



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 12:10 AM BST

PDB ID : 2H35  
Title : Solution structure of Human normal adult hemoglobin  
Authors : Fan, J.S.; Yang, D.  
Deposited on : 2006-05-22

This is a Full wwPDB NMR 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/NMRValidationReportHelp>  
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:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

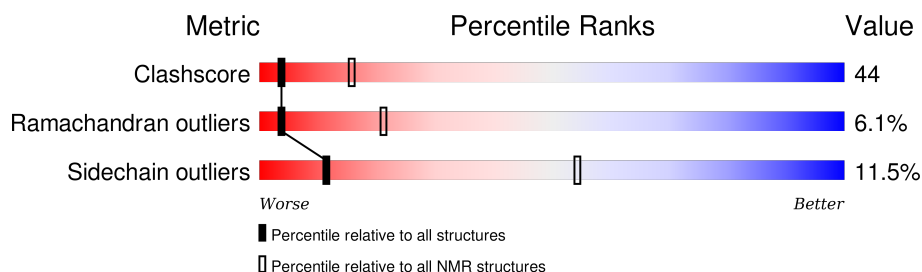
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 114402                      | 11133                     |
| Ramachandran outliers | 111179                      | 9975                      |
| Sidechain outliers    | 111093                      | 9958                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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  $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 141    |                  |
| 1   | C     | 141    |                  |
| 2   | B     | 146    |                  |
| 2   | D     | 146    |                  |

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues |   |                   |              |
|--------------------------------------|---|-------------------|--------------|
| Well-defined core                    | Residue range (total)   | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:1-A:41, A:45-A:138,<br>B:2-B:146, C:1-C:41, C:45-<br>C:138, D:2-D:146 (560) | 0.57              | 5            |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 4 single-model clusters were found.

| Cluster number        | Models                                |
|-----------------------|---------------------------------------|
| 1                     | 4, 5, 6, 7, 8, 10, 11, 12, 16, 17, 18 |
| 2                     | 9, 13, 14                             |
| 3                     | 3, 15                                 |
| Single-model clusters | 1; 2; 19; 20                          |

### 3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9104 atoms, of which 4548 are hydrogens and 0 are deuteriums.

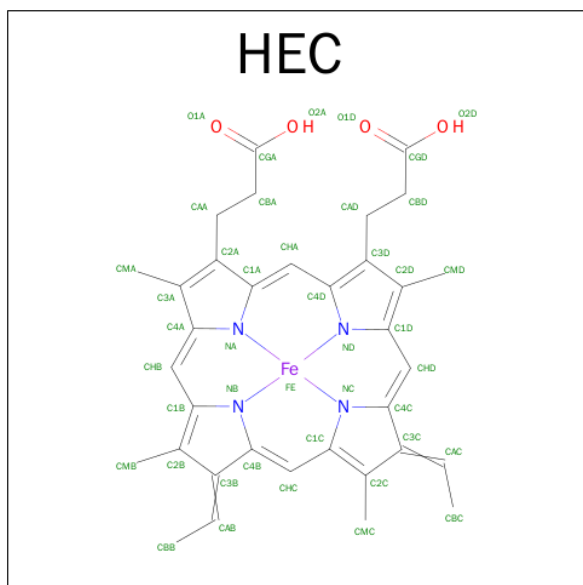
- Molecule 1 is a protein called Hemoglobin alpha subunit.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 141      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2152  | 685 | 1083 | 187 | 194 | 3 |       |
| 1   | C     | 141      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2152  | 685 | 1083 | 187 | 194 | 3 |       |

- Molecule 2 is a protein called Hemoglobin beta subunit.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 2   | B     | 146      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2250  | 724 | 1127 | 195 | 201 | 3 |       |
| 2   | D     | 146      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 2250  | 724 | 1127 | 195 | 201 | 3 |       |

- Molecule 3 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms |    |    |    |   |   |
|-----|-------|----------|-------|----|----|----|---|---|
| 3   | A     | 1        | Total | C  | Fe | H  | N | O |
|     |       |          | 75    | 34 | 1  | 32 | 4 | 4 |
| 3   | B     | 1        | Total | C  | Fe | H  | N | O |
|     |       |          | 75    | 34 | 1  | 32 | 4 | 4 |

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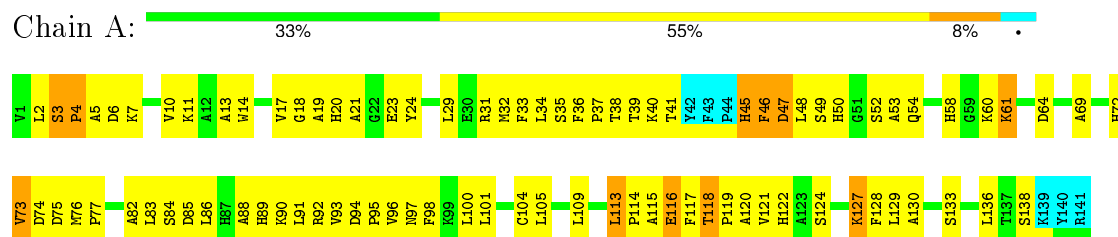
| Mol | Chain | Residues | Atoms |    |    |    |   |   |
|-----|-------|----------|-------|----|----|----|---|---|
|     |       |          | Total | C  | Fe | H  | N | O |
| 3   | C     | 1        | 75    | 34 | 1  | 32 | 4 | 4 |
| 3   | D     | 1        | 75    | 34 | 1  | 32 | 4 | 4 |

## 4 Residue-property plots

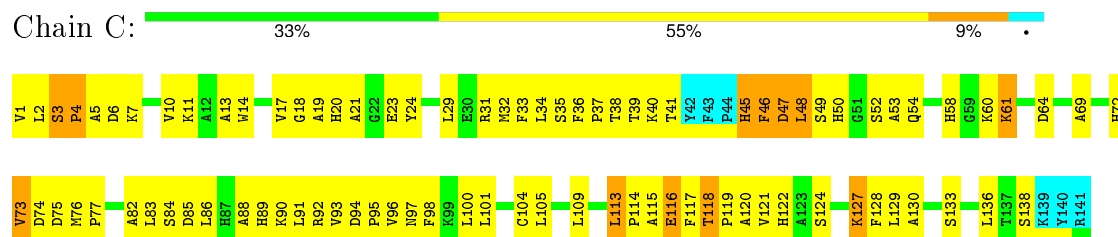
### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

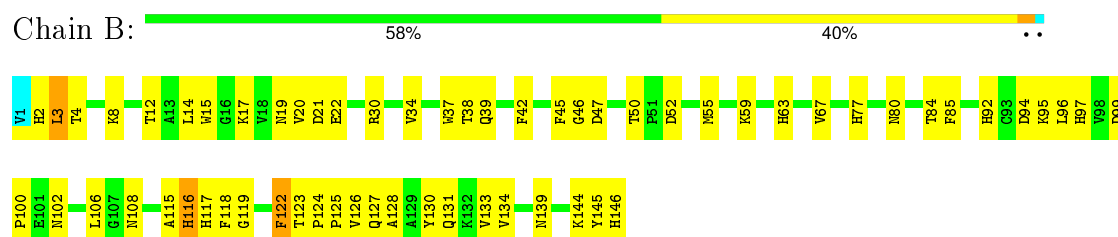
- Molecule 1: Hemoglobin alpha subunit



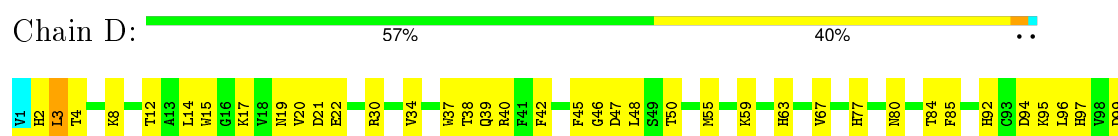
- Molecule 1: Hemoglobin alpha subunit

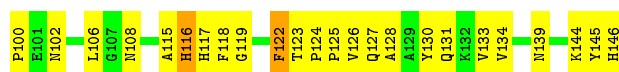


- Molecule 2: Hemoglobin beta subunit



- Molecule 2: Hemoglobin beta subunit





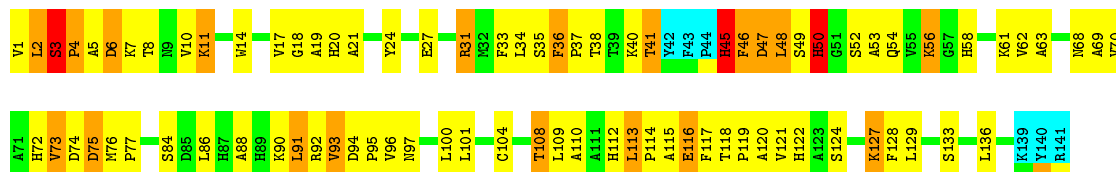
## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

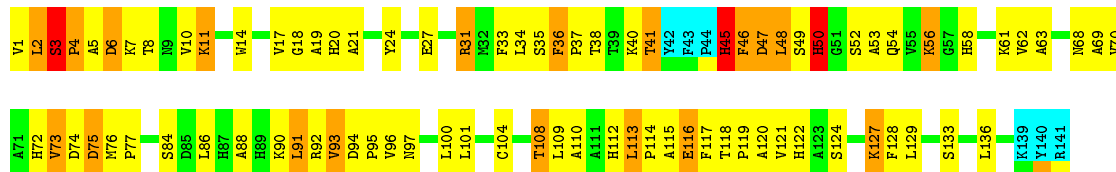
- Molecule 1: Hemoglobin alpha subunit

Chain A: 36% 44% 13% . .



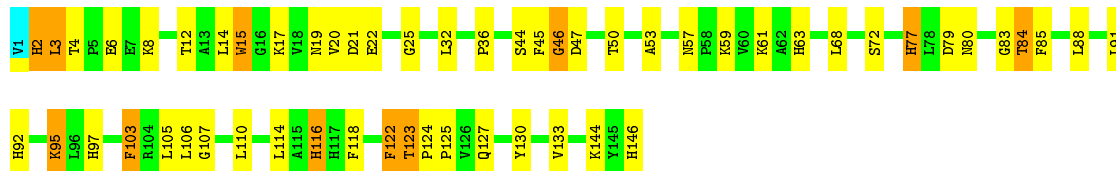
- Molecule 1: Hemoglobin alpha subunit

Chain C: 36% 44% 13% . .



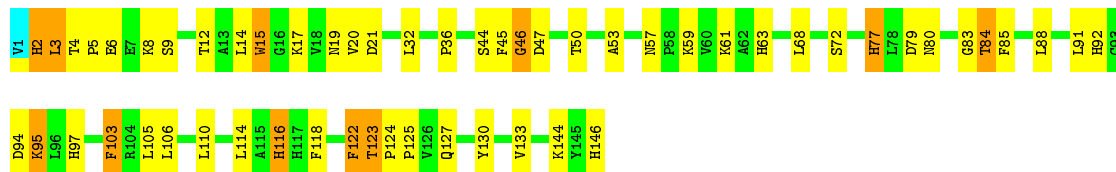
- Molecule 2: Hemoglobin beta subunit

Chain B: 61% 31% 8% .



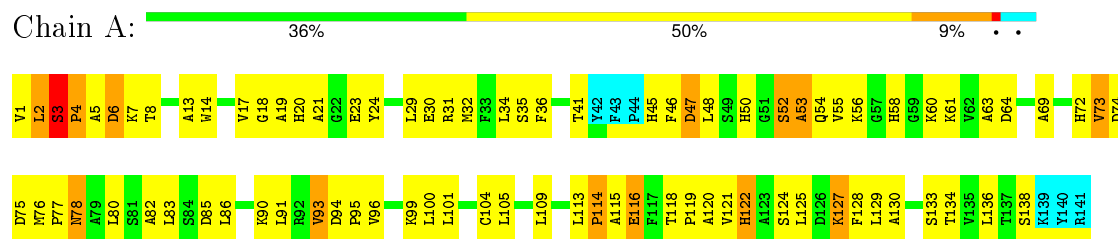
- Molecule 2: Hemoglobin beta subunit

Chain D: 61% 31% 8% .

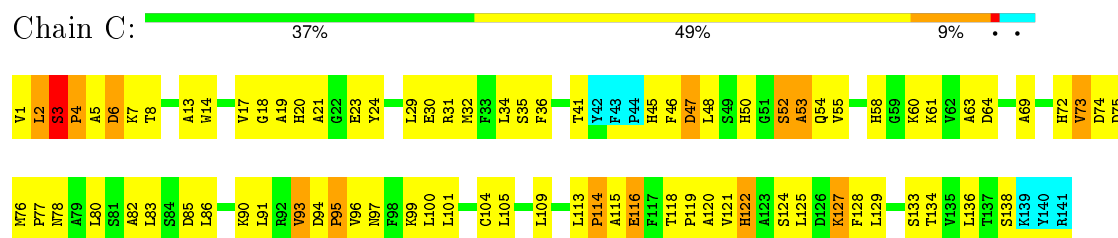


### 4.2.2 Score per residue for model 2

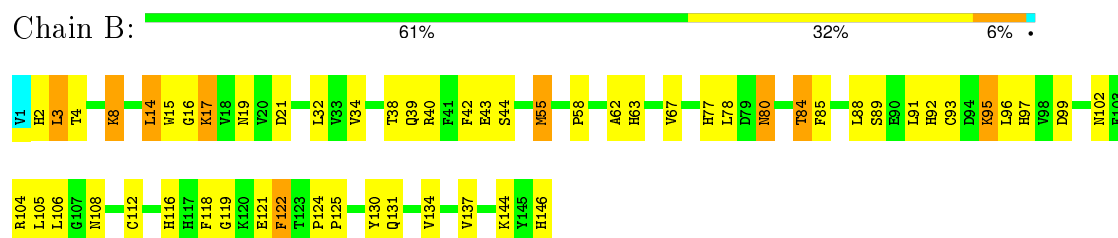
#### • Molecule 1: Hemoglobin alpha subunit



