  | 1:D:381:ARG:NH1  | 2.30                     | 0.47              |
| 1:D:90:ILE:HD13  | 1:D:312:VAL:HG13 | 1.96                     | 0.47              |
| 1:B:65:ARG:O     | 1:D:389:GLY:HA2  | 2.15                     | 0.47              |
| 1:D:52:GLN:CB    | 4:D:3005:HOH:O   | 2.21                     | 0.47              |
| 1:C:211:MET:HG2  | 1:C:212:ASP:N    | 2.29                     | 0.47              |
| 1:C:396:ASN:O    | 1:C:397:GLN:HB2  | 2.15                     | 0.47              |
| 1:B:329:GLU:OE1  | 1:B:329:GLU:HA   | 2.14                     | 0.47              |
| 1:C:142:TRP:HB2  | 1:C:339:PRO:HD3  | 1.96                     | 0.47              |
| 1:C:394:MET:HB3  | 4:C:2089:HOH:O   | 2.15                     | 0.47              |
| 1:D:335:PRO:HD3  | 1:D:357:TYR:CG   | 2.50                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:90:ILE:O     | 1:D:92:ARG:N      | 2.47                     | 0.47              |
| 1:A:23:PRO:CB    | 1:C:412:GLU:HG2   | 2.45                     | 0.47              |
| 1:A:358:PRO:HB2  | 1:A:362:ARG:HH12  | 1.80                     | 0.47              |
| 1:B:446:TYR:CE1  | 1:B:455:ARG:HG2   | 2.49                     | 0.47              |
| 1:D:86:VAL:HG23  | 1:D:104:LYS:O     | 2.14                     | 0.47              |
| 1:A:15:LYS:NZ    | 4:A:3112:HOH:O    | 2.44                     | 0.47              |
| 1:A:500:ASN:O    | 1:A:501:GLU:O     | 2.33                     | 0.47              |
| 1:B:274:PRO:HB2  | 1:B:276:TRP:CZ3   | 2.50                     | 0.47              |
| 1:A:43:VAL:HG21  | 1:B:43:VAL:HG21   | 1.97                     | 0.47              |
| 1:B:71:ARG:HG2   | 3:B:2001:HEM:O2A  | 2.14                     | 0.47              |
| 3:C:2002:HEM:HHC | 3:C:2002:HEM:HMC1 | 1.48                     | 0.47              |
| 1:C:476:LYS:HB3  | 1:C:476:LYS:NZ    | 2.30                     | 0.47              |
| 1:B:16:GLU:O     | 1:B:18:ARG:N      | 2.48                     | 0.47              |
| 1:B:404:TYR:OH   | 1:B:413:HIS:CD2   | 2.67                     | 0.47              |
| 1:B:4:ARG:NH2    | 1:C:179:ASP:OD2   | 2.48                     | 0.47              |
| 1:C:256:ASP:OD2  | 1:C:259:TYR:HA    | 2.15                     | 0.47              |
| 1:C:72:VAL:HG13  | 1:C:73:VAL:HG22   | 1.96                     | 0.47              |
| 1:A:455:ARG:NE   | 4:A:3196:HOH:O    | 2.48                     | 0.47              |
| 1:A:487:GLU:OE1  | 1:A:491:ARG:HD2   | 2.15                     | 0.47              |
| 1:D:145:VAL:HG12 | 3:D:2003:HEM:HMD2 | 1.96                     | 0.47              |
| 1:B:310:ILE:HD12 | 1:B:310:ILE:N     | 2.31                     | 0.46              |
| 1:C:368:ASN:O    | 1:C:371:GLN:HB2   | 2.14                     | 0.46              |
| 1:A:152:PHE:HA   | 1:A:194:GLN:HG3   | 1.97                     | 0.46              |
| 1:B:123:ASP:O    | 1:B:125:VAL:N     | 2.48                     | 0.46              |
| 1:C:74:HIS:NE2   | 3:C:2002:HEM:ND   | 2.63                     | 0.46              |
| 1:C:209:ARG:O    | 1:C:210:HIS:ND1   | 2.47                     | 0.46              |
| 1:C:432:ASN:HD22 | 1:C:432:ASN:C     | 2.15                     | 0.46              |
| 1:A:234:HIS:O    | 1:A:278:LEU:HD12  | 2.15                     | 0.46              |
| 1:A:237:THR:HA   | 1:A:276:TRP:CD1   | 2.50                     | 0.46              |
| 1:A:43:VAL:HG12  | 1:A:50:LEU:CD2    | 2.44                     | 0.46              |
| 1:B:160:PHE:CD1  | 3:B:2001:HEM:HAB  | 2.50                     | 0.46              |
| 1:D:26:LEU:HB3   | 1:D:34:VAL:CG2    | 2.45                     | 0.46              |
| 1:B:229:VAL:HG23 | 1:B:284:THR:HA    | 1.98                     | 0.46              |
| 1:B:217:HIS:CD2  | 1:B:353:ARG:NH1   | 2.82                     | 0.46              |
| 1:C:52:GLN:O     | 1:C:54:VAL:N      | 2.49                     | 0.46              |
| 1:D:154:ILE:HG13 | 1:D:349:MET:HE2   | 1.97                     | 0.46              |
| 1:D:223:ASN:OD1  | 1:D:225:ASP:N     | 2.48                     | 0.46              |
| 1:D:450:LEU:O    | 1:D:455:ARG:NH1   | 2.45                     | 0.46              |
| 1:A:37:LYS:NZ    | 1:A:37:LYS:O      | 2.41                     | 0.46              |
| 1:B:152:PHE:HB3  | 1:B:298:LEU:CD2   | 2.44                     | 0.46              |
| 1:B:212:ASP:OD1  | 1:B:236:LYS:HA    | 2.15                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:174:HIS:HA   | 4:D:3042:HOH:O    | 2.16                     | 0.46              |
| 1:D:460:GLU:HA   | 1:D:495:LEU:CD1   | 2.45                     | 0.46              |
| 1:B:188:ARG:NE   | 1:B:190:GLU:OE2   | 2.44                     | 0.46              |
| 1:B:472:PHE:CZ   | 1:B:473:ILE:HG13  | 2.51                     | 0.46              |
| 1:B:9:ASP:O      | 1:B:12:LYS:HB3    | 2.15                     | 0.46              |
| 1:C:129:ARG:HB3  | 1:C:211:MET:HE1   | 1.94                     | 0.46              |
| 1:D:323:ASN:ND2  | 4:D:3007:HOH:O    | 2.48                     | 0.46              |
| 1:D:90:ILE:HD11  | 1:D:99:PHE:CD1    | 2.50                     | 0.46              |
| 1:A:439:VAL:O    | 1:A:440:THR:C     | 2.54                     | 0.46              |
| 1:B:122:ALA:HB2  | 1:B:257:PRO:HB3   | 1.97                     | 0.46              |
| 1:B:46:ARG:NH1   | 1:C:294:ASN:HB2   | 2.31                     | 0.46              |
| 1:D:190:GLU:HA   | 1:D:438:ASN:CB    | 2.38                     | 0.46              |
| 1:D:235:TYR:CD1  | 1:D:235:TYR:N     | 2.83                     | 0.46              |
| 1:D:485:HIS:CE1  | 1:D:486:PRO:HG2   | 2.51                     | 0.46              |
| 1:A:298:LEU:HD22 | 3:A:2000:HEM:HBC1 | 1.91                     | 0.46              |
| 1:A:141:ASN:O    | 1:A:337:ASN:HB3   | 2.15                     | 0.46              |
| 1:D:368:ASN:O    | 1:D:371:GLN:HB2   | 2.15                     | 0.46              |
| 1:A:391:MET:CE   | 1:A:393:MET:CE    | 2.92                     | 0.46              |
| 1:B:129:ARG:HB2  | 1:B:148:ASN:ND2   | 2.31                     | 0.46              |
| 1:B:43:VAL:HG13  | 1:B:48:PRO:HD2    | 1.98                     | 0.46              |
| 1:C:291:PHE:CD2  | 1:C:293:PHE:O     | 2.69                     | 0.46              |
| 1:C:414:GLN:HA   | 1:C:415:PRO:HD2   | 1.82                     | 0.46              |
| 1:D:209:ARG:HG2  | 1:D:274:PRO:HB3   | 1.97                     | 0.46              |
| 1:D:442:VAL:HG12 | 1:D:484:VAL:HG11  | 1.98                     | 0.46              |
| 1:A:110:VAL:HA   | 1:A:132:ALA:O     | 2.16                     | 0.46              |
| 1:A:126:ARG:CA   | 1:A:204:ILE:HG12  | 2.46                     | 0.46              |
| 1:A:452:GLU:O    | 1:A:453:GLU:C     | 2.54                     | 0.46              |
| 1:B:26:LEU:HA    | 1:D:383:ALA:O     | 2.16                     | 0.46              |
| 1:B:332:ALA:HB1  | 1:B:361:HIS:ND1   | 2.31                     | 0.46              |
| 1:C:40:SER:HB3   | 1:C:49:LEU:CD1    | 2.46                     | 0.46              |
| 1:A:421:ARG:CD   | 1:B:429:GLN:HG2   | 2.46                     | 0.45              |
| 1:B:41:LEU:O     | 1:B:50:LEU:HD23   | 2.15                     | 0.45              |
| 1:D:246:VAL:HG23 | 1:D:247:GLU:OE1   | 2.16                     | 0.45              |
| 1:A:18:ARG:HG2   | 1:A:18:ARG:HH11   | 1.81                     | 0.45              |
| 1:A:153:PHE:CD1  | 1:A:194:GLN:HB3   | 2.52                     | 0.45              |
| 1:A:451:ASN:N    | 1:A:454:GLN:NE2   | 2.56                     | 0.45              |
| 1:B:403:TYR:CD1  | 1:B:403:TYR:N     | 2.85                     | 0.45              |
| 1:B:78:ALA:O     | 1:B:111:ARG:HA    | 2.15                     | 0.45              |
| 1:C:130:GLY:HA2  | 1:C:147:ASN:CB    | 2.46                     | 0.45              |
| 1:D:145:VAL:CG1  | 3:D:2003:HEM:C2D  | 2.99                     | 0.45              |
| 1:D:284:THR:OG1  | 1:D:287:GLU:HG3   | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:300:LYS:HA   | 1:C:441:GLN:OE1  | 2.16                     | 0.45              |
| 1:D:182:TRP:CD2  | 1:D:466:LEU:HD13 | 2.51                     | 0.45              |
| 1:B:13:HIS:O     | 1:B:17:GLN:HG2   | 2.17                     | 0.45              |
| 1:B:140:GLY:HA3  | 1:D:32:ASN:ND2   | 2.30                     | 0.45              |
| 1:D:60:MET:HE3   | 1:D:63:PHE:HB3   | 1.98                     | 0.45              |
| 1:A:90:ILE:HD13  | 1:A:312:VAL:HG22 | 1.97                     | 0.45              |
| 1:B:239:GLN:N    | 1:B:239:GLN:CD   | 2.70                     | 0.45              |
| 1:B:41:LEU:CB    | 1:B:53:ASP:HB2   | 2.47                     | 0.45              |
| 1:B:474:GLN:O    | 1:B:477:ALA:HB3  | 2.17                     | 0.45              |
| 1:D:26:LEU:HB3   | 1:D:34:VAL:HG22  | 1.99                     | 0.45              |
| 1:B:154:ILE:HG13 | 1:B:349:MET:CE   | 2.47                     | 0.45              |
| 1:C:308:PRO:O    | 1:C:310:ILE:CD1  | 2.64                     | 0.45              |
| 1:C:467:LYS:HD3  | 1:C:499:TYR:CD1  | 2.51                     | 0.45              |
| 1:A:74:HIS:HE1   | 4:A:3009:HOH:O   | 2.00                     | 0.45              |
| 1:B:86:VAL:CG1   | 1:B:102:ILE:HD13 | 2.45                     | 0.45              |
| 1:C:151:ILE:CG2  | 1:C:301:VAL:HG13 | 2.47                     | 0.45              |
| 1:A:428:VAL:O    | 4:A:3193:HOH:O   | 2.20                     | 0.45              |
| 1:A:445:PHE:HA   | 1:A:449:VAL:CG2  | 2.46                     | 0.45              |
| 1:A:455:ARG:HD2  | 4:A:3196:HOH:O   | 2.16                     | 0.45              |
| 1:B:476:LYS:HB2  | 1:B:476:LYS:HE3  | 1.63                     | 0.45              |
| 1:C:395:ASP:C    | 1:C:395:ASP:OD2  | 2.46                     | 0.45              |
| 1:D:339:PRO:HD2  | 1:D:342:ILE:HD12 | 1.98                     | 0.45              |
| 1:C:395:ASP:CG   | 1:C:395:ASP:O    | 2.55                     | 0.45              |
| 1:A:154:ILE:HG13 | 1:A:349:MET:CE   | 2.47                     | 0.45              |
| 1:A:378:TYR:CD1  | 1:A:378:TYR:C    | 2.91                     | 0.45              |
| 1:B:374:VAL:HG23 | 4:B:2178:HOH:O   | 2.17                     | 0.45              |
| 1:B:41:LEU:HB2   | 1:B:53:ASP:OD2   | 2.17                     | 0.45              |
| 1:C:126:ARG:HH11 | 1:C:126:ARG:HG2  | 1.82                     | 0.45              |
| 1:C:152:PHE:HB3  | 1:C:298:LEU:CD2  | 2.47                     | 0.45              |
| 4:A:3200:HOH:O   | 1:C:409:SER:HB3  | 2.17                     | 0.45              |
| 1:D:90:ILE:HD11  | 1:D:99:PHE:CD2   | 2.52                     | 0.45              |
| 1:A:338:MET:HB3  | 1:A:342:ILE:O    | 2.17                     | 0.44              |
| 1:B:99:PHE:O     | 1:B:100:GLU:C    | 2.55                     | 0.44              |
| 1:C:275:SER:HA   | 1:C:315:LEU:O    | 2.17                     | 0.44              |
| 1:C:362:ARG:NH1  | 4:C:2008:HOH:O   | 2.50                     | 0.44              |
| 1:D:151:ILE:HD13 | 1:D:193:HIS:CG   | 2.52                     | 0.44              |
| 1:A:418:LEU:HB3  | 1:A:419:GLU:H    | 1.55                     | 0.44              |
| 1:B:192:LEU:HD13 | 1:B:484:VAL:CG2  | 2.47                     | 0.44              |
| 1:B:467:LYS:HG3  | 1:B:468:ASP:N    | 2.32                     | 0.44              |
| 1:C:99:PHE:O     | 1:C:100:GLU:C    | 2.55                     | 0.44              |
| 1:D:11:MET:O     | 1:D:12:LYS:C     | 2.55                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:280:ILE:O    | 1:D:280:ILE:HD13 | 2.17                     | 0.44              |
| 1:D:378:TYR:HD1  | 1:D:378:TYR:C    | 2.21                     | 0.44              |
| 1:A:18:ARG:CD    | 4:A:3200:HOH:O   | 2.65                     | 0.44              |
| 1:A:229:VAL:HG11 | 1:A:282:VAL:CG1  | 2.46                     | 0.44              |