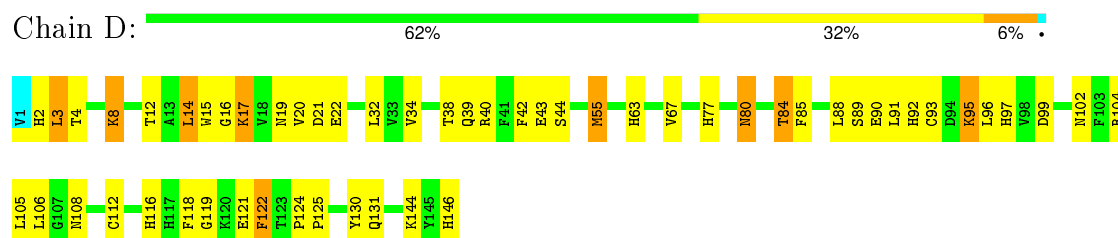
#### • Molecule 1: Hemoglobin alpha subunit



#### • Molecule 2: Hemoglobin beta subunit

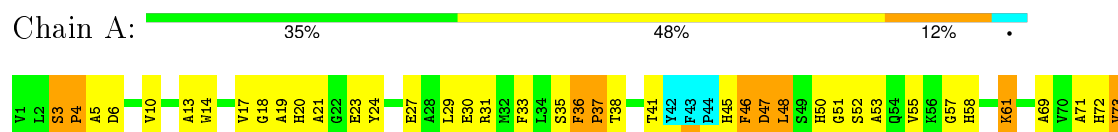


#### • Molecule 2: Hemoglobin beta subunit

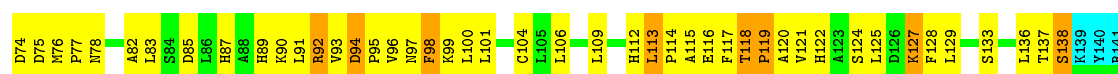


### 4.2.3 Score per residue for model 3

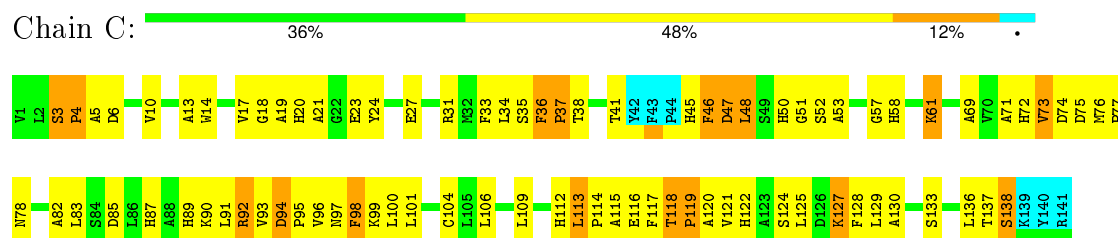
#### • Molecule 1: Hemoglobin alpha subunit



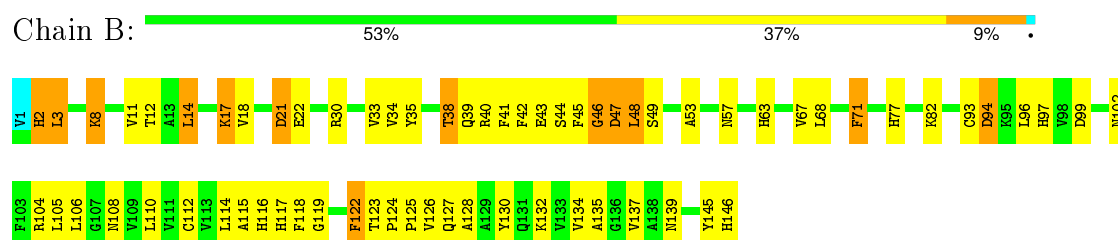




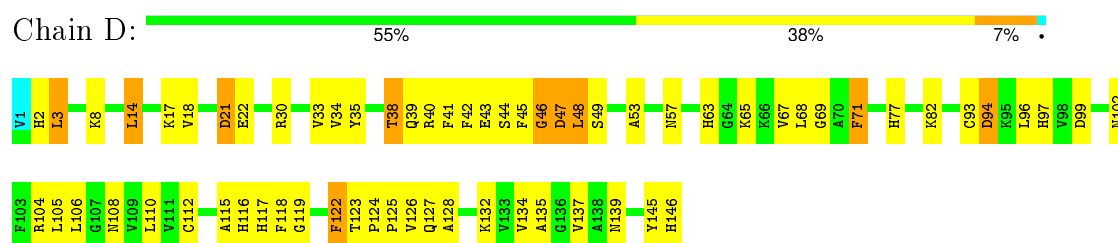
• Molecule 1: Hemoglobin alpha subunit



• Molecule 2: Hemoglobin beta subunit

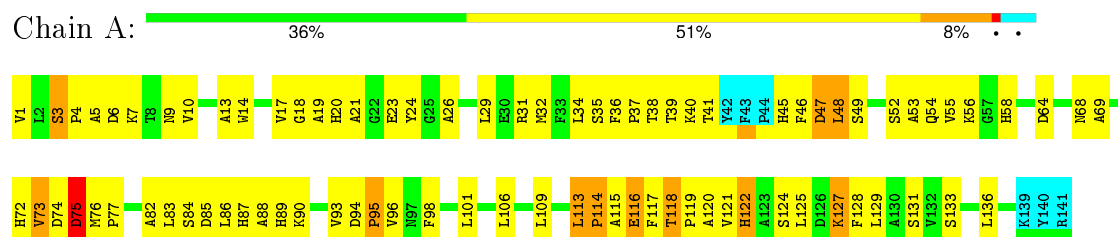


• Molecule 2: Hemoglobin beta subunit



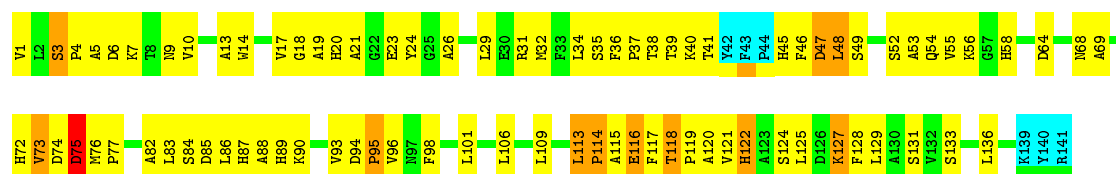
#### 4.2.4 Score per residue for model 4