| 1:A:384:ASN:OD1  | 1:A:386:GLN:HB2  | 2.16                     | 0.44              |
| 1:B:455:ARG:HG3  | 1:B:455:ARG:HH11 | 1.82                     | 0.44              |
| 1:B:467:LYS:HD3  | 1:B:499:TYR:CD1  | 2.53                     | 0.44              |
| 1:C:247:GLU:O    | 1:C:250:ALA:HB3  | 2.17                     | 0.44              |
| 1:C:297:ASP:OD1  | 1:C:300:LYS:HG2  | 2.17                     | 0.44              |
| 1:A:363:HIS:CD2  | 1:D:65:ARG:HA    | 2.52                     | 0.44              |
| 1:B:129:ARG:H    | 1:B:148:ASN:CG   | 2.21                     | 0.44              |
| 1:B:81:PHE:CZ    | 1:B:327:GLU:HB3  | 2.53                     | 0.44              |
| 1:D:304:HIS:CD2  | 1:D:309:LEU:HD11 | 2.52                     | 0.44              |
| 1:D:96:ALA:C     | 1:D:98:VAL:H     | 2.21                     | 0.44              |
| 1:B:122:ALA:HB1  | 1:B:257:PRO:HA   | 1.99                     | 0.44              |
| 1:B:374:VAL:HG22 | 4:B:2178:HOH:O   | 2.18                     | 0.44              |
| 1:B:410:ALA:HB1  | 1:B:411:PRO:HD2  | 1.98                     | 0.44              |
| 1:C:237:THR:HA   | 1:C:276:TRP:CD1  | 2.52                     | 0.44              |
| 1:C:92:ARG:HH11  | 1:C:92:ARG:HG3   | 1.82                     | 0.44              |
| 1:D:15:LYS:O     | 1:D:18:ARG:HB3   | 2.18                     | 0.44              |
| 1:D:404:TYR:CD1  | 1:D:405:PRO:HA   | 2.52                     | 0.44              |
| 1:B:285:PHE:O    | 1:B:289:GLU:HG3  | 2.18                     | 0.44              |
| 1:B:456:LYS:HB2  | 1:B:491:ARG:HH22 | 1.83                     | 0.44              |
| 1:C:155:ARG:NH2  | 1:C:438:ASN:ND2  | 2.65                     | 0.44              |
| 1:C:485:HIS:HA   | 1:C:486:PRO:HD2  | 1.66                     | 0.44              |
| 1:D:107:PRO:HG2  | 1:D:136:TYR:HB2  | 1.99                     | 0.44              |
| 1:D:112:PHE:CD1  | 1:D:208:HIS:HB3  | 2.52                     | 0.44              |
| 1:A:6:PRO:HG2    | 1:A:270:THR:CG2  | 2.48                     | 0.44              |
| 1:B:361:HIS:NE2  | 3:B:2001:HEM:O1A | 2.49                     | 0.44              |
| 1:D:285:PHE:N    | 1:D:285:PHE:CD1  | 2.86                     | 0.44              |
| 1:D:296:PHE:HB3  | 1:D:347:ASP:HA   | 1.99                     | 0.44              |
| 1:A:485:HIS:HD2  | 1:A:487:GLU:CB   | 2.26                     | 0.44              |
| 1:C:155:ARG:HH22 | 1:C:438:ASN:ND2  | 2.15                     | 0.44              |
| 1:C:293:PHE:CD1  | 1:C:293:PHE:N    | 2.85                     | 0.44              |
| 1:D:451:ASN:OD1  | 1:D:451:ASN:C    | 2.56                     | 0.44              |
| 1:D:60:MET:CE    | 1:D:63:PHE:HD2   | 2.31                     | 0.44              |
| 1:A:229:VAL:HG11 | 1:A:282:VAL:HG13 | 1.99                     | 0.44              |
| 1:B:100:GLU:HB3  | 1:B:101:HIS:H    | 1.62                     | 0.44              |
| 1:B:315:LEU:HD23 | 1:B:315:LEU:HA   | 1.89                     | 0.44              |
| 1:B:454:GLN:HA   | 1:B:457:ARG:HH12 | 1.82                     | 0.44              |
| 1:C:129:ARG:CG   | 1:C:211:MET:HE1  | 2.46                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:279:TYR:CD1  | 1:C:311:PRO:HA   | 2.53                     | 0.44              |
| 1:A:450:LEU:HD22 | 1:A:454:GLN:HB3  | 1.99                     | 0.43              |
| 1:B:163:PHE:O    | 1:B:166:SER:N    | 2.51                     | 0.43              |
| 1:A:427:ASP:HA   | 1:B:423:HIS:HA   | 2.00                     | 0.43              |
| 1:B:71:ARG:HG3   | 4:B:2159:HOH:O   | 2.18                     | 0.43              |
| 1:C:241:ILE:H    | 1:C:241:ILE:HD12 | 1.83                     | 0.43              |
| 1:C:402:ASN:OD1  | 1:D:165:HIS:HB3  | 2.18                     | 0.43              |
| 1:D:221:LEU:HB2  | 1:D:229:VAL:HG23 | 1.98                     | 0.43              |
| 1:D:220:LYS:HA   | 1:D:229:VAL:O    | 2.18                     | 0.43              |
| 1:A:88:HIS:CD2   | 1:A:311:PRO:HG2  | 2.53                     | 0.43              |
| 1:B:262:ARG:HG3  | 1:B:266:ASN:ND2  | 2.32                     | 0.43              |
| 1:C:406:ASN:ND2  | 1:C:410:ALA:HB3  | 2.19                     | 0.43              |
| 1:A:455:ARG:CD   | 4:A:3196:HOH:O   | 2.67                     | 0.43              |
| 1:B:273:TYR:HA   | 1:B:274:PRO:HD3  | 1.79                     | 0.43              |
| 1:B:351:GLN:O    | 1:B:354:LEU:HB2  | 2.18                     | 0.43              |
| 1:C:451:ASN:OD1  | 1:C:454:GLN:HG3  | 2.19                     | 0.43              |
| 1:A:273:TYR:HA   | 1:A:274:PRO:HD3  | 1.87                     | 0.43              |
| 1:B:139:ASP:HB3  | 1:B:340:PRO:HD2  | 2.01                     | 0.43              |
| 1:C:234:HIS:O    | 1:C:278:LEU:HA   | 2.18                     | 0.43              |
| 1:C:421:ARG:HD2  | 1:D:429:GLN:HB2  | 2.00                     | 0.43              |
| 1:A:410:ALA:HB1  | 1:A:411:PRO:HD2  | 2.00                     | 0.43              |
| 1:A:485:HIS:CD2  | 1:A:487:GLU:CB   | 2.98                     | 0.43              |
| 1:C:456:LYS:O    | 1:C:460:GLU:HG3  | 2.18                     | 0.43              |
| 1:D:101:HIS:CD2  | 4:D:3063:HOH:O   | 2.72                     | 0.43              |
| 1:D:237:THR:HA   | 1:D:276:TRP:CD1  | 2.54                     | 0.43              |
| 1:B:160:PHE:N    | 1:B:161:PRO:CD   | 2.82                     | 0.43              |
| 1:C:12:LYS:HG2   | 1:C:16:GLU:OE2   | 2.17                     | 0.43              |
| 1:C:182:TRP:CD2  | 1:C:466:LEU:HD13 | 2.53                     | 0.43              |
| 1:C:244:LEU:HB3  | 1:C:249:ALA:HB2  | 2.00                     | 0.43              |
| 1:C:152:PHE:HB3  | 1:C:298:LEU:HD23 | 2.01                     | 0.43              |
| 1:A:391:MET:HE2  | 1:A:393:MET:CE   | 2.49                     | 0.43              |
| 1:B:357:TYR:CZ   | 3:B:2001:HEM:NA  | 2.86                     | 0.43              |
| 1:B:446:TYR:CE2  | 1:B:488:TYR:HB2  | 2.54                     | 0.43              |