• Molecule 1: Hemoglobin alpha subunit



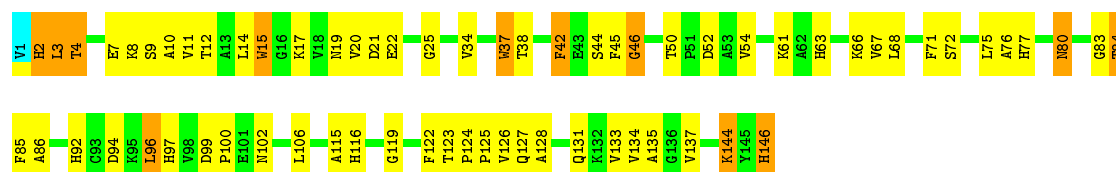
• Molecule 1: Hemoglobin alpha subunit





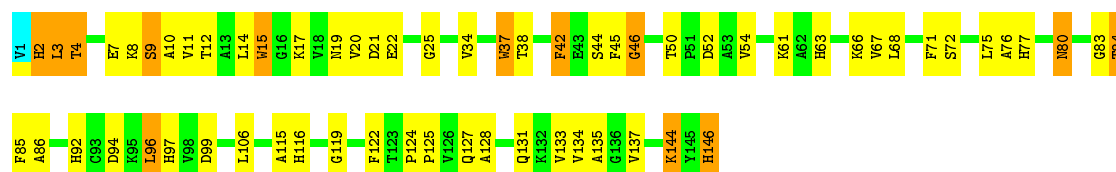
• Molecule 2: Hemoglobin beta subunit

Chain B: 53% 38% 8%



• Molecule 2: Hemoglobin beta subunit

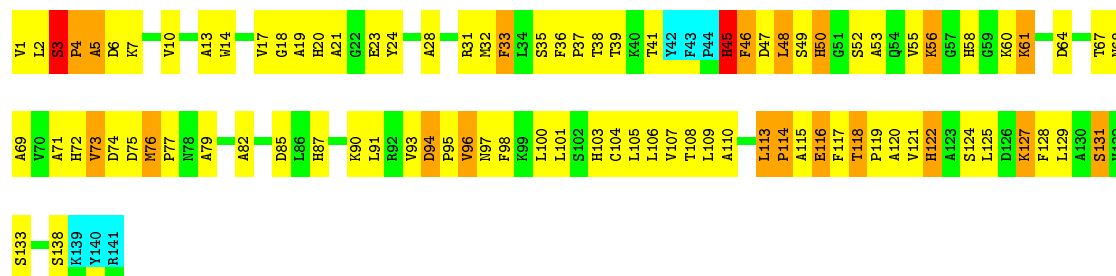
Chain D: 56% 34% 9%



#### 4.2.5 Score per residue for model 5 (medoid)

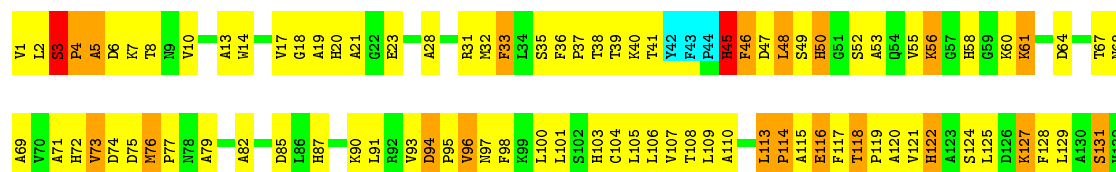
• Molecule 1: Hemoglobin alpha subunit

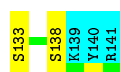
Chain A: 31% 50% 13%



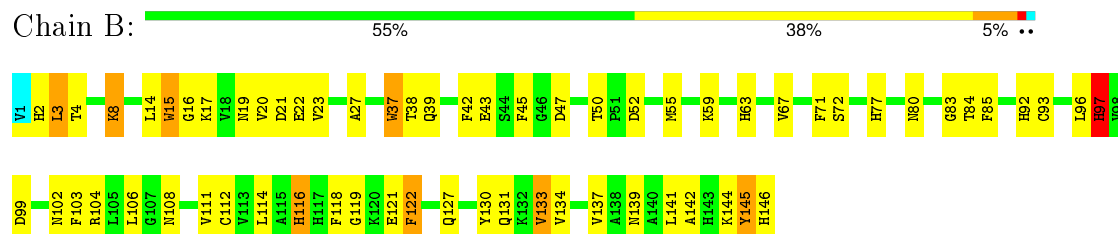
• Molecule 1: Hemoglobin alpha subunit

Chain C: 30% 50% 13%

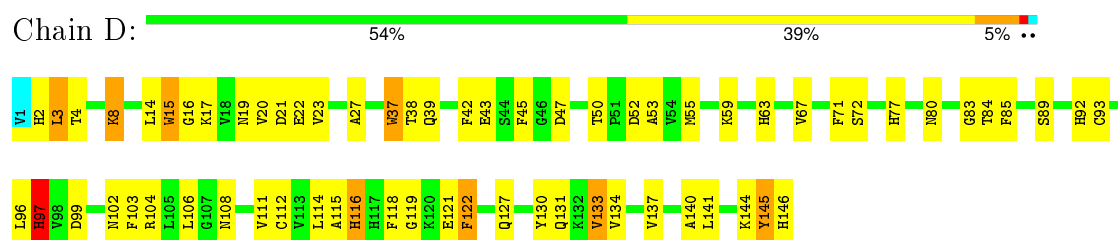




• Molecule 2: Hemoglobin beta subunit

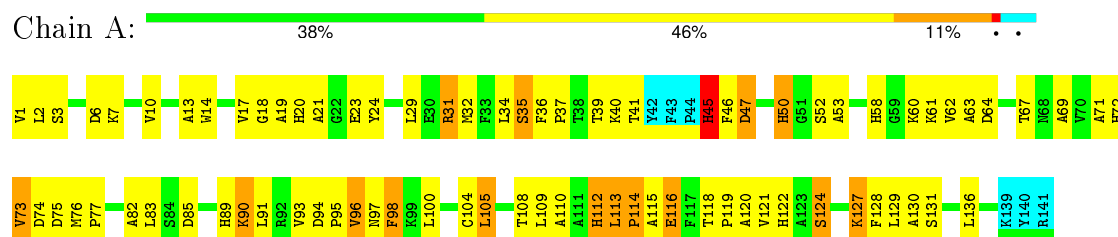


• Molecule 2: Hemoglobin beta subunit

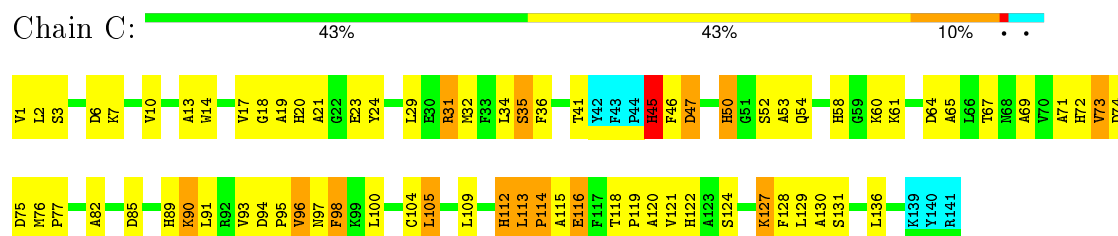


#### 4.2.6 Score per residue for model 6

• Molecule 1: Hemoglobin alpha subunit

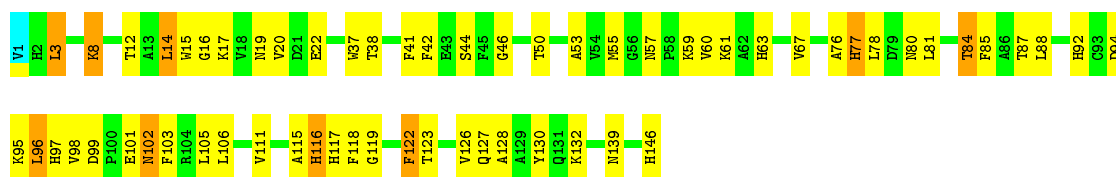


• Molecule 1: Hemoglobin alpha subunit



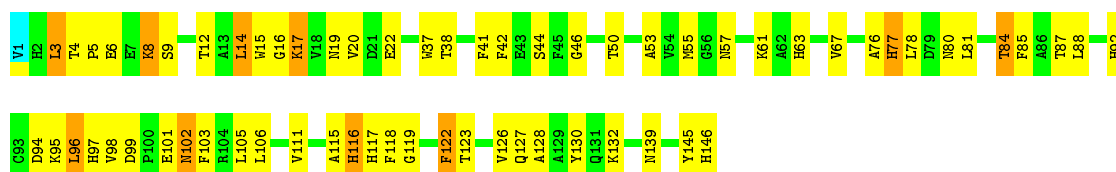
• Molecule 2: Hemoglobin beta subunit





- Molecule 2: Hemoglobin beta subunit

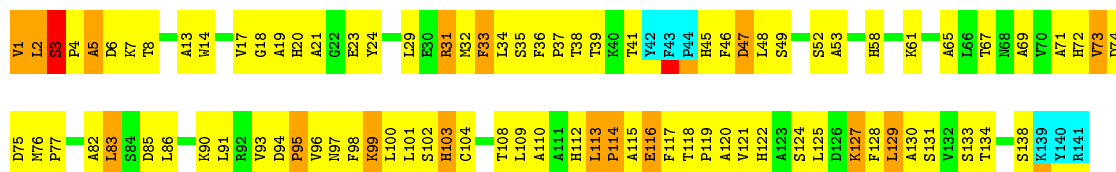
Chain D: 55% 37% 7%



#### 4.2.7 Score per residue for model 7

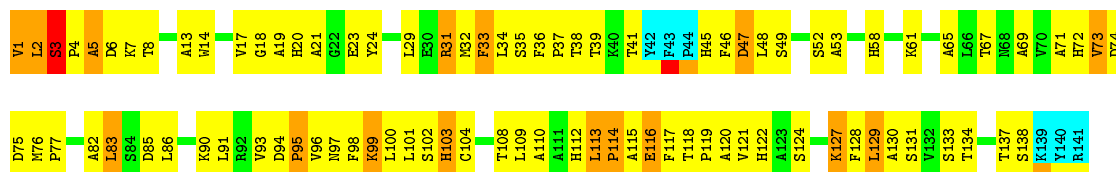
- Molecule 1: Hemoglobin alpha subunit

Chain A: 33% 51% 11%



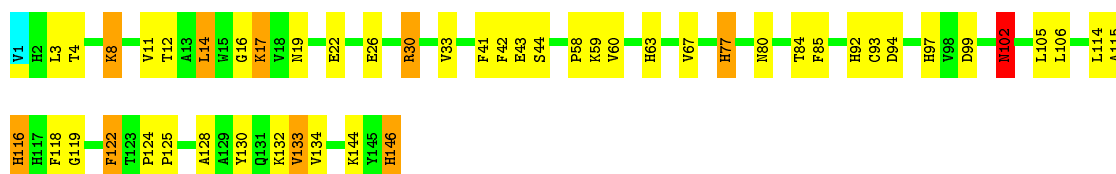
- Molecule 1: Hemoglobin alpha subunit

Chain C: 33% 51% 11%



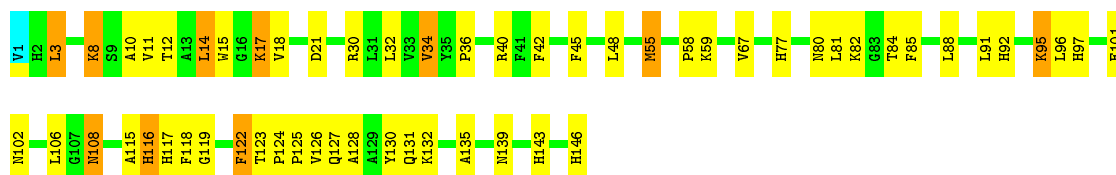
- Molecule 2: Hemoglobin beta subunit

Chain B: 66% 27% 6%



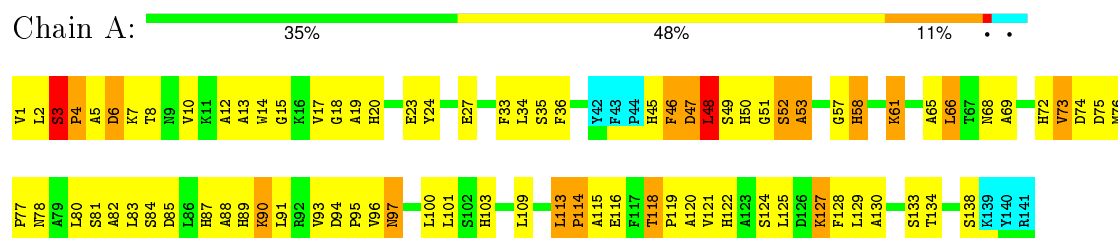
- Molecule 2: Hemoglobin beta subunit



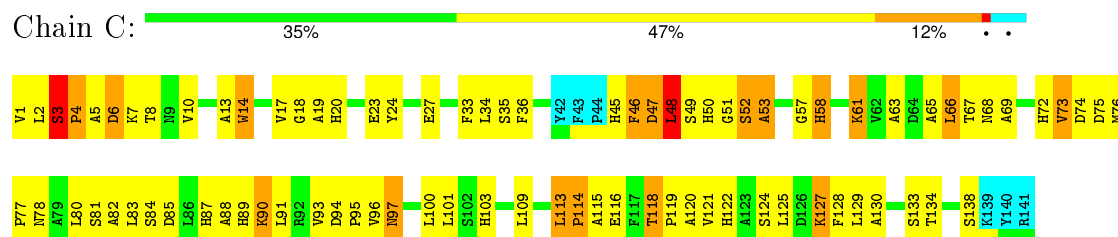


#### 4.2.9 Score per residue for model 9

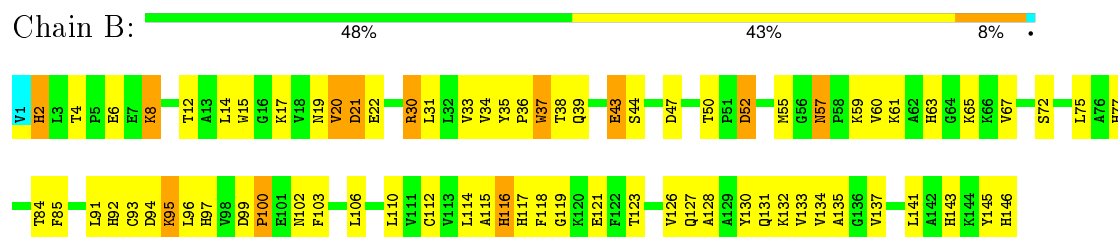
- Molecule 1: Hemoglobin alpha subunit



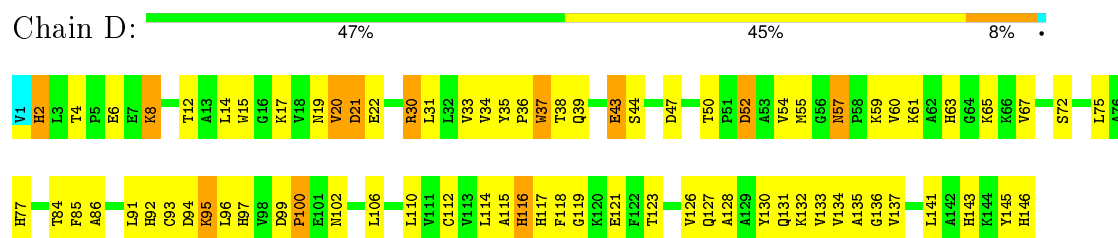
- Molecule 1: Hemoglobin alpha subunit



- Molecule 2: Hemoglobin beta subunit

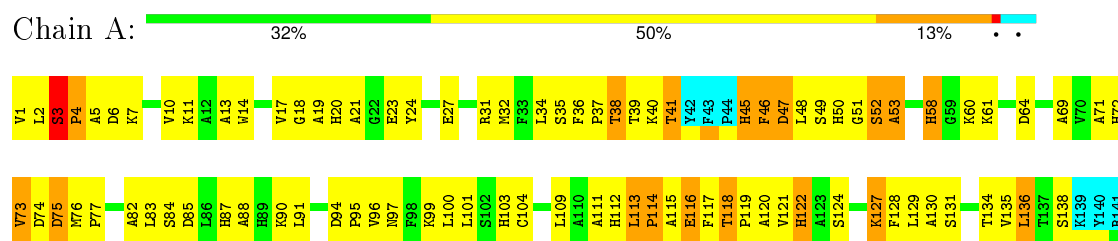


- Molecule 2: Hemoglobin beta subunit

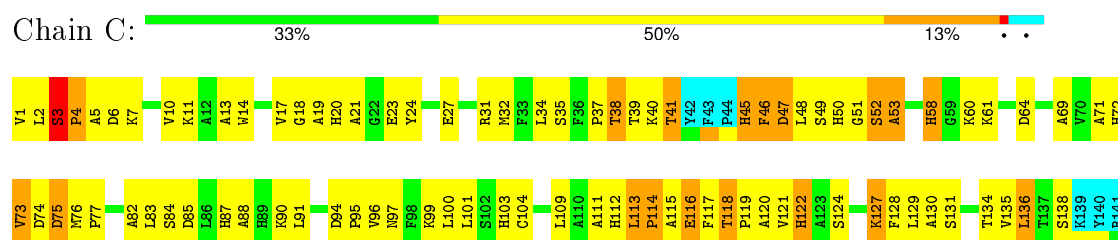


### 4.2.10 Score per residue for model 10

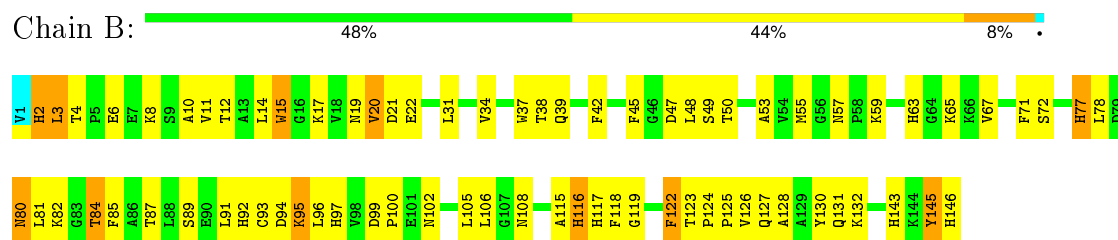
#### • Molecule 1: Hemoglobin alpha subunit



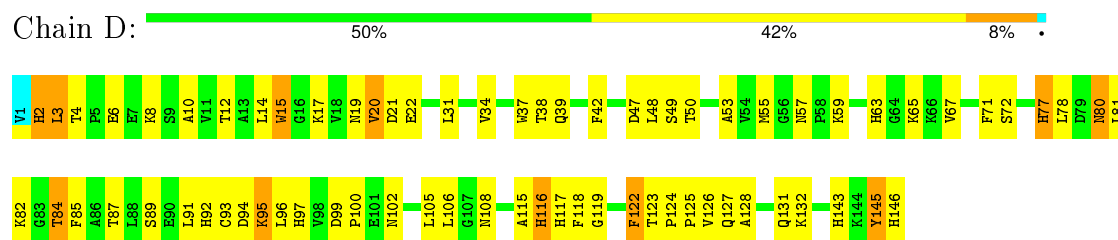
#### • Molecule 1: Hemoglobin alpha subunit



#### • Molecule 2: Hemoglobin beta subunit

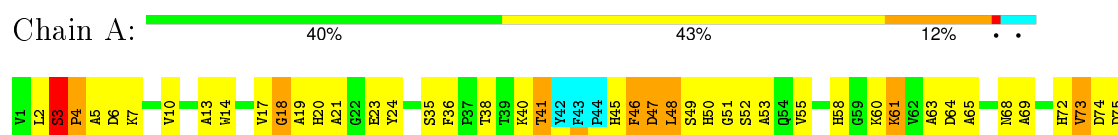


#### • Molecule 2: Hemoglobin beta subunit



### 4.2.11 Score per residue for model 11

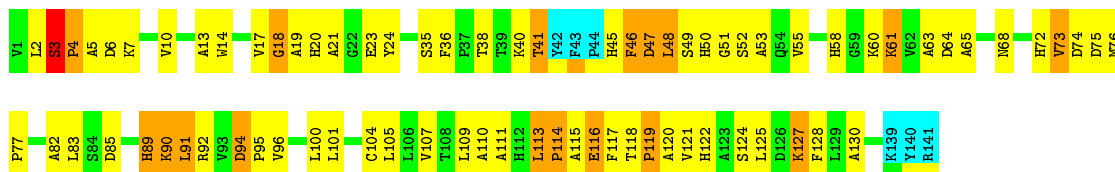
#### • Molecule 1: Hemoglobin alpha subunit





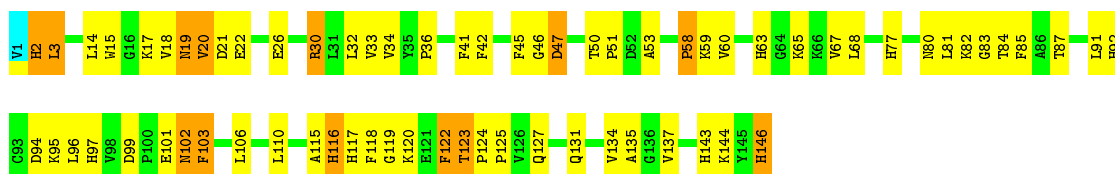
• Molecule 1: Hemoglobin alpha subunit

Chain C: 41% 42% 12%



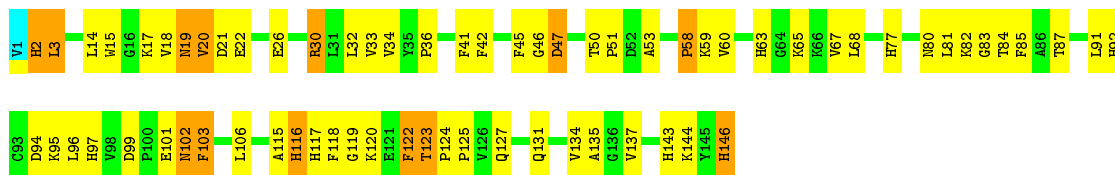
• Molecule 2: Hemoglobin beta subunit

Chain B: 52% 38% 9%



• Molecule 2: Hemoglobin beta subunit

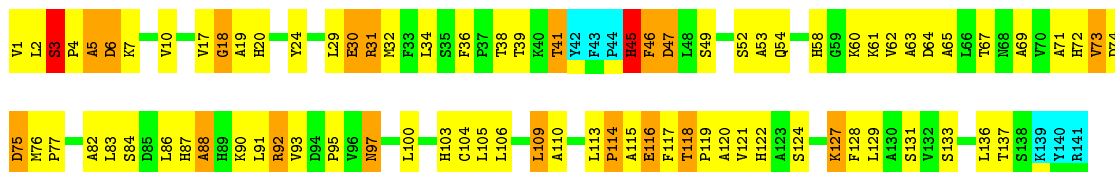
Chain D: 53% 38% 9%



#### 4.2.12 Score per residue for model 12

• Molecule 1: Hemoglobin alpha subunit

Chain A: 38% 44% 13%

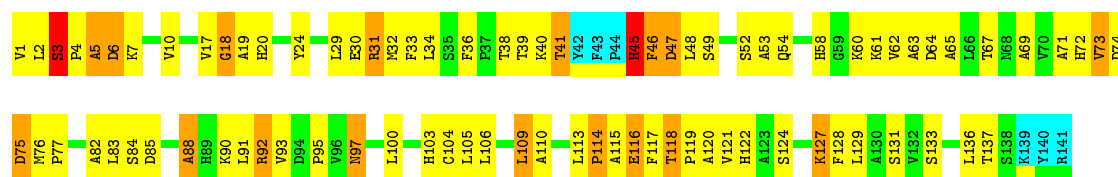


• Molecule 1: Hemoglobin alpha subunit

Chain C: 36% 46% 12%

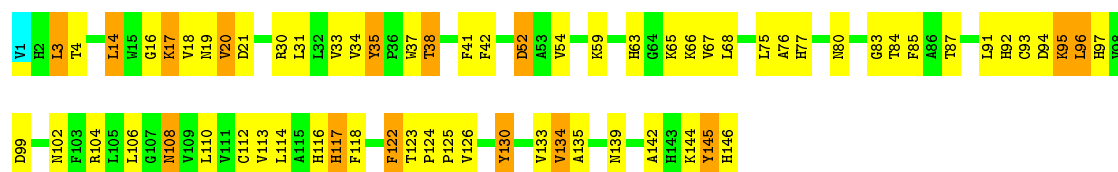






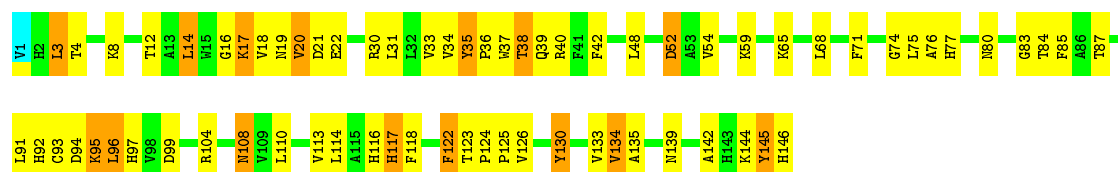
- Molecule 2: Hemoglobin beta subunit

Chain B: 53% 36% 10%



- Molecule 2: Hemoglobin beta subunit

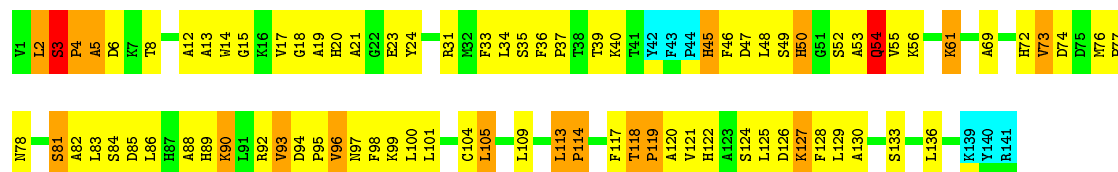
Chain D: 52% 37% 10%



#### 4.2.13 Score per residue for model 13

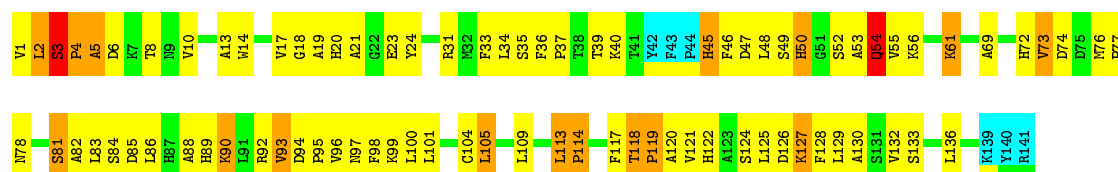
- Molecule 1: Hemoglobin alpha subunit

Chain A: 37% 45% 12%

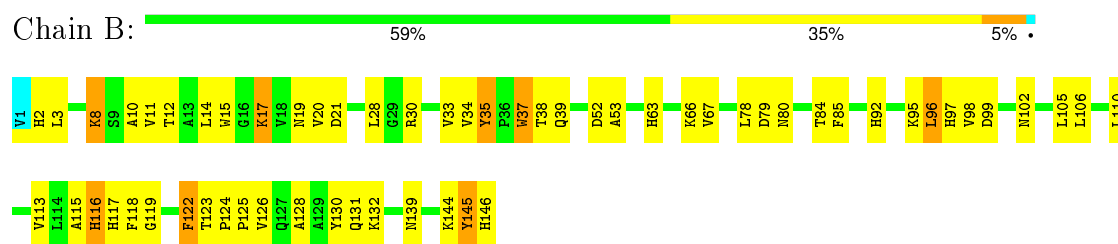


- Molecule 1: Hemoglobin alpha subunit

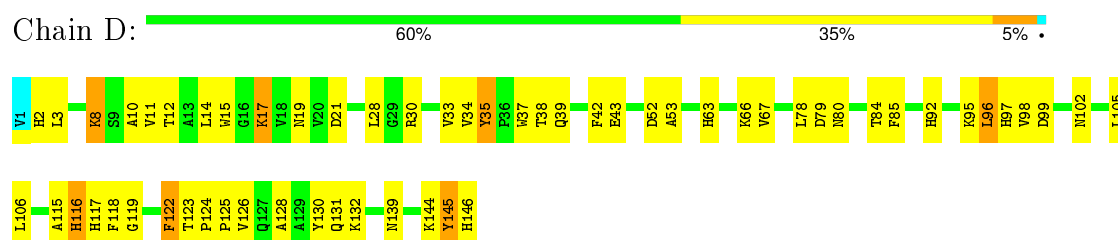
Chain C: 36% 47% 11%



- Molecule 2: Hemoglobin beta subunit

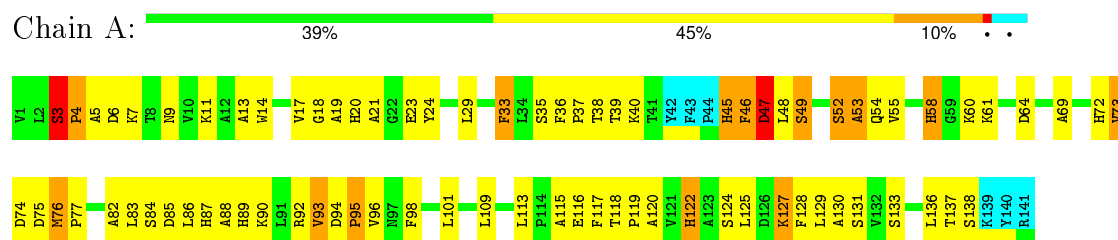


- Molecule 2: Hemoglobin beta subunit

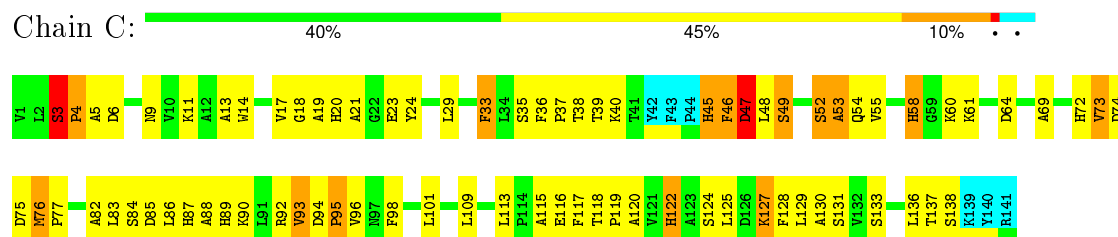


#### 4.2.14 Score per residue for model 14

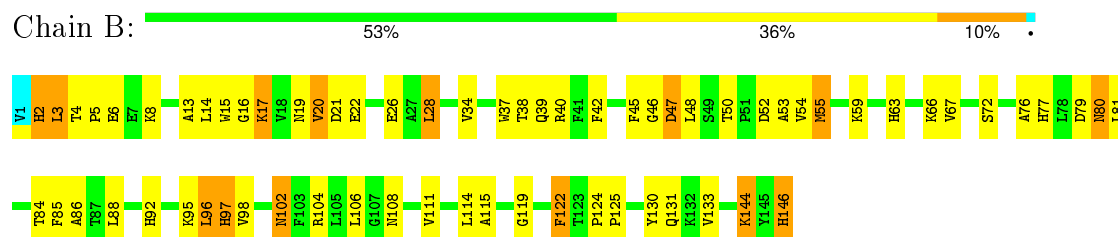
- Molecule 1: Hemoglobin alpha subunit



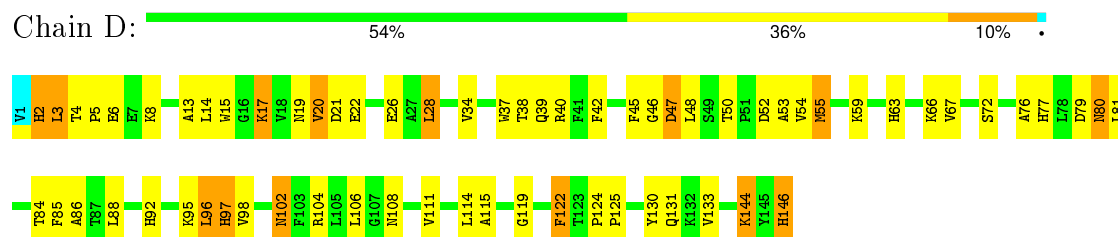
- Molecule 1: Hemoglobin alpha subunit



- Molecule 2: Hemoglobin beta subunit

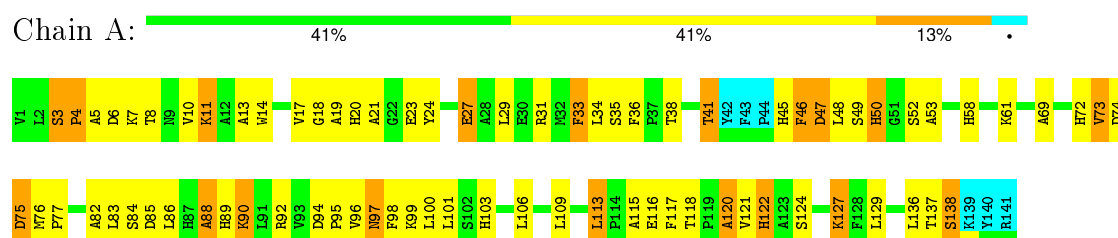


- Molecule 2: Hemoglobin beta subunit

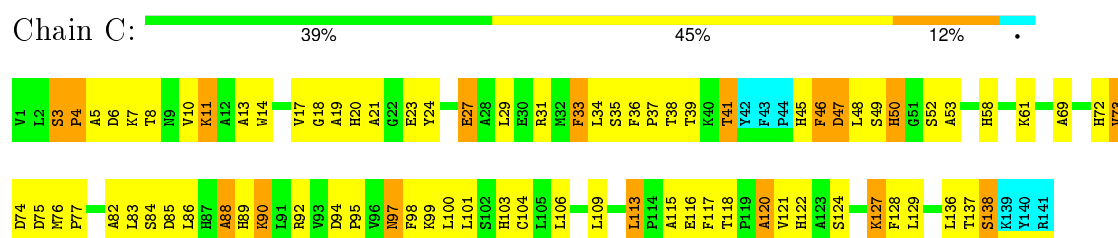