| 1:C:156:ASP:OD2  | 1:C:348:LYS:HD3  | 2.18                     | 0.43              |
| 1:C:81:PHE:CD1   | 1:C:81:PHE:N     | 2.86                     | 0.43              |
| 1:D:212:ASP:OD1  | 1:D:236:LYS:HA   | 2.19                     | 0.43              |
| 1:B:82:GLY:HA3   | 1:B:317:LEU:HA   | 2.01                     | 0.43              |
| 1:B:296:PHE:CE1  | 1:B:346:PRO:HD2  | 2.54                     | 0.43              |
| 1:C:232:LYS:O    | 1:C:280:ILE:HA   | 2.18                     | 0.43              |
| 1:D:170:ASN:ND2  | 1:D:173:THR:H    | 2.16                     | 0.43              |
| 1:D:377:PRO:HG2  | 1:D:382:VAL:CG2  | 2.49                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:21:GLN:HG3   | 1:B:21:GLN:H      | 1.54                     | 0.43              |
| 1:B:353:ARG:NH1  | 3:B:2001:HEM:CBC  | 2.82                     | 0.43              |
| 1:B:487:GLU:O    | 1:B:491:ARG:HG3   | 2.19                     | 0.43              |
| 1:C:281:GLN:CG   | 1:C:309:LEU:HD12  | 2.49                     | 0.43              |
| 1:C:381:ARG:HB2  | 1:C:381:ARG:HH11  | 1.84                     | 0.43              |
| 1:B:90:ILE:HD13  | 1:B:312:VAL:HB    | 2.00                     | 0.43              |
| 1:C:279:TYR:HD1  | 1:C:311:PRO:HA    | 1.84                     | 0.43              |
| 1:C:402:ASN:N    | 1:C:402:ASN:ND2   | 2.46                     | 0.43              |
| 1:B:41:LEU:HD23  | 1:C:430:ARG:CZ    | 2.49                     | 0.43              |
| 1:C:469:ALA:O    | 1:C:470:GLN:C     | 2.58                     | 0.43              |
| 1:D:160:PHE:CE1  | 1:D:164:ILE:HD11  | 2.54                     | 0.42              |
| 1:D:160:PHE:HB3  | 1:D:161:PRO:HD3   | 2.01                     | 0.42              |
| 1:D:357:TYR:HB2  | 1:D:358:PRO:HD3   | 1.99                     | 0.42              |
| 1:A:83:TYR:CD1   | 1:A:105:ARG:HD2   | 2.53                     | 0.42              |
| 1:A:309:LEU:N    | 1:A:309:LEU:CD2   | 2.78                     | 0.42              |
| 1:A:388:ASP:H    | 1:A:396:ASN:HD21  | 1.67                     | 0.42              |
| 1:B:18:ARG:O     | 1:B:19:ALA:C      | 2.57                     | 0.42              |
| 1:B:430:ARG:HD3  | 1:C:36:ASP:HB3    | 2.00                     | 0.42              |
| 1:C:355:PHE:O    | 1:C:358:PRO:HD2   | 2.19                     | 0.42              |
| 1:D:137:THR:O    | 1:D:379:ARG:HB2   | 2.19                     | 0.42              |
| 1:D:220:LYS:O    | 1:D:221:LEU:HD23  | 2.19                     | 0.42              |
| 1:D:43:VAL:HG13  | 1:D:43:VAL:O      | 2.19                     | 0.42              |
| 2:A:3000:CYN:N   | 3:A:2000:HEM:NC   | 2.62                     | 0.42              |
| 1:B:149:THR:OG1  | 1:B:150:PRO:HD2   | 2.19                     | 0.42              |
| 1:B:145:VAL:HB   | 1:B:353:ARG:NH2   | 2.35                     | 0.42              |
| 1:B:4:ARG:HD2    | 1:B:8:SER:CB      | 2.49                     | 0.42              |
| 1:D:422:THR:HG22 | 1:D:423:HIS:N     | 2.33                     | 0.42              |
| 1:A:82:GLY:HA3   | 1:A:317:LEU:HA    | 2.00                     | 0.42              |
| 1:B:188:ARG:NH2  | 1:B:190:GLU:OE2   | 2.47                     | 0.42              |
| 1:B:452:GLU:OE2  | 1:B:491:ARG:NH1   | 2.45                     | 0.42              |
| 1:C:131:PHE:CE1  | 1:C:235:TYR:HE2   | 2.37                     | 0.42              |
| 1:D:391:MET:HB3  | 1:D:391:MET:HE3   | 1.86                     | 0.42              |
| 1:A:332:ALA:CB   | 1:A:361:HIS:NE2   | 2.82                     | 0.42              |
| 1:A:410:ALA:HB1  | 1:A:411:PRO:CD    | 2.49                     | 0.42              |
| 1:B:223:ASN:C    | 1:B:225:ASP:H     | 2.21                     | 0.42              |
| 1:D:160:PHE:CE2  | 1:D:164:ILE:HG13  | 2.55                     | 0.42              |
| 1:B:264:LEU:HG   | 4:B:2055:HOH:O    | 2.19                     | 0.42              |
| 1:D:106:THR:O    | 1:D:108:ILE:HG23  | 2.20                     | 0.42              |
| 1:D:145:VAL:HB   | 1:D:353:ARG:NH2   | 2.35                     | 0.42              |
| 1:A:197:PHE:O    | 1:A:200:SER:OG    | 2.27                     | 0.42              |
| 1:B:217:HIS:CE1  | 3:B:2001:HEM:HBC1 | 2.55                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:293:PHE:CE1  | 1:D:437:ASP:OD2  | 2.73                     | 0.42              |
| 1:A:268:ILE:HB   | 1:A:320:ASN:HD21 | 1.85                     | 0.42              |
| 1:B:393:MET:HE2  | 1:D:373:PRO:CD   | 2.48                     | 0.42              |
| 1:B:402:ASN:HD22 | 1:B:402:ASN:C    | 2.23                     | 0.42              |
| 1:B:66:GLU:HA    | 1:D:389:GLY:N    | 2.35                     | 0.42              |
| 1:C:210:HIS:HD2  | 1:C:242:LYS:HB3  | 1.82                     | 0.42              |
| 1:C:444:THR:HG22 | 1:C:444:THR:O    | 2.19                     | 0.42              |
| 1:D:129:ARG:O    | 1:D:147:ASN:HA   | 2.20                     | 0.42              |
| 1:A:273:TYR:CD1  | 1:A:318:ASN:HA   | 2.55                     | 0.42              |
| 1:A:357:TYR:O    | 1:A:360:THR:HG22 | 2.20                     | 0.42              |
| 1:A:284:THR:OG1  | 1:A:287:GLU:CG   | 2.64                     | 0.42              |
| 1:A:41:LEU:HB3   | 1:A:53:ASP:HB2   | 2.01                     | 0.42              |
| 1:C:95:LYS:HG2   | 1:C:222:VAL:O    | 2.19                     | 0.42              |
| 1:C:22:LYS:HD3   | 1:C:23:PRO:N     | 2.35                     | 0.42              |
| 1:C:422:THR:HG22 | 1:C:423:HIS:N    | 2.35                     | 0.42              |
| 1:C:182:TRP:NE1  | 1:C:465:HIS:ND1  | 2.64                     | 0.42              |
| 1:D:154:ILE:HB   | 4:D:3132:HOH:O   | 2.19                     | 0.42              |
| 1:A:172:GLN:NE2  | 1:D:322:VAL:HA   | 2.30                     | 0.42              |
| 1:B:71:ARG:CG    | 1:B:71:ARG:NH1   | 2.77                     | 0.41              |