#### 4.2.15 Score per residue for model 15

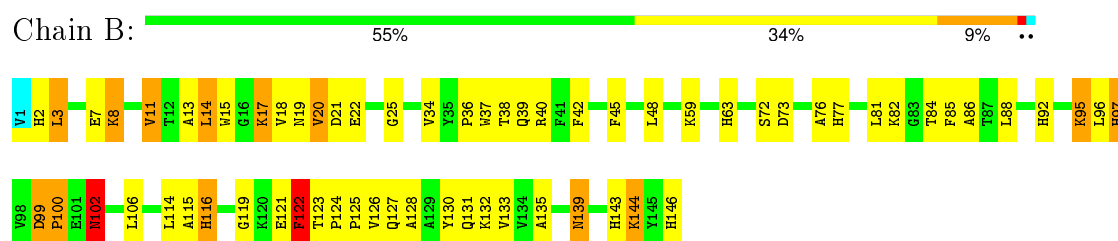
- Molecule 1: Hemoglobin alpha subunit



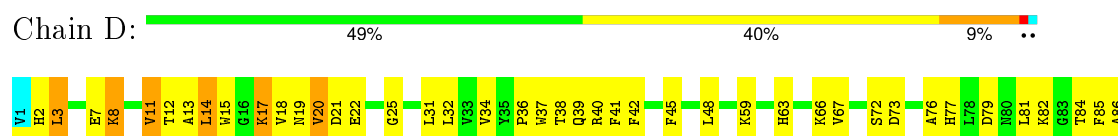
- Molecule 1: Hemoglobin alpha subunit



- Molecule 2: Hemoglobin beta subunit



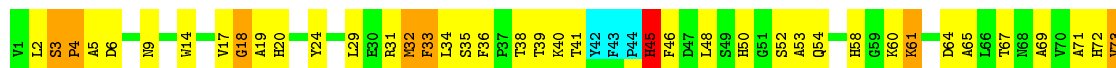
- Molecule 2: Hemoglobin beta subunit



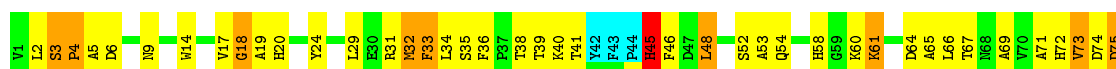


#### 4.2.16 Score per residue for model 16

- Molecule 1: Hemoglobin alpha subunit



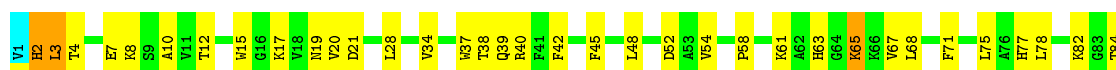
- Molecule 1: Hemoglobin alpha subunit



- Molecule 2: Hemoglobin beta subunit

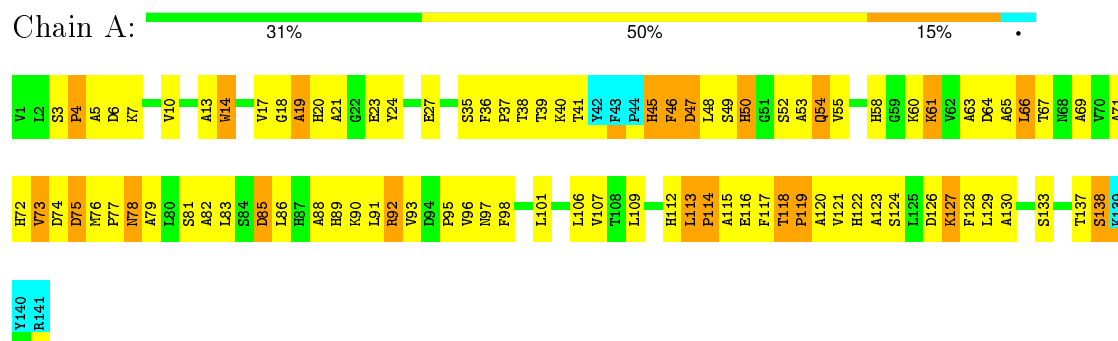


- Molecule 2: Hemoglobin beta subunit

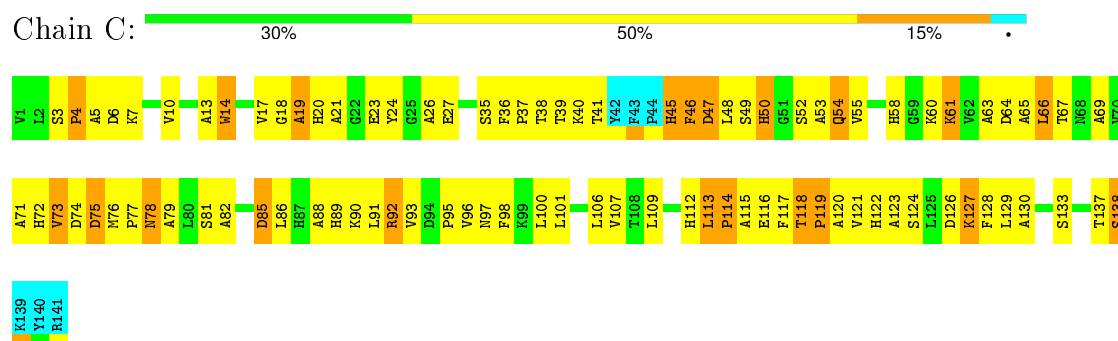


#### 4.2.17 Score per residue for model 17

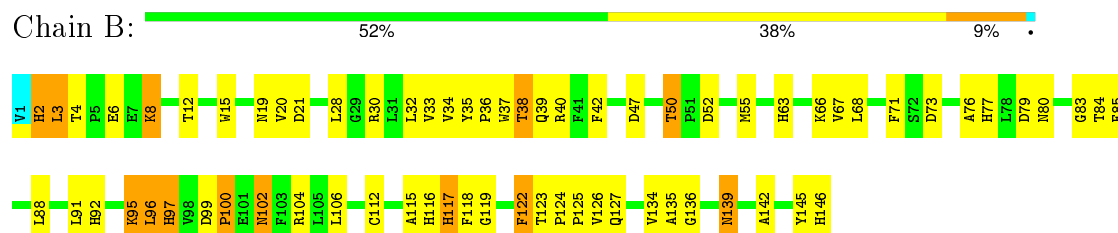
- Molecule 1: Hemoglobin alpha subunit



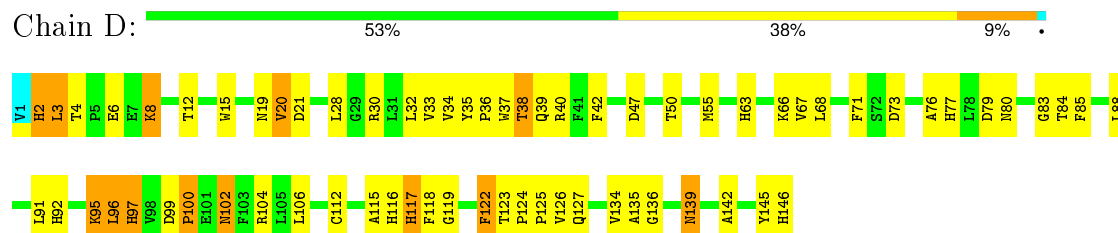
- Molecule 1: Hemoglobin alpha subunit



- Molecule 2: Hemoglobin beta subunit



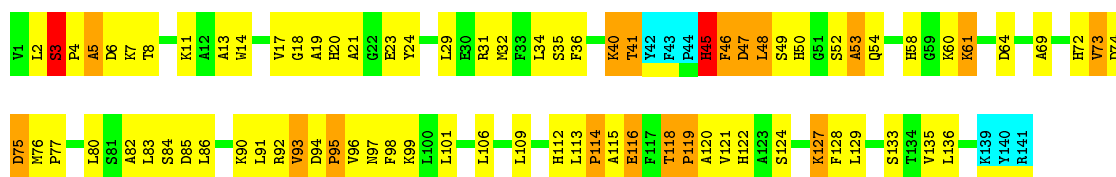
- Molecule 2: Hemoglobin beta subunit



#### 4.2.18 Score per residue for model 18

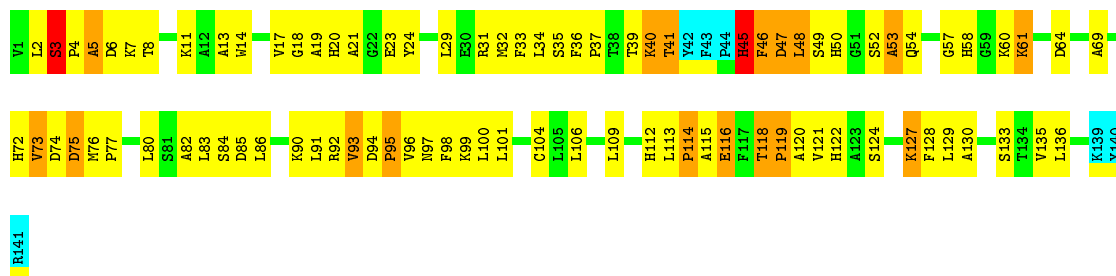
- Molecule 1: Hemoglobin alpha subunit





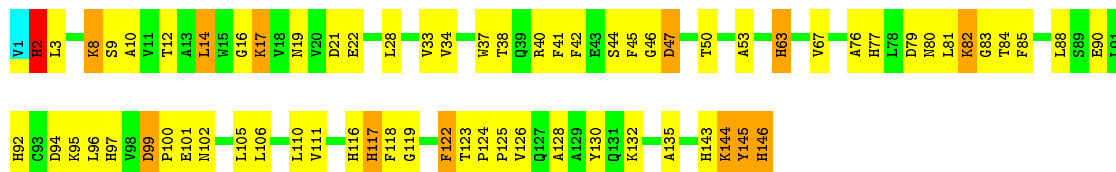
• Molecule 1: Hemoglobin alpha subunit

Chain C: 33% 49% 12% ..



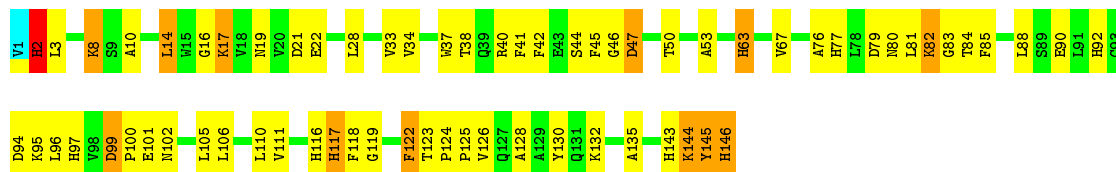
• Molecule 2: Hemoglobin beta subunit

Chain B: 52% 38% 8% ..



• Molecule 2: Hemoglobin beta subunit

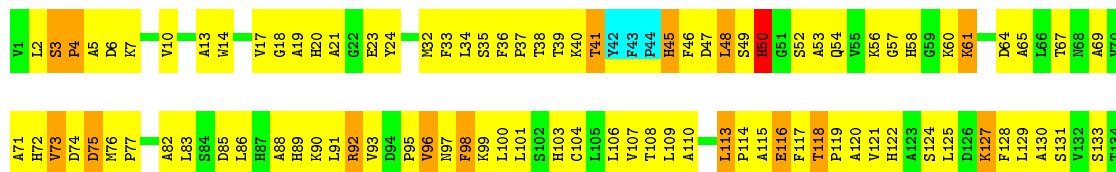
Chain D: 53% 37% 8% ..

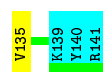


#### 4.2.19 Score per residue for model 19

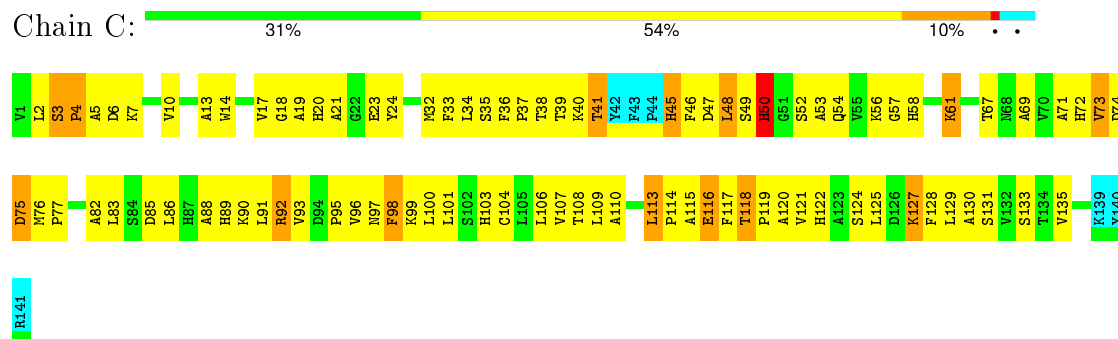
• Molecule 1: Hemoglobin alpha subunit

Chain A: 29% 55% 11% ..