| 1:D:87:THR:C     | 1:D:88:HIS:ND1   | 2.73                     | 0.41              |
| 1:A:439:VAL:HG23 | 1:A:440:THR:N    | 2.36                     | 0.41              |
| 1:A:455:ARG:NH1  | 4:A:3196:HOH:O   | 2.52                     | 0.41              |
| 1:B:472:PHE:C    | 1:B:472:PHE:CD2  | 2.94                     | 0.41              |
| 1:A:50:LEU:CD1   | 1:B:48:PRO:HB2   | 2.50                     | 0.41              |
| 1:B:74:HIS:CD2   | 3:B:2001:HEM:C4D | 3.08                     | 0.41              |
| 1:C:414:GLN:NE2  | 1:C:417:ALA:HB2  | 2.33                     | 0.41              |
| 1:C:480:ASN:O    | 1:C:484:VAL:HG23 | 2.20                     | 0.41              |
| 1:A:430:ARG:HE   | 1:B:419:GLU:CD   | 2.23                     | 0.41              |
| 1:C:223:ASN:O    | 1:C:225:ASP:N    | 2.53                     | 0.41              |
| 1:C:467:LYS:HE2  | 1:C:468:ASP:OD2  | 2.20                     | 0.41              |
| 1:D:189:PRO:HB2  | 1:D:438:ASN:HD22 | 1.85                     | 0.41              |
| 1:D:71:ARG:HH22  | 1:D:329:GLU:C    | 2.22                     | 0.41              |
| 1:A:158:LEU:HD21 | 1:D:56:PHE:HA    | 2.03                     | 0.41              |
| 1:A:15:LYS:HD2   | 1:C:408:PHE:HA   | 2.03                     | 0.41              |
| 1:A:452:GLU:HA   | 1:A:455:ARG:HH11 | 1.85                     | 0.41              |
| 1:B:432:ASN:HA   | 1:C:39:ASN:OD1   | 2.20                     | 0.41              |
| 1:B:470:GLN:OE1  | 1:B:472:PHE:HE1  | 2.03                     | 0.41              |
| 1:B:475:LYS:O    | 1:B:476:LYS:C    | 2.57                     | 0.41              |
| 1:B:493:GLN:O    | 1:B:494:ALA:C    | 2.59                     | 0.41              |
| 1:C:209:ARG:NH2  | 1:C:267:ALA:HB2  | 2.29                     | 0.41              |
| 1:C:332:ALA:HB1  | 1:C:361:HIS:ND1  | 2.35                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:499:TYR:C    | 1:C:501:GLU:H     | 2.23                     | 0.41              |
| 1:D:298:LEU:HD21 | 3:D:2003:HEM:HMC3 | 2.03                     | 0.41              |
| 1:A:452:GLU:N    | 1:A:455:ARG:NH1   | 2.69                     | 0.41              |
| 1:B:26:LEU:HD21  | 1:B:37:LYS:HD2    | 2.01                     | 0.41              |
| 1:B:487:GLU:C    | 1:B:489:GLY:H     | 2.23                     | 0.41              |
| 1:B:92:ARG:H     | 1:B:92:ARG:HG3    | 1.62                     | 0.41              |
| 1:D:94:SER:HB2   | 1:D:221:LEU:HB3   | 2.01                     | 0.41              |
| 1:D:209:ARG:O    | 1:D:239:GLN:HB2   | 2.20                     | 0.41              |
| 1:B:193:HIS:HA   | 1:B:442:VAL:HG22  | 2.01                     | 0.41              |
| 1:C:395:ASP:OD2  | 1:C:395:ASP:O     | 2.39                     | 0.41              |
| 1:B:165:HIS:NE2  | 1:C:66:GLU:OE2    | 2.37                     | 0.41              |
| 3:B:2001:HEM:CGD | 4:B:2179:HOH:O    | 2.68                     | 0.41              |
| 1:D:179:ASP:O    | 1:D:183:ASP:HB2   | 2.20                     | 0.41              |
| 1:D:217:HIS:CD2  | 1:D:353:ARG:HH11  | 2.39                     | 0.41              |
| 1:A:69:PRO:O     | 1:A:364:ARG:HG3   | 2.21                     | 0.41              |
| 1:A:385:TYR:OH   | 1:A:410:ALA:HB3   | 2.21                     | 0.41              |
| 1:B:43:VAL:HG22  | 1:B:43:VAL:O      | 2.21                     | 0.41              |
| 1:B:177:ASP:C    | 1:B:177:ASP:OD1   | 2.59                     | 0.41              |
| 1:B:332:ALA:N    | 1:B:375:ASN:OD1   | 2.54                     | 0.41              |
| 1:A:421:ARG:NH2  | 1:B:429:GLN:NE2   | 2.69                     | 0.41              |
| 1:D:114:THR:HB   | 1:D:115:VAL:H     | 1.74                     | 0.41              |
| 1:D:291:PHE:HA   | 1:D:292:PRO:HD3   | 1.83                     | 0.41              |
| 1:D:346:PRO:O    | 1:D:347:ASP:C     | 2.58                     | 0.41              |
| 1:A:242:LYS:HD3  | 1:A:242:LYS:C     | 2.41                     | 0.41              |
| 1:A:453:GLU:OE2  | 1:A:457:ARG:NH1   | 2.54                     | 0.41              |
| 1:B:408:PHE:O    | 1:B:409:SER:HB2   | 2.20                     | 0.41              |
| 1:B:442:VAL:O    | 1:B:445:PHE:HB3   | 2.20                     | 0.41              |
| 1:C:115:VAL:HB   | 1:C:127:ASP:OD1   | 2.20                     | 0.41              |
| 1:C:131:PHE:C    | 1:C:131:PHE:CD1   | 2.94                     | 0.41              |
| 1:C:281:GLN:HG2  | 1:C:309:LEU:HD12  | 2.03                     | 0.41              |
| 1:C:221:LEU:HA   | 1:C:341:GLY:O     | 2.20                     | 0.41              |
| 1:D:147:ASN:OD1  | 3:D:2003:HEM:C4C  | 2.74                     | 0.41              |
| 1:B:153:PHE:N    | 1:B:153:PHE:CD1   | 2.88                     | 0.41              |
| 1:B:19:ALA:HB3   | 1:B:21:GLN:NE2    | 2.09                     | 0.41              |
| 1:B:357:TYR:HB2  | 1:B:358:PRO:HD3   | 2.02                     | 0.41              |
| 1:B:414:GLN:HA   | 1:B:415:PRO:HD2   | 1.89                     | 0.41              |
| 1:B:301:VAL:HG22 | 1:B:441:GLN:OE1   | 2.21                     | 0.41              |
| 1:B:442:VAL:HG12 | 1:B:484:VAL:CG1   | 2.51                     | 0.41              |
| 1:C:202:ARG:HA   | 1:C:243:ASN:OD1   | 2.20                     | 0.41              |
| 1:C:284:THR:HA   | 4:C:2136:HOH:O    | 2.20                     | 0.41              |
| 1:C:487:GLU:HG2  | 1:C:491:ARG:HD2   | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:220:LYS:HE3  | 1:B:343:GLU:OE1  | 2.21                     | 0.40              |
| 1:B:252:LEU:O    | 1:B:253:ALA:C    | 2.59                     | 0.40              |
| 1:B:50:LEU:N     | 1:B:50:LEU:CD2   | 2.83                     | 0.40              |
| 1:C:448:LYS:HD2  | 4:C:2115:HOH:O   | 2.22                     | 0.40              |
| 1:B:139:ASP:O    | 1:D:32:ASN:HA    | 2.21                     | 0.40              |
| 1:D:347:ASP:OD1  | 1:D:349:MET:HB2  | 2.20                     | 0.40              |
| 1:D:500:ASN:O    | 1:D:501:GLU:C    | 2.60                     | 0.40              |
| 1:A:413:HIS:O    | 1:A:413:HIS:HD2  | 2.04                     | 0.40              |
| 1:B:252:LEU:CD1  | 1:B:252:LEU:N    | 2.84                     | 0.40              |
| 1:B:220:LYS:N    | 1:B:343:GLU:O    | 2.52                     | 0.40              |
| 1:B:371:GLN:OE1  | 1:B:393:MET:N    | 2.54                     | 0.40              |
| 1:B:447:LEU:O    | 1:B:447:LEU:HD12 | 2.21                     | 0.40              |
| 4:A:3145:HOH:O   | 1:C:37:LYS:N     | 2.08                     | 0.40              |
| 1:D:145:VAL:CG1  | 3:D:2003:HEM:CMD | 2.98                     | 0.40              |
| 1:D:280:ILE:HD13 | 1:D:310:ILE:HB   | 2.03                     | 0.40              |
| 1:D:452:GLU:HA   | 1:D:452:GLU:OE1  | 2.22                     | 0.40              |
| 1:A:265:PHE:CE2  | 1:D:173:THR:HG22 | 2.56                     | 0.40              |
| 1:A:395:ASP:OD2  | 1:A:398:GLY:HA2  | 2.21                     | 0.40              |
| 1:B:83:TYR:N     | 1:B:108:ILE:HG12 | 2.36                     | 0.40              |
| 1:B:296:PHE:CD2  | 1:B:346:PRO:HG2  | 2.56                     | 0.40              |
| 1:B:458:LEU:HG   | 1:B:459:CYS:N    | 2.35                     | 0.40              |
| 1:C:71:ARG:NE    | 3:C:2002:HEM:O2D | 2.50                     | 0.40              |
| 1:A:323:ASN:CG   | 1:C:396:ASN:HB3  | 2.42                     | 0.40              |
| 1:B:177:ASP:OD1  | 1:B:179:ASP:HB2  | 2.21                     | 0.40              |
| 1:B:436:ASP:O    | 1:B:437:ASP:O    | 2.39                     | 0.40              |
| 1:C:233:PHE:N    | 4:C:2020:HOH:O   | 2.54                     | 0.40              |
| 1:D:218:THR:HG23 | 1:D:302:TRP:CZ2  | 2.56                     | 0.40              |
| 1:D:335:PRO:HD2  | 1:D:357:TYR:CG   | 2.56                     | 0.40              |
| 1:D:478:VAL:HG21 | 1:D:493:GLN:OE1  | 2.22                     | 0.40              |
| 1:A:280:ILE:HG12 | 1:A:310:ILE:HB   | 2.03                     | 0.40              |
| 1:A:332:ALA:N    | 1:A:375:ASN:OD1  | 2.53                     | 0.40              |
| 1:B:444:THR:O    | 1:B:448:LYS:CB   | 2.61                     | 0.40              |
| 1:B:10:GLN:NE2   | 1:C:172:GLN:HE21 | 2.19                     | 0.40              |
| 1:C:446:TYR:CE2  | 1:C:455:ARG:HD3  | 2.57                     | 0.40              |
| 1:C:463:ALA:O    | 1:C:467:LYS:HB3  | 2.21                     | 0.40              |
| 1:D:170:ASN:HD22 | 1:D:172:GLN:N    | 2.09                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 497/506 (98%)   | 450 (90%)  | 39 (8%)   | 8 (2%)   | 11          | 36 |
| 1   | B     | 497/506 (98%)   | 425 (86%)  | 58 (12%)  | 14 (3%)  | 6           | 19 |
| 1   | C     | 497/506 (98%)   | 427 (86%)  | 54 (11%)  | 16 (3%)  | 5           | 16 |
| 1   | D     | 497/506 (98%)   | 438 (88%)  | 50 (10%)  | 9 (2%)   | 10          | 32 |
| All | All   | 1988/2024 (98%) | 1740 (88%) | 201 (10%) | 47 (2%)  | 7           | 23 |

All (47) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 43  | VAL  |
| 1   | A     | 100 | GLU  |
| 1   | B     | 4   | ARG  |
| 1   | B     | 100 | GLU  |
| 1   | B     | 124 | THR  |
| 1   | B     | 437 | ASP  |
| 1   | C     | 206 | ASP  |
| 1   | C     | 209 | ARG  |
| 1   | D     | 100 | GLU  |
| 1   | D     | 413 | HIS  |
| 1   | A     | 19  | ALA  |
| 1   | A     | 20  | ALA  |
| 1   | B     | 17  | GLN  |
| 1   | B     | 448 | LYS  |
| 1   | C     | 19  | ALA  |
| 1   | C     | 53  | ASP  |
| 1   | C     | 100 | GLU  |
| 1   | C     | 211 | MET  |
| 1   | C     | 224 | ALA  |
| 1   | C     | 240 | GLY  |
| 1   | D     | 91  | THR  |
| 1   | D     | 271 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 101 | HIS  |
| 1   | A     | 437 | ASP  |
| 1   | A     | 500 | ASN  |
| 1   | B     | 19  | ALA  |
| 1   | C     | 440 | THR  |
| 1   | C     | 470 | GLN  |
| 1   | D     | 19  | ALA  |
| 1   | D     | 411 | PRO  |
| 1   | B     | 16  | GLU  |
| 1   | D     | 437 | ASP  |
| 1   | A     | 498 | LYS  |
| 1   | B     | 18  | ARG  |
| 1   | B     | 270 | THR  |
| 1   | B     | 325 | PHE  |
| 1   | C     | 346 | PRO  |
| 1   | D     | 36  | ASP  |
| 1   | D     | 216 | SER  |
| 1   | B     | 347 | ASP  |
| 1   | C     | 304 | HIS  |
| 1   | C     | 373 | PRO  |
| 1   | B     | 203 | GLY  |
| 1   | B     | 115 | VAL  |
| 1   | C     | 127 | ASP  |
| 1   | C     | 181 | VAL  |
| 1   | C     | 439 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 431/437 (99%)   | 400 (93%)  | 31 (7%)  | 17          | 43 |
| 1   | B     | 431/437 (99%)   | 392 (91%)  | 39 (9%)  | 11          | 32 |
| 1   | C     | 431/437 (99%)   | 388 (90%)  | 43 (10%) | 9           | 26 |
| 1   | D     | 431/437 (99%)   | 404 (94%)  | 27 (6%)  | 21          | 51 |
| All | All   | 1724/1748 (99%) | 1584 (92%) | 140 (8%) | 14          | 37 |

All (140) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | ARG  |
| 1   | A     | 18  | ARG  |
| 1   | A     | 26  | LEU  |
| 1   | A     | 37  | LYS  |
| 1   | A     | 43  | VAL  |
| 1   | A     | 49  | LEU  |
| 1   | A     | 54  | VAL  |
| 1   | A     | 106 | THR  |
| 1   | A     | 131 | PHE  |
| 1   | A     | 137 | THR  |
| 1   | A     | 148 | ASN  |
| 1   | A     | 191 | SER  |
| 1   | A     | 194 | GLN  |
| 1   | A     | 202 | ARG  |
| 1   | A     | 235 | TYR  |
| 1   | A     | 263 | ASP  |
| 1   | A     | 309 | LEU  |
| 1   | A     | 336 | SER  |
| 1   | A     | 361 | HIS  |
| 1   | A     | 379 | ARG  |
| 1   | A     | 394 | MET  |
| 1   | A     | 402 | ASN  |
| 1   | A     | 407 | SER  |
| 1   | A     | 413 | HIS  |
| 1   | A     | 421 | ARG  |
| 1   | A     | 435 | ASN  |
| 1   | A     | 436 | ASP  |
| 1   | A     | 456 | LYS  |
| 1   | A     | 476 | LYS  |
| 1   | A     | 488 | TYR  |
| 1   | A     | 496 | LEU  |
| 1   | B     | 18  | ARG  |
| 1   | B     | 21  | GLN  |
| 1   | B     | 32  | ASN  |
| 1   | B     | 37  | LYS  |
| 1   | B     | 41  | LEU  |
| 1   | B     | 46  | ARG  |