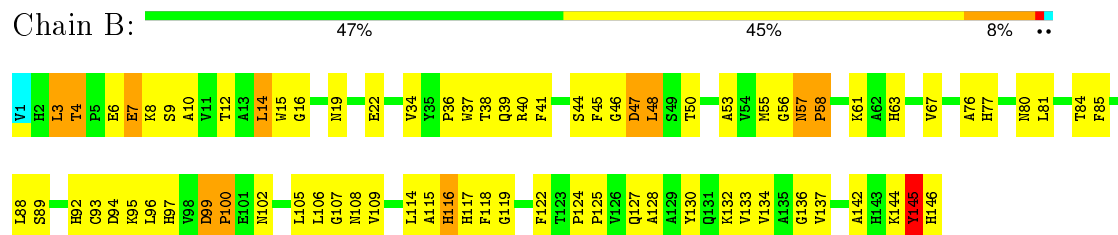




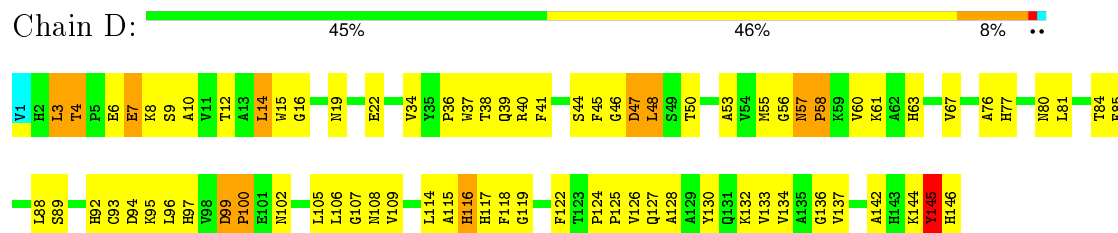
- Molecule 1: Hemoglobin alpha subunit



- Molecule 2: Hemoglobin beta subunit

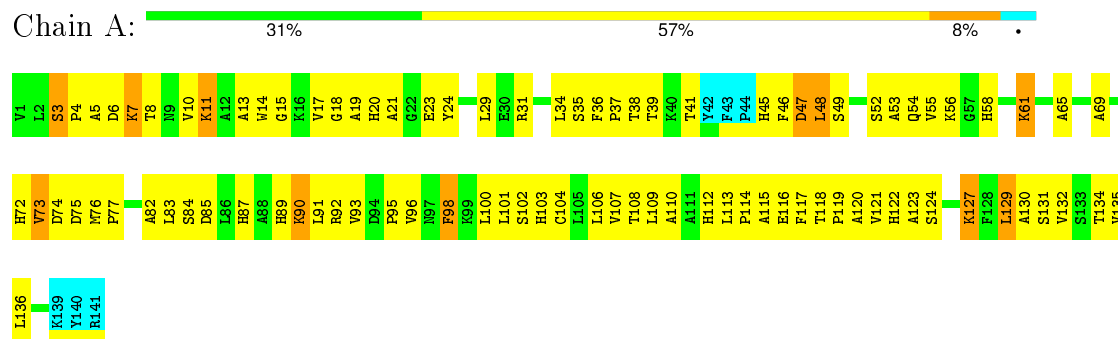


- Molecule 2: Hemoglobin beta subunit

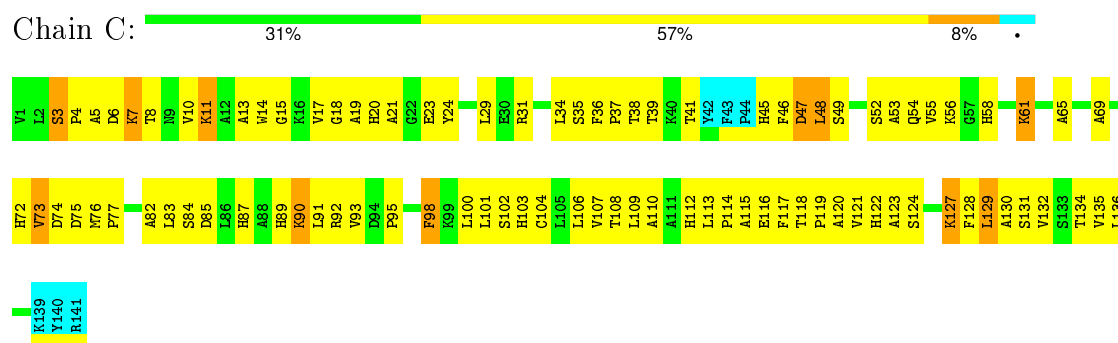


#### 4.2.20 Score per residue for model 20

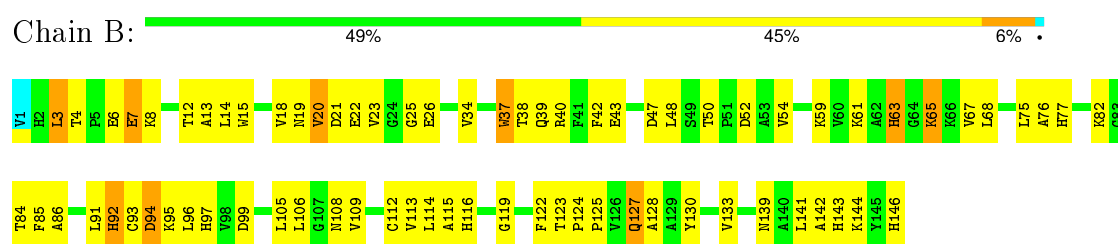
- Molecule 1: Hemoglobin alpha subunit



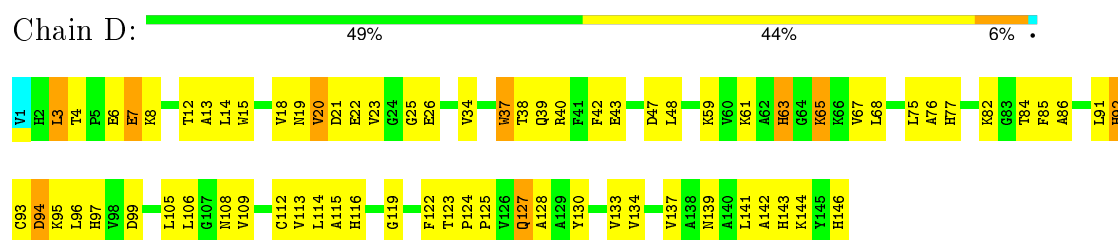
- Molecule 1: Hemoglobin alpha subunit



- Molecule 2: Hemoglobin beta subunit



- Molecule 2: Hemoglobin beta subunit





## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry, structures with the least restraint violations, structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| xplor-nih     | structure solution | 2.14    |
| xplor-nih     | refinement         | 2.14    |

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 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 each 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 averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 1006  | 1023     | 1013     | 112±18  |
| 1   | C     | 1006  | 1023     | 1013     | 112±22  |
| 2   | B     | 1116  | 1116     | 1107     | 98±24   |
| 2   | D     | 1116  | 1116     | 1107     | 102±28  |
| 3   | A     | 43    | 32       | 32       | 10±5    |
| 3   | B     | 43    | 32       | 32       | 23±11   |
| 3   | C     | 43    | 32       | 32       | 13±11   |
| 3   | D     | 43    | 32       | 32       | 23±14   |
| All | All   | 88320 | 88120    | 87310    | 7771    |

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 44.