| 1   | B     | 51  | VAL  |
| 1   | B     | 67  | ARG  |
| 1   | B     | 92  | ARG  |
| 1   | B     | 95  | LYS  |
| 1   | B     | 101 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 114 | THR  |
| 1   | B     | 124 | THR  |
| 1   | B     | 126 | ARG  |
| 1   | B     | 131 | PHE  |
| 1   | B     | 137 | THR  |
| 1   | B     | 149 | THR  |
| 1   | B     | 168 | LYS  |
| 1   | B     | 193 | HIS  |
| 1   | B     | 202 | ARG  |
| 1   | B     | 220 | LYS  |
| 1   | B     | 232 | LYS  |
| 1   | B     | 235 | TYR  |
| 1   | B     | 262 | ARG  |
| 1   | B     | 272 | ASN  |
| 1   | B     | 290 | ILE  |
| 1   | B     | 312 | VAL  |
| 1   | B     | 336 | SER  |
| 1   | B     | 374 | VAL  |
| 1   | B     | 381 | ARG  |
| 1   | B     | 393 | MET  |
| 1   | B     | 394 | MET  |
| 1   | B     | 402 | ASN  |
| 1   | B     | 412 | GLU  |
| 1   | B     | 416 | SER  |
| 1   | B     | 427 | ASP  |
| 1   | B     | 447 | LEU  |
| 1   | B     | 457 | ARG  |
| 1   | B     | 466 | LEU  |
| 1   | C     | 3   | ASN  |
| 1   | C     | 4   | ARG  |
| 1   | C     | 18  | ARG  |
| 1   | C     | 26  | LEU  |
| 1   | C     | 34  | VAL  |
| 1   | C     | 46  | ARG  |
| 1   | C     | 52  | GLN  |
| 1   | C     | 88  | HIS  |
| 1   | C     | 92  | ARG  |
| 1   | C     | 105 | ARG  |
| 1   | C     | 131 | PHE  |
| 1   | C     | 147 | ASN  |
| 1   | C     | 149 | THR  |
| 1   | C     | 179 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 194 | GLN  |
| 1   | C     | 200 | SER  |
| 1   | C     | 201 | ASP  |
| 1   | C     | 202 | ARG  |
| 1   | C     | 206 | ASP  |
| 1   | C     | 209 | ARG  |
| 1   | C     | 210 | HIS  |
| 1   | C     | 235 | TYR  |
| 1   | C     | 237 | THR  |
| 1   | C     | 239 | GLN  |
| 1   | C     | 248 | ASP  |
| 1   | C     | 293 | PHE  |
| 1   | C     | 304 | HIS  |
| 1   | C     | 331 | LEU  |
| 1   | C     | 345 | SER  |
| 1   | C     | 381 | ARG  |
| 1   | C     | 402 | ASN  |
| 1   | C     | 412 | GLU  |
| 1   | C     | 413 | HIS  |
| 1   | C     | 414 | GLN  |
| 1   | C     | 418 | LEU  |
| 1   | C     | 432 | ASN  |
| 1   | C     | 436 | ASP  |
| 1   | C     | 438 | ASN  |
| 1   | C     | 451 | ASN  |
| 1   | C     | 467 | LYS  |
| 1   | C     | 472 | PHE  |
| 1   | C     | 488 | TYR  |
| 1   | C     | 501 | GLU  |
| 1   | D     | 18  | ARG  |
| 1   | D     | 22  | LYS  |
| 1   | D     | 105 | ARG  |
| 1   | D     | 111 | ARG  |
| 1   | D     | 124 | THR  |
| 1   | D     | 127 | ASP  |
| 1   | D     | 131 | PHE  |
| 1   | D     | 138 | GLU  |
| 1   | D     | 147 | ASN  |
| 1   | D     | 148 | ASN  |
| 1   | D     | 193 | HIS  |
| 1   | D     | 235 | TYR  |
| 1   | D     | 247 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 261 | LEU  |
| 1   | D     | 263 | ASP  |
| 1   | D     | 280 | ILE  |
| 1   | D     | 301 | VAL  |
| 1   | D     | 368 | ASN  |
| 1   | D     | 378 | TYR  |
| 1   | D     | 397 | GLN  |
| 1   | D     | 412 | GLU  |
| 1   | D     | 413 | HIS  |
| 1   | D     | 421 | ARG  |
| 1   | D     | 438 | ASN  |
| 1   | D     | 467 | LYS  |
| 1   | D     | 479 | LYS  |
| 1   | D     | 488 | TYR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 17  | GLN  |
| 1   | A     | 148 | ASN  |
| 1   | A     | 167 | GLN  |
| 1   | A     | 254 | HIS  |
| 1   | A     | 320 | ASN  |
| 1   | A     | 337 | ASN  |
| 1   | A     | 423 | HIS  |
| 1   | A     | 429 | GLN  |
| 1   | A     | 454 | GLN  |
| 1   | A     | 470 | GLN  |
| 1   | A     | 485 | HIS  |
| 1   | B     | 17  | GLN  |
| 1   | B     | 21  | GLN  |
| 1   | B     | 32  | ASN  |
| 1   | B     | 62  | HIS  |
| 1   | B     | 272 | ASN  |
| 1   | B     | 320 | ASN  |
| 1   | B     | 337 | ASN  |
| 1   | B     | 361 | HIS  |
| 1   | B     | 363 | HIS  |
| 1   | B     | 402 | ASN  |
| 1   | B     | 414 | GLN  |
| 1   | B     | 429 | GLN  |
| 1   | B     | 435 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 461 | ASN  |
| 1   | C     | 17  | GLN  |
| 1   | C     | 52  | GLN  |
| 1   | C     | 167 | GLN  |
| 1   | C     | 172 | GLN  |
| 1   | C     | 239 | GLN  |
| 1   | C     | 272 | ASN  |
| 1   | C     | 337 | ASN  |
| 1   | C     | 402 | ASN  |
| 1   | C     | 414 | GLN  |
| 1   | C     | 432 | ASN  |
| 1   | C     | 435 | ASN  |
| 1   | C     | 438 | ASN  |
| 1   | C     | 454 | GLN  |
| 1   | C     | 461 | ASN  |
| 1   | C     | 474 | GLN  |
| 1   | C     | 500 | ASN  |
| 1   | D     | 32  | ASN  |
| 1   | D     | 52  | GLN  |
| 1   | D     | 148 | ASN  |
| 1   | D     | 167 | GLN  |
| 1   | D     | 170 | ASN  |
| 1   | D     | 193 | HIS  |
| 1   | D     | 239 | GLN  |
| 1   | D     | 337 | ASN  |
| 1   | D     | 368 | ASN  |
| 1   | D     | 413 | HIS  |
| 1   | D     | 480 | ASN  |
| 1   | D     | 500 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

6 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |       |          | Bond angles |       |          |
|-----|------|-------|------|------|--------------|-------|----------|-------------|-------|----------|
|     |      |       |      |      | Counts       | RMSZ  | # Z  > 2 | Counts      | RMSZ  | # Z  > 2 |
| 3   | HEM  | A     | 2000 | 1    | 28,50,50     | 12.50 | 9 (32%)  | 17,82,82    | 13.02 | 2 (11%)  |
| 2   | CYN  | A     | 3000 | -    | 0,1,1        | 0.00  | -        | 0,0,0       | 0.00  | -        |
| 3   | HEM  | B     | 2001 | 1    | 28,50,50     | 12.98 | 11 (39%) | 17,82,82    | 14.53 | 6 (35%)  |
| 3   | HEM  | C     | 2002 | 1    | 28,50,50     | 1.92  | 7 (25%)  | 17,82,82    | 2.82  | 2 (11%)  |
| 3   | HEM  | D     | 2003 | 1,2  | 28,50,50     | 2.04  | 9 (32%)  | 17,82,82    | 10.95 | 5 (29%)  |
| 2   | CYN  | D     | 3001 | 3    | 0,1,1        | 0.00  | -        | 0,0,0       | 0.00  | -        |

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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 3   | HEM  | A     | 2000 | 1    | -       | 0/6/54/54 | 0/0/8/8 |
| 2   | CYN  | A     | 3000 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 3   | HEM  | B     | 2001 | 1    | -       | 0/6/54/54 | 0/0/8/8 |
| 3   | HEM  | C     | 2002 | 1    | -       | 0/6/54/54 | 0/0/8/8 |