All unique clashes are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:40:ARG:CD    | 1:C:92:ARG:HD3   | 1.59     | 1.25        | 18     | 2     |
| 2:B:146:HIS:CD2  | 2:D:139:ASN:HD21 | 1.58     | 1.16        | 6      | 2     |
| 2:B:139:ASN:HD21 | 2:D:146:HIS:CD2  | 1.57     | 1.16        | 6      | 2     |
| 2:B:106:LEU:HD22 | 3:B:147:HEC:CBB  | 1.57     | 1.16        | 19     | 1     |
| 1:A:92:ARG:HD3   | 2:D:40:ARG:CD    | 1.57     | 1.19        | 18     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:146:HIS:CD2  | 2:D:2:HIS:NE2    | 1.57     | 1.73        | 15     | 1     |
| 2:D:106:LEU:CD2  | 3:D:147:HEC:HBB3 | 1.55     | 1.31        | 19     | 1     |
| 2:D:106:LEU:HD22 | 3:D:147:HEC:CBB  | 1.55     | 1.16        | 19     | 1     |
| 2:B:106:LEU:CD1  | 3:B:147:HEC:HAB  | 1.55     | 1.32        | 18     | 2     |
| 2:B:106:LEU:CD2  | 3:B:147:HEC:HBB3 | 1.54     | 1.31        | 19     | 1     |
| 2:B:2:HIS:NE2    | 2:D:146:HIS:CD2  | 1.52     | 1.77        | 15     | 1     |
| 1:A:101:LEU:HD22 | 3:A:142:HEC:CBB  | 1.52     | 1.35        | 15     | 2     |
| 1:A:41:THR:HG21  | 2:D:97:HIS:CD2   | 1.51     | 1.37        | 11     | 5     |
| 1:A:117:PHE:CZ   | 2:B:116:HIS:NE2  | 1.50     | 1.79        | 13     | 3     |
| 2:D:106:LEU:CD1  | 3:D:147:HEC:HAB  | 1.50     | 1.32        | 18     | 2     |
| 1:C:34:LEU:CD1   | 2:D:128:ALA:HB2  | 1.49     | 1.34        | 18     | 4     |
| 1:C:117:PHE:CZ   | 2:D:116:HIS:NE2  | 1.49     | 1.79        | 13     | 3     |
| 1:C:101:LEU:HD22 | 3:C:142:HEC:CBB  | 1.49     | 1.35        | 15     | 2     |
| 2:B:146:HIS:HD2  | 2:D:139:ASN:ND2  | 1.48     | 0.98        | 6      | 1     |
| 1:A:34:LEU:CD1   | 2:B:128:ALA:HB2  | 1.48     | 1.34        | 18     | 4     |
| 2:B:97:HIS:CD2   | 1:C:41:THR:HG21  | 1.47     | 1.44        | 11     | 5     |
| 2:D:67:VAL:HG13  | 3:D:147:HEC:C1B  | 1.46     | 1.41        | 19     | 11    |
| 2:B:139:ASN:ND2  | 2:D:146:HIS:HD2  | 1.46     | 0.98        | 6      | 1     |
| 1:A:92:ARG:CG    | 2:D:40:ARG:NH2   | 1.46     | 1.79        | 16     | 1     |
| 1:C:48:LEU:HD11  | 3:C:142:HEC:CHA  | 1.45     | 1.41        | 12     | 1     |
| 1:A:92:ARG:CD    | 2:D:40:ARG:NH2   | 1.45     | 1.69        | 16     | 1     |
| 2:B:67:VAL:HG13  | 3:B:147:HEC:C1B  | 1.45     | 1.41        | 19     | 12    |
| 2:B:42:PHE:CZ    | 3:B:147:HEC:CBC  | 1.42     | 2.02        | 17     | 4     |
| 1:A:92:ARG:NE    | 2:D:40:ARG:HB2   | 1.40     | 1.30        | 19     | 1     |
| 2:D:42:PHE:CZ    | 3:D:147:HEC:CBC  | 1.40     | 2.02        | 17     | 3     |
| 1:C:34:LEU:HD12  | 2:D:128:ALA:CB   | 1.40     | 1.45        | 18     | 1     |
| 1:A:92:ARG:HD3   | 2:D:40:ARG:NE    | 1.39     | 1.27        | 16     | 2     |
| 1:A:34:LEU:HD12  | 2:B:128:ALA:CB   | 1.39     | 1.45        | 18     | 1     |
| 2:D:42:PHE:HB3   | 3:D:147:HEC:CMA  | 1.36     | 1.49        | 12     | 1     |
| 3:B:147:HEC:CHC  | 2:D:106:LEU:CD1  | 1.35     | 2.02        | 15     | 1     |
| 2:D:38:THR:C     | 3:D:147:HEC:C1C  | 1.35     | 1.93        | 12     | 1     |
| 1:A:92:ARG:NH2   | 2:D:40:ARG:HE    | 1.35     | 1.17        | 15     | 1     |
| 1:A:92:ARG:CD    | 2:D:40:ARG:HD2   | 1.35     | 1.49        | 18     | 2     |
| 2:B:40:ARG:HB2   | 1:C:92:ARG:NE    | 1.33     | 1.35        | 19     | 1     |
| 1:A:41:THR:HG21  | 2:D:97:HIS:ND1   | 1.33     | 1.31        | 17     | 2     |
| 2:B:146:HIS:CD2  | 2:D:139:ASN:ND2  | 1.31     | 1.80        | 6      | 2     |
| 2:B:97:HIS:ND1   | 1:C:41:THR:HG21  | 1.31     | 1.37        | 17     | 2     |
| 1:A:96:VAL:HG11  | 2:D:99:ASP:OD2   | 1.31     | 1.24        | 11     | 1     |
| 1:A:92:ARG:NH2   | 2:D:40:ARG:NE    | 1.31     | 1.78        | 15     | 1     |
| 2:B:40:ARG:HE    | 1:C:92:ARG:NH2   | 1.31     | 1.21        | 15     | 1     |
| 2:D:42:PHE:O     | 3:D:147:HEC:HMA2 | 1.31     | 1.13        | 12     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 2:B:139:ASN:ND2 | 2:D:146:HIS:CD2  | 1.30     | 1.82        | 6      | 2     |
| 2:B:40:ARG:HD2  | 1:C:92:ARG:CD    | 1.30     | 1.55        | 18     | 2     |
| 2:B:82:LYS:NZ   | 2:D:82:LYS:HZ1   | 1.28     | 1.23        | 15     | 1     |
| 2:D:42:PHE:CB   | 3:D:147:HEC:CMA  | 1.28     | 2.10        | 12     | 1     |
| 1:A:92:ARG:NE   | 2:D:40:ARG:CB    | 1.28     | 1.97        | 19     | 1     |
| 2:B:82:LYS:NZ   | 2:D:82:LYS:NZ    | 1.27     | 1.81        | 15     | 1     |
| 2:D:32:LEU:O    | 3:D:147:HEC:HMB1 | 1.27     | 1.09        | 15     | 1     |
| 2:D:63:HIS:NE2  | 3:D:147:HEC:CHA  | 1.26     | 1.99        | 16     | 8     |
| 1:A:92:ARG:NH2  | 3:D:147:HEC:HBD2 | 1.26     | 1.43        | 12     | 1     |
| 2:B:40:ARG:CB   | 1:C:92:ARG:NE    | 1.25     | 1.99        | 19     | 1     |
| 2:B:99:ASP:OD2  | 1:C:96:VAL:HG11  | 1.25     | 1.24        | 11     | 1     |
| 2:B:40:ARG:NE   | 1:C:92:ARG:NH2   | 1.25     | 1.85        | 15     | 1     |
| 1:A:41:THR:CG2  | 2:D:97:HIS:CE1   | 1.25     | 2.10        | 17     | 3     |
| 2:D:42:PHE:CZ   | 3:D:147:HEC:HBC3 | 1.25     | 1.64        | 17     | 5     |
| 2:B:40:ARG:CZ   | 1:C:92:ARG:CB    | 1.24     | 2.15        | 17     | 2     |
| 1:A:111:ALA:HB2 | 2:B:122:PHE:CE2  | 1.24     | 1.67        | 8      | 3     |
| 1:A:38:THR:HG22 | 2:D:97:HIS:ND1   | 1.24     | 1.48        | 7      | 1     |
| 2:D:38:THR:N    | 3:D:147:HEC:CHC  | 1.23     | 1.74        | 12     | 1     |
| 2:B:97:HIS:CE1  | 1:C:41:THR:HG21  | 1.23     | 1.63        | 17     | 3     |
| 2:B:63:HIS:NE2  | 3:B:147:HEC:CHA  | 1.23     | 1.99        | 16     | 9     |
| 1:A:101:LEU:CD2 | 3:A:142:HEC:CBB  | 1.23     | 2.17        | 15     | 4     |
| 1:A:92:ARG:CD   | 2:D:40:ARG:CD    | 1.23     | 2.09        | 18     | 1     |
| 1:C:111:ALA:HB2 | 2:D:122:PHE:CE2  | 1.23     | 1.67        | 8      | 3     |
| 2:D:38:THR:N    | 3:D:147:HEC:HHC  | 1.22     | 1.27        | 12     | 1     |
| 2:B:146:HIS:CE1 | 2:D:139:ASN:OD1  | 1.22     | 1.92        | 8      | 1     |
| 2:B:42:PHE:CE1  | 3:B:147:HEC:HBC1 | 1.22     | 1.68        | 17     | 2     |
| 2:B:40:ARG:CD   | 1:C:92:ARG:CD    | 1.22     | 2.15        | 18     | 1     |
| 1:A:96:VAL:HG21 | 2:D:99:ASP:CB    | 1.22     | 1.63        | 18     | 2     |
| 1:A:41:THR:HG21 | 2:D:97:HIS:CE1   | 1.21     | 1.58        | 17     | 2     |
| 2:B:40:ARG:NH1  | 1:C:92:ARG:HB3   | 1.21     | 1.49        | 17     | 1     |
| 1:C:101:LEU:CD2 | 3:C:142:HEC:CBB  | 1.21     | 2.17        | 15     | 4     |
| 2:D:42:PHE:CE1  | 3:D:147:HEC:HBC1 | 1.21     | 1.68        | 17     | 1     |
| 1:A:117:PHE:CD1 | 2:B:30:ARG:NH2   | 1.21     | 2.08        | 3      | 3     |
| 1:A:92:ARG:CB   | 2:D:40:ARG:CZ    | 1.21     | 2.17        | 17     | 2     |
| 1:A:117:PHE:CZ  | 2:B:116:HIS:CD2  | 1.21     | 2.28        | 13     | 1     |
| 2:D:38:THR:CA   | 3:D:147:HEC:CHC  | 1.21     | 2.09        | 12     | 1     |
| 2:D:42:PHE:CB   | 3:D:147:HEC:HMA1 | 1.20     | 1.65        | 12     | 1     |
| 1:A:96:VAL:CG1  | 2:D:99:ASP:OD2   | 1.20     | 1.89        | 11     | 1     |
| 1:C:101:LEU:CD2 | 3:C:142:HEC:HBB3 | 1.20     | 1.67        | 15     | 7     |
| 2:D:42:PHE:CE2  | 3:D:147:HEC:HMD3 | 1.20     | 1.72        | 2      | 1     |
| 1:C:117:PHE:CD1 | 2:D:30:ARG:NH2   | 1.19     | 2.08        | 3      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:C:117:PHE:CZ   | 2:D:116:HIS:CD2  | 1.19     | 2.28        | 13     | 1     |
| 1:A:41:THR:HG21  | 2:D:97:HIS:CG    | 1.19     | 1.71        | 12     | 4     |
| 1:A:101:LEU:CD2  | 3:A:142:HEC:HBB3 | 1.18     | 1.67        | 15     | 7     |
| 1:C:45:HIS:N     | 3:C:142:HEC:HMA2 | 1.18     | 1.22        | 12     | 1     |
| 2:B:106:LEU:HD21 | 3:B:147:HEC:CHC  | 1.18     | 1.67        | 2      | 1     |
| 1:A:92:ARG:HB3   | 2:D:40:ARG:NH1   | 1.18     | 1.50        | 17     | 1     |
| 2:B:99:ASP:OD2   | 1:C:96:VAL:CG1   | 1.18     | 1.92        | 11     | 1     |
| 2:D:106:LEU:HD21 | 3:D:147:HEC:CHC  | 1.18     | 1.66        | 2      | 1     |
| 1:A:92:ARG:HH21  | 2:D:40:ARG:NE    | 1.18     | 1.31        | 15     | 1     |
| 2:B:42:PHE:CE2   | 3:B:147:HEC:HMD3 | 1.18     | 1.72        | 2      | 1     |
| 2:D:39:GLN:N     | 3:D:147:HEC:C4B  | 1.18     | 1.94        | 12     | 1     |
| 2:B:99:ASP:CB    | 1:C:96:VAL:HG21  | 1.17     | 1.69        | 18     | 1     |
| 1:A:92:ARG:HD3   | 2:D:40:ARG:CZ    | 1.17     | 1.62        | 16     | 1     |
| 1:C:32:MET:HE2   | 3:C:142:HEC:CAB  | 1.17     | 1.70        | 12     | 1     |
| 2:B:139:ASN:OD1  | 2:D:146:HIS:CE1  | 1.17     | 1.95        | 8      | 1     |
| 2:D:106:LEU:CD1  | 3:D:147:HEC:CHC  | 1.17     | 2.23        | 9      | 13    |
| 2:B:106:LEU:CD2  | 3:B:147:HEC:HHC  | 1.17     | 1.69        | 2      | 1     |
| 1:C:32:MET:CE    | 3:C:142:HEC:HAB  | 1.16     | 1.67        | 12     | 1     |
| 2:D:106:LEU:CD2  | 3:D:147:HEC:HHC  | 1.16     | 1.69        | 2      | 1     |
| 2:B:42:PHE:CZ    | 3:B:147:HEC:HBC3 | 1.16     | 1.64        | 17     | 6     |
| 2:B:97:HIS:ND1   | 1:C:38:THR:HG22  | 1.16     | 1.53        | 7      | 1     |
| 2:D:106:LEU:CG   | 3:D:147:HEC:CAB  | 1.16     | 2.24        | 18     | 1     |
| 2:B:97:HIS:CE1   | 1:C:41:THR:CG2   | 1.15     | 2.16        | 17     | 3     |
| 2:D:42:PHE:HB2   | 3:D:147:HEC:C4A  | 1.15     | 1.69        | 12     | 1     |
| 2:B:106:LEU:CG   | 3:B:147:HEC:CAB  | 1.15     | 2.24        | 18     | 1     |
| 2:B:106:LEU:CD1  | 3:B:147:HEC:CHC  | 1.15     | 2.23        | 9      | 14    |
| 2:B:97:HIS:CG    | 1:C:41:THR:HG21  | 1.15     | 1.75        | 12     | 3     |
| 1:C:48:LEU:CD1   | 3:C:142:HEC:CHA  | 1.15     | 2.22        | 12     | 1     |
| 2:B:2:HIS:NE2    | 2:D:146:HIS:HD2  | 1.15     | 1.16        | 15     | 1     |
| 2:D:32:LEU:O     | 3:D:147:HEC:CMB  | 1.15     | 1.93        | 15     | 1     |
| 1:A:96:VAL:HG11  | 2:D:99:ASP:CG    | 1.15     | 1.60        | 11     | 1     |
| 3:B:147:HEC:CHC  | 2:D:106:LEU:HD13 | 1.14     | 1.60        | 15     | 1     |
| 2:D:42:PHE:HB2   | 3:D:147:HEC:CHB  | 1.14     | 1.72        | 12     | 1     |
| 2:B:82:LYS:HZ1   | 2:D:82:LYS:NZ    | 1.14     | 1.34        | 15     | 1     |
| 2:B:42:PHE:HZ    | 3:B:147:HEC:CBC  | 1.14     | 1.41        | 17     | 2     |
| 1:C:117:PHE:HZ   | 2:D:116:HIS:NE2  | 1.13     | 1.21        | 13     | 1     |
| 2:B:106:LEU:CD1  | 3:B:147:HEC:CAB  | 1.13     | 2.26        | 18     | 2     |
| 2:D:106:LEU:HD12 | 3:D:147:HEC:CAB  | 1.13     | 1.72        | 18     | 1     |
| 2:D:106:LEU:CG   | 3:D:147:HEC:HAB  | 1.13     | 1.72        | 18     | 1     |
| 2:D:42:PHE:HZ    | 3:D:147:HEC:CBC  | 1.13     | 1.41        | 17     | 1     |
| 2:D:106:LEU:CD1  | 3:D:147:HEC:CAB  | 1.12     | 2.26        | 18     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:146:HIS:HD2  | 2:D:2:HIS:NE2    | 1.12     | 1.15        | 15     | 1     |
| 3:B:147:HEC:HHC  | 2:D:106:LEU:CD1  | 1.12     | 1.74        | 15     | 1     |
| 2:B:106:LEU:HD12 | 3:B:147:HEC:CAB  | 1.12     | 1.72        | 18     | 1     |
| 1:A:92:ARG:HH22  | 3:D:147:HEC:CBD  | 1.12     | 1.55        | 12     | 1     |
| 2:B:106:LEU:CG   | 3:B:147:HEC:HAB  | 1.12     | 1.72        | 18     | 1     |
| 2:D:38:THR:C     | 3:D:147:HEC:CHC  | 1.12     | 2.17        | 12     | 1     |
| 1:A:41:THR:CG2   | 2:D:97:HIS:CD2   | 1.12     | 2.33        | 11     | 3     |
| 1:A:92:ARG:HG3   | 2:D:40:ARG:NH2   | 1.12     | 1.45        | 16     | 1     |
| 2:D:106:LEU:CD2  | 3:D:147:HEC:CHC  | 1.11     | 2.27        | 2      | 1     |
| 2:D:106:LEU:HD22 | 3:D:147:HEC:HAB  | 1.11     | 1.17        | 10     | 12    |
| 1:C:101:LEU:HD13 | 3:C:142:HEC:CHC  | 1.11     | 1.75        | 15     | 5     |
| 1:C:48:LEU:HD11  | 3:C:142:HEC:C1A  | 1.11     | 1.75        | 12     | 1     |
| 2:D:63:HIS:NE2   | 3:D:147:HEC:HAD2 | 1.11     | 1.59        | 19     | 4     |
| 1:A:101:LEU:HD13 | 3:A:142:HEC:CHC  | 1.11     | 1.75        | 15     | 5     |
| 2:B:63:HIS:NE2   | 3:B:147:HEC:HAD2 | 1.11     | 1.59        | 19     | 4     |
| 2:B:99:ASP:CG    | 1:C:96:VAL:HG11  | 1.11     | 1.65        | 11     | 1     |
| 1:C:101:LEU:CD1  | 3:C:142:HEC:CHC  | 1.11     | 2.29        | 19     | 5     |
| 2:B:146:HIS:NE2  | 2:D:139:ASN:ND2  | 1.10     | 1.99        | 8      | 2     |
| 1:A:92:ARG:CZ    | 2:D:40:ARG:HB2   | 1.10     | 1.77        | 19     | 1     |
| 2:B:67:VAL:HG13  | 3:B:147:HEC:C2B  | 1.10     | 1.76        | 9      | 17    |
| 2:B:139:ASN:ND2  | 2:D:146:HIS:NE2  | 1.10     | 1.99        | 8      | 2     |
| 2:B:42:PHE:CE1   | 3:B:147:HEC:CBC  | 1.10     | 2.33        | 12     | 3     |
| 2:D:106:LEU:HD21 | 3:D:147:HEC:HHC  | 1.10     | 1.16        | 2      | 1     |
| 2:D:67:VAL:HG13  | 3:D:147:HEC:C2B  | 1.09     | 1.76        | 9      | 16    |
| 2:B:40:ARG:HB2   | 1:C:92:ARG:CZ    | 1.09     | 1.76        | 19     | 1     |