| 3   | HEM  | D     | 2003 | 1,2  | -       | 0/6/54/54 | 0/0/8/8 |
| 2   | CYN  | D     | 3001 | 3    | -       | 0/0/0/0   | 0/0/0/0 |

All (36) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | B     | 2001 | HEM  | C3B-CAB | -4.59 | 1.38        | 1.47     |
| 3   | C     | 2002 | HEM  | C3B-CAB | -4.57 | 1.38        | 1.47     |
| 3   | D     | 2003 | HEM  | C3B-CAB | -4.54 | 1.38        | 1.47     |
| 3   | A     | 2000 | HEM  | C3B-CAB | -4.46 | 1.39        | 1.47     |
| 3   | A     | 2000 | HEM  | C3B-C2B | -4.03 | 1.35        | 1.40     |
| 3   | D     | 2003 | HEM  | C3B-C2B | -4.03 | 1.35        | 1.40     |
| 3   | C     | 2002 | HEM  | C3B-C2B | -3.96 | 1.35        | 1.40     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | B     | 2001 | HEM  | C3B-C2B | -3.92 | 1.35        | 1.40     |
| 3   | A     | 2000 | HEM  | C3C-C2C | -3.28 | 1.36        | 1.40     |
| 3   | B     | 2001 | HEM  | C3C-C2C | -3.20 | 1.36        | 1.40     |
| 3   | B     | 2001 | HEM  | C4B-CHC | -2.69 | 1.33        | 1.40     |
| 3   | C     | 2002 | HEM  | C3C-C2C | -2.60 | 1.36        | 1.40     |
| 3   | D     | 2003 | HEM  | C3C-C2C | -2.54 | 1.37        | 1.40     |
| 3   | B     | 2001 | HEM  | CAA-C2A | 2.10  | 1.55        | 1.52     |
| 3   | B     | 2001 | HEM  | C1C-NC  | 2.20  | 1.39        | 1.36     |
| 3   | D     | 2003 | HEM  | C3C-CAC | 2.37  | 1.52        | 1.47     |
| 3   | D     | 2003 | HEM  | C1A-CHA | 2.40  | 1.46        | 1.40     |
| 3   | C     | 2002 | HEM  | C1C-NC  | 2.61  | 1.39        | 1.36     |
| 3   | D     | 2003 | HEM  | C1C-NC  | 2.75  | 1.40        | 1.36     |
| 3   | A     | 2000 | HEM  | C1C-NC  | 2.84  | 1.40        | 1.36     |
| 3   | D     | 2003 | HEM  | C1B-NB  | 3.11  | 1.40        | 1.36     |
| 3   | A     | 2000 | HEM  | C1B-NB  | 3.11  | 1.40        | 1.36     |
| 3   | B     | 2001 | HEM  | C1B-NB  | 3.11  | 1.40        | 1.36     |
| 3   | C     | 2002 | HEM  | C1B-NB  | 3.13  | 1.40        | 1.36     |
| 3   | B     | 2001 | HEM  | CBC-CAC | 3.14  | 1.51        | 1.28     |
| 3   | D     | 2003 | HEM  | CBC-CAC | 3.27  | 1.51        | 1.28     |
| 3   | C     | 2002 | HEM  | CBC-CAC | 3.31  | 1.52        | 1.28     |
| 3   | A     | 2000 | HEM  | CBC-CAC | 3.34  | 1.52        | 1.28     |
| 3   | D     | 2003 | HEM  | C4C-NC  | 3.55  | 1.41        | 1.36     |
| 3   | C     | 2002 | HEM  | C4C-NC  | 3.57  | 1.41        | 1.36     |
| 3   | B     | 2001 | HEM  | C4C-NC  | 3.68  | 1.41        | 1.36     |
| 3   | A     | 2000 | HEM  | C4C-NC  | 3.94  | 1.41        | 1.36     |
| 3   | A     | 2000 | HEM  | C3C-CAC | 39.27 | 2.25        | 1.47     |
| 3   | B     | 2001 | HEM  | C3C-CAC | 43.62 | 2.34        | 1.47     |
| 3   | B     | 2001 | HEM  | CMC-C2C | 51.96 | 2.62        | 1.51     |
| 3   | A     | 2000 | HEM  | CMC-C2C | 52.17 | 2.62        | 1.51     |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 3   | A     | 2000 | HEM  | CMC-C2C-C3C | -53.59 | 25.47       | 124.89   |
| 3   | B     | 2001 | HEM  | CMC-C2C-C3C | -53.04 | 26.48       | 124.89   |
| 3   | B     | 2001 | HEM  | CBA-CAA-C2A | -4.31  | 104.23      | 112.48   |
| 3   | D     | 2003 | HEM  | CAD-C3D-C2D | -4.25  | 116.86      | 129.00   |
| 3   | C     | 2002 | HEM  | CBA-CAA-C2A | -2.29  | 108.11      | 112.48   |
| 3   | A     | 2000 | HEM  | CBA-CAA-C2A | -2.28  | 108.13      | 112.48   |
| 3   | B     | 2001 | HEM  | CAA-C2A-C3A | 3.45   | 138.85      | 129.00   |
| 3   | D     | 2003 | HEM  | CAD-CBD-CGD | 10.40  | 130.43      | 112.66   |
| 3   | C     | 2002 | HEM  | CMC-C2C-C3C | 11.17  | 145.62      | 124.89   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | D     | 2003 | HEM  | CBD-CAD-C3D | 14.89 | 140.87      | 112.47   |
| 3   | B     | 2001 | HEM  | CAD-CBD-CGD | 15.07 | 138.42      | 112.66   |
| 3   | B     | 2001 | HEM  | CBD-CAD-C3D | 15.95 | 142.90      | 112.47   |
| 3   | B     | 2001 | HEM  | CAA-CBA-CGA | 16.14 | 140.25      | 112.66   |
| 3   | D     | 2003 | HEM  | CBA-CAA-C2A | 23.15 | 156.75      | 112.48   |
| 3   | D     | 2003 | HEM  | CAA-CBA-CGA | 33.81 | 170.43      | 112.66   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 88 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | A     | 2000 | HEM  | 16      | 0            |
| 2   | A     | 3000 | CYN  | 6       | 0            |
| 3   | B     | 2001 | HEM  | 25      | 0            |
| 3   | C     | 2002 | HEM  | 26      | 0            |
| 3   | D     | 2003 | HEM  | 21      | 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     | 499/506 (98%)   | -0.62  | 2 (0%) 92 90 | 9, 29, 55, 85         | 0      |
| 1   | B     | 499/506 (98%)   | -0.49  | 2 (0%) 92 90 | 12, 37, 64, 97        | 0      |
| 1   | C     | 499/506 (98%)   | -0.49  | 3 (0%) 89 86 | 12, 33, 65, 90        | 1 (0%) |
| 1   | D     | 499/506 (98%)   | -0.49  | 0 100 100    | 10, 35, 69, 89        | 0      |
| All | All   | 1996/2024 (98%) | -0.52  | 7 (0%) 92 90 | 9, 34, 64, 97         | 1 (0%) |

All (7) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 3   | ASN  | 2.8  |
| 1   | A     | 3   | ASN  | 2.6  |
| 1   | C     | 20  | ALA  | 2.6  |
| 1   | A     | 20  | ALA  | 2.4  |
| 1   | C     | 471 | LEU  | 2.4  |
| 1   | B     | 20  | ALA  | 2.2  |
| 1   | C     | 415 | PRO  | 2.2  |

### 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 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 3   | HEM  | B     | 2001 | 43/43 | 0.92 | 0.25 | 3.09 | 20,37,58,100               | 0     |
| 3   | HEM  | D     | 2003 | 43/43 | 0.93 | 0.27 | 2.96 | 21,48,68,78                | 0     |
| 3   | HEM  | C     | 2002 | 43/43 | 0.94 | 0.21 | 2.53 | 22,37,54,101               | 0     |
| 3   | HEM  | A     | 2000 | 43/43 | 0.97 | 0.18 | 0.56 | 7,26,38,101                | 0     |
| 2   | CYN  | D     | 3001 | 2/2   | 0.99 | 0.12 | -    | 57,57,57,63                | 0     |
| 2   | CYN  | A     | 3000 | 2/2   | 1.00 | 0.17 | -    | 41,41,41,48                | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.