| 1:A:101:LEU:CD1  | 3:A:142:HEC:CHC  | 1.08     | 2.29        | 19     | 5     |
| 1:C:117:PHE:CE1  | 2:D:30:ARG:NH2   | 1.08     | 2.21        | 3      | 2     |
| 2:D:67:VAL:HG22  | 3:D:147:HEC:C1B  | 1.08     | 1.77        | 9      | 12    |
| 1:A:117:PHE:CE1  | 2:B:30:ARG:NH2   | 1.08     | 2.21        | 3      | 2     |
| 1:A:96:VAL:HG21  | 2:D:99:ASP:HB3   | 1.08     | 1.21        | 18     | 2     |
| 1:A:92:ARG:CD    | 2:D:40:ARG:CZ    | 1.08     | 2.20        | 16     | 2     |
| 2:D:63:HIS:CE1   | 3:D:147:HEC:CHA  | 1.08     | 2.36        | 2      | 13    |
| 1:A:94:ASP:OD1   | 2:D:40:ARG:NH1   | 1.08     | 1.87        | 3      | 1     |
| 2:B:63:HIS:CE1   | 3:B:147:HEC:CHA  | 1.08     | 2.36        | 2      | 14    |
| 2:B:67:VAL:HG22  | 3:B:147:HEC:C1B  | 1.07     | 1.77        | 9      | 13    |
| 1:C:45:HIS:N     | 3:C:142:HEC:CMA  | 1.07     | 2.17        | 12     | 1     |
| 2:B:40:ARG:CZ    | 1:C:92:ARG:HB2   | 1.07     | 1.78        | 17     | 2     |
| 2:B:139:ASN:ND2  | 2:D:139:ASN:ND2  | 1.07     | 2.01        | 3      | 1     |
| 2:B:146:HIS:O    | 2:D:132:LYS:HD3  | 1.06     | 1.50        | 15     | 1     |
| 2:B:67:VAL:HG22  | 3:B:147:HEC:CHB  | 1.06     | 1.80        | 9      | 13    |
| 1:C:31:ARG:NH1   | 2:D:127:GLN:CG   | 1.06     | 2.19        | 16     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:C:86:LEU:HD11  | 3:C:142:HEC:HBD2 | 1.06     | 1.13        | 7      | 2     |
| 2:B:135:ALA:O    | 2:D:146:HIS:CD2  | 1.06     | 2.08        | 17     | 1     |
| 2:B:106:LEU:CD2  | 3:B:147:HEC:CHC  | 1.06     | 2.27        | 2      | 1     |
| 2:B:40:ARG:NE    | 1:C:92:ARG:HH21  | 1.06     | 1.39        | 15     | 1     |
| 2:D:106:LEU:HD12 | 3:D:147:HEC:CHC  | 1.05     | 1.81        | 9      | 6     |
| 1:A:31:ARG:NH1   | 2:B:127:GLN:CG   | 1.05     | 2.18        | 16     | 2     |
| 2:B:97:HIS:CD2   | 1:C:41:THR:CG2   | 1.05     | 2.40        | 11     | 3     |
| 1:A:92:ARG:HB3   | 2:D:40:ARG:CZ    | 1.05     | 1.76        | 17     | 1     |
| 2:D:67:VAL:HG22  | 3:D:147:HEC:CHB  | 1.05     | 1.80        | 9      | 12    |
| 2:D:42:PHE:O     | 3:D:147:HEC:CMA  | 1.05     | 2.04        | 12     | 1     |
| 2:B:106:LEU:HD22 | 3:B:147:HEC:HAB  | 1.04     | 1.17        | 10     | 13    |
| 2:D:42:PHE:C     | 3:D:147:HEC:HMA2 | 1.04     | 1.71        | 12     | 1     |
| 2:D:42:PHE:HE2   | 3:D:147:HEC:HMD3 | 1.04     | 1.01        | 2      | 1     |
| 2:D:42:PHE:CE1   | 3:D:147:HEC:CBC  | 1.04     | 2.35        | 17     | 2     |
| 2:B:40:ARG:CD    | 1:C:92:ARG:HE    | 1.04     | 1.64        | 19     | 1     |
| 1:C:86:LEU:HD11  | 3:C:142:HEC:CBD  | 1.04     | 1.82        | 7      | 2     |
| 3:B:147:HEC:CHC  | 2:D:106:LEU:HD12 | 1.04     | 1.77        | 15     | 1     |
| 2:B:132:LYS:HD3  | 2:D:146:HIS:O    | 1.04     | 1.50        | 15     | 1     |
| 3:B:147:HEC:C4B  | 2:D:106:LEU:HD13 | 1.04     | 1.83        | 15     | 1     |
| 2:D:63:HIS:HE1   | 3:D:147:HEC:CHA  | 1.03     | 1.66        | 19     | 8     |
| 2:B:106:LEU:HD13 | 3:B:147:HEC:CHC  | 1.03     | 1.83        | 12     | 15    |
| 2:B:40:ARG:NH1   | 1:C:94:ASP:OD1   | 1.03     | 1.91        | 3      | 1     |
| 2:B:146:HIS:CD2  | 2:D:135:ALA:O    | 1.03     | 2.10        | 17     | 1     |
| 2:B:63:HIS:HE1   | 3:B:147:HEC:CHA  | 1.03     | 1.66        | 19     | 8     |
| 1:A:86:LEU:HD11  | 3:A:142:HEC:CBD  | 1.03     | 1.82        | 7      | 2     |
| 2:B:146:HIS:HD2  | 2:D:139:ASN:CG   | 1.03     | 1.56        | 6      | 1     |
| 1:A:34:LEU:CD1   | 2:B:128:ALA:CB   | 1.03     | 2.20        | 18     | 1     |
| 2:D:42:PHE:HB2   | 3:D:147:HEC:C3A  | 1.03     | 1.83        | 12     | 1     |
| 2:B:106:LEU:HD12 | 3:B:147:HEC:CHC  | 1.02     | 1.81        | 9      | 7     |
| 1:A:96:VAL:CB    | 2:D:99:ASP:OD2   | 1.02     | 2.06        | 11     | 2     |
| 2:B:63:HIS:NE2   | 3:B:147:HEC:C4D  | 1.02     | 2.22        | 16     | 10    |
| 2:D:63:HIS:NE2   | 3:D:147:HEC:C4D  | 1.02     | 2.22        | 16     | 9     |
| 2:B:67:VAL:CG1   | 3:B:147:HEC:C1B  | 1.02     | 2.37        | 19     | 2     |
| 2:D:67:VAL:CG1   | 3:D:147:HEC:C1B  | 1.02     | 2.37        | 19     | 2     |
| 1:A:48:LEU:HD13  | 1:A:48:LEU:H     | 1.02     | 1.13        | 11     | 1     |
| 1:C:48:LEU:HD13  | 1:C:48:LEU:H     | 1.02     | 1.13        | 11     | 1     |
| 2:B:106:LEU:HG   | 3:B:147:HEC:CAB  | 1.02     | 1.84        | 18     | 1     |
| 2:B:99:ASP:HB3   | 1:C:96:VAL:HG21  | 1.01     | 1.26        | 18     | 2     |
| 1:C:36:PHE:CZ    | 2:D:131:GLN:NE2  | 1.01     | 2.28        | 13     | 1     |
| 2:D:39:GLN:N     | 3:D:147:HEC:C1C  | 1.01     | 2.23        | 12     | 1     |
| 1:A:117:PHE:CE1  | 2:B:116:HIS:CD2  | 1.01     | 2.48        | 13     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:111:ALA:CB   | 2:B:122:PHE:CE2  | 1.01     | 2.44        | 8      | 3     |
| 1:A:92:ARG:CD    | 2:D:40:ARG:NE    | 1.00     | 2.21        | 16     | 2     |
| 1:A:86:LEU:HD11  | 3:A:142:HEC:HBD2 | 1.00     | 1.13        | 7      | 2     |
| 1:A:48:LEU:H     | 1:A:48:LEU:HD13  | 1.00     | 1.13        | 9      | 1     |
| 1:C:117:PHE:CE1  | 2:D:116:HIS:CD2  | 1.00     | 2.48        | 13     | 1     |
| 1:A:36:PHE:CZ    | 2:B:131:GLN:NE2  | 1.00     | 2.28        | 13     | 1     |
| 2:B:42:PHE:HE2   | 3:B:147:HEC:HMD3 | 1.00     | 1.01        | 2      | 1     |
| 2:B:40:ARG:CZ    | 1:C:92:ARG:HB3   | 1.00     | 1.75        | 17     | 1     |
| 2:B:146:HIS:CD2  | 2:D:139:ASN:CG   | 1.00     | 2.33        | 6      | 2     |
| 2:D:106:LEU:HG   | 3:D:147:HEC:CAB  | 1.00     | 1.84        | 18     | 1     |
| 1:C:34:LEU:HD13  | 2:D:128:ALA:HB2  | 1.00     | 1.34        | 8      | 7     |
| 2:B:106:LEU:HD21 | 3:B:147:HEC:HHC  | 1.00     | 1.16        | 2      | 1     |
| 1:A:92:ARG:HE    | 2:D:40:ARG:CD    | 0.99     | 1.68        | 19     | 1     |
| 2:B:40:ARG:HD3   | 1:C:92:ARG:HE    | 0.99     | 1.15        | 19     | 1     |
| 1:A:41:THR:HG21  | 2:D:97:HIS:NE2   | 0.99     | 1.71        | 11     | 2     |
| 1:A:101:LEU:HD13 | 3:A:142:HEC:HHC  | 0.99     | 1.28        | 15     | 4     |
| 2:D:42:PHE:CZ    | 3:D:147:HEC:HMB2 | 0.99     | 1.91        | 12     | 1     |
| 1:A:101:LEU:HD22 | 3:A:142:HEC:HBB3 | 0.99     | 1.02        | 15     | 2     |
| 1:C:111:ALA:CB   | 2:D:122:PHE:CE2  | 0.99     | 2.44        | 8      | 3     |
| 1:A:34:LEU:HD13  | 2:B:128:ALA:HB2  | 0.99     | 1.34        | 8      | 7     |
| 1:C:48:LEU:H     | 1:C:48:LEU:HD13  | 0.99     | 1.12        | 9      | 1     |
| 2:D:38:THR:C     | 3:D:147:HEC:NC   | 0.99     | 2.13        | 12     | 1     |
| 1:C:32:MET:CE    | 3:C:142:HEC:CAB  | 0.98     | 2.37        | 12     | 1     |
| 1:C:34:LEU:CD1   | 2:D:128:ALA:CB   | 0.98     | 2.20        | 18     | 1     |
| 1:C:101:LEU:HD22 | 3:C:142:HEC:HBB3 | 0.98     | 1.02        | 15     | 2     |
| 2:D:106:LEU:HD13 | 3:D:147:HEC:CHC  | 0.98     | 1.87        | 6      | 14    |
| 1:C:101:LEU:HD13 | 3:C:142:HEC:HHC  | 0.98     | 1.28        | 15     | 4     |
| 1:C:31:ARG:NH1   | 2:D:127:GLN:HG2  | 0.98     | 1.72        | 16     | 2     |
| 2:B:106:LEU:CD2  | 3:B:147:HEC:CBB  | 0.98     | 2.10        | 19     | 1     |
| 1:A:92:ARG:HB2   | 2:D:40:ARG:CZ    | 0.98     | 1.82        | 17     | 2     |
| 2:D:106:LEU:CD2  | 3:D:147:HEC:CBB  | 0.98     | 2.10        | 19     | 1     |
| 1:A:92:ARG:HD3   | 2:D:40:ARG:HD3   | 0.97     | 1.31        | 18     | 1     |
| 1:A:92:ARG:HD3   | 2:D:40:ARG:HD2   | 0.97     | 1.01        | 17     | 2     |
| 2:B:139:ASN:CG   | 2:D:146:HIS:HD2  | 0.97     | 1.62        | 6      | 1     |
| 2:B:42:PHE:HE1   | 3:B:147:HEC:HBC1 | 0.97     | 1.15        | 12     | 3     |
| 2:B:40:ARG:HD2   | 1:C:92:ARG:HD3   | 0.97     | 0.99        | 17     | 2     |
| 2:D:106:LEU:CD1  | 3:D:147:HEC:HHC  | 0.97     | 1.90        | 5      | 11    |
| 1:A:92:ARG:HE    | 2:D:40:ARG:HD3   | 0.97     | 1.20        | 19     | 1     |
| 1:A:117:PHE:HZ   | 2:B:116:HIS:NE2  | 0.96     | 1.21        | 13     | 1     |
| 2:B:139:ASN:CG   | 2:D:146:HIS:CD2  | 0.96     | 2.39        | 6      | 2     |
| 2:B:99:ASP:OD2   | 1:C:96:VAL:CB    | 0.96     | 2.13        | 11     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:D:42:PHE:CB    | 3:D:147:HEC:CHB  | 0.96     | 2.43        | 12     | 1     |
| 2:B:106:LEU:HD13 | 3:B:147:HEC:CAB  | 0.96     | 1.91        | 9      | 10    |
| 1:C:101:LEU:CD2  | 3:C:142:HEC:HHC  | 0.96     | 1.90        | 4      | 3     |
| 2:D:106:LEU:HD13 | 3:D:147:HEC:CAB  | 0.96     | 1.91        | 9      | 9     |
| 2:B:106:LEU:CD1  | 3:B:147:HEC:HHC  | 0.95     | 1.90        | 5      | 11    |
| 2:D:42:PHE:CE1   | 3:D:147:HEC:HMB2 | 0.95     | 1.95        | 12     | 1     |
| 1:A:31:ARG:NH1   | 2:B:127:GLN:HG2  | 0.95     | 1.72        | 16     | 2     |
| 1:A:101:LEU:CD2  | 3:A:142:HEC:HHC  | 0.95     | 1.90        | 4      | 3     |
| 1:C:40:LYS:O     | 3:C:142:HEC:C3D  | 0.95     | 2.15        | 12     | 1     |
| 1:A:34:LEU:HB3   | 2:B:128:ALA:HB2  | 0.94     | 1.40        | 15     | 5     |
| 1:A:41:THR:CG2   | 2:D:97:HIS:ND1   | 0.94     | 2.26        | 17     | 1     |
| 2:B:3:LEU:H      | 2:B:3:LEU:HD12   | 0.94     | 1.22        | 6      | 9     |
| 1:C:34:LEU:HB3   | 2:D:128:ALA:HB2  | 0.94     | 1.39        | 15     | 5     |
| 2:B:139:ASN:OD1  | 2:D:146:HIS:ND1  | 0.94     | 2.01        | 8      | 1     |
| 2:D:106:LEU:HD13 | 3:D:147:HEC:C3B  | 0.94     | 1.92        | 9      | 8     |
| 2:B:146:HIS:CG   | 2:D:139:ASN:OD1  | 0.94     | 2.20        | 8      | 1     |
| 2:B:139:ASN:OD1  | 2:D:146:HIS:CG   | 0.94     | 2.21        | 8      | 1     |
| 2:B:146:HIS:CD2  | 2:D:139:ASN:OD1  | 0.93     | 2.21        | 8      | 2     |
| 2:B:63:HIS:CE1   | 3:B:147:HEC:O1A  | 0.93     | 2.21        | 5      | 1     |
| 2:B:42:PHE:HE1   | 3:B:147:HEC:CBC  | 0.93     | 1.75        | 18     | 1     |
| 1:C:36:PHE:CZ    | 2:D:131:GLN:OE1  | 0.93     | 2.21        | 2      | 4     |
| 1:A:36:PHE:CZ    | 2:B:131:GLN:OE1  | 0.93     | 2.21        | 2      | 4     |
| 1:C:31:ARG:HH12  | 2:D:127:GLN:CG   | 0.93     | 1.75        | 16     | 1     |
| 2:D:42:PHE:CB    | 3:D:147:HEC:C3A  | 0.93     | 2.47        | 12     | 1     |
| 1:A:101:LEU:CD2  | 3:A:142:HEC:CHC  | 0.93     | 2.47        | 4      | 3     |
| 2:B:106:LEU:HD13 | 3:B:147:HEC:C3B  | 0.93     | 1.92        | 9      | 9     |
| 1:A:111:ALA:CB   | 2:B:122:PHE:CZ   | 0.93     | 2.52        | 8      | 1     |
| 2:D:3:LEU:H      | 2:D:3:LEU:HD12   | 0.93     | 1.24        | 4      | 8     |
| 2:B:146:HIS:O    | 2:D:132:LYS:HG3  | 0.93     | 1.62        | 9      | 1     |
| 1:C:111:ALA:CB   | 2:D:122:PHE:CZ   | 0.92     | 2.52        | 8      | 1     |
| 2:D:63:HIS:CE1   | 3:D:147:HEC:O1A  | 0.92     | 2.21        | 5      | 1     |
| 2:B:106:LEU:HD11 | 3:B:147:HEC:HAB  | 0.92     | 1.40        | 2      | 1     |
| 2:B:146:HIS:ND1  | 2:D:139:ASN:OD1  | 0.92     | 2.01        | 8      | 1     |
| 1:C:101:LEU:CD1  | 3:C:142:HEC:HHC  | 0.92     | 1.94        | 7      | 3     |
| 1:A:101:LEU:CD1  | 3:A:142:HEC:HHC  | 0.92     | 1.94        | 7      | 3     |
| 2:B:132:LYS:HG3  | 2:D:146:HIS:O    | 0.92     | 1.64        | 9      | 1     |
| 2:D:3:LEU:HD12   | 2:D:3:LEU:H      | 0.92     | 1.22        | 6      | 7     |
| 2:D:38:THR:CG2   | 3:D:147:HEC:HBC1 | 0.92     | 1.95        | 20     | 1     |
| 1:A:38:THR:CG2   | 2:D:97:HIS:ND1   | 0.91     | 2.32        | 7      | 1     |
| 1:C:46:PHE:CD1   | 3:C:142:HEC:HMA3 | 0.91     | 2.01        | 12     | 1     |
| 1:C:101:LEU:CD2  | 3:C:142:HEC:CHC  | 0.91     | 2.47        | 4      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:C:40:LYS:O     | 3:C:142:HEC:C4D  | 0.91     | 2.18        | 12     | 1     |
| 1:A:41:THR:CG2   | 2:D:97:HIS:NE2   | 0.91     | 2.33        | 11     | 2     |
| 2:B:38:THR:CG2   | 3:B:147:HEC:HBC1 | 0.91     | 1.95        | 20     | 1     |
| 2:B:97:HIS:NE2   | 1:C:41:THR:HG21  | 0.91     | 1.79        | 11     | 2     |
| 1:C:36:PHE:HZ    | 2:D:131:GLN:OE1  | 0.91     | 1.47        | 9      | 2     |
| 1:A:31:ARG:HH12  | 2:B:127:GLN:CG   | 0.90     | 1.75        | 16     | 1     |
| 1:C:117:PHE:CZ   | 2:D:116:HIS:CE1  | 0.90     | 2.60        | 4      | 1     |
| 1:A:36:PHE:HZ    | 2:B:131:GLN:OE1  | 0.90     | 1.47        | 9      | 2     |
| 1:A:92:ARG:HB2   | 2:D:40:ARG:NE    | 0.90     | 1.81        | 17     | 1     |
| 2:D:42:PHE:HE1   | 3:D:147:HEC:CBC  | 0.90     | 1.75        | 18     | 1     |
| 2:D:106:LEU:HD11 | 3:D:147:HEC:HAB  | 0.90     | 1.40        | 2      | 1     |
| 1:A:117:PHE:CZ   | 2:B:116:HIS:CE1  | 0.90     | 2.60        | 4      | 1     |
| 1:C:101:LEU:HD22 | 3:C:142:HEC:HBB1 | 0.89     | 1.44        | 15     | 1     |
| 2:B:3:LEU:HD12   | 2:B:3:LEU:H      | 0.89     | 1.24        | 4      | 6     |
| 1:A:92:ARG:HD2   | 2:D:40:ARG:HG2   | 0.89     | 1.40        | 3      | 2     |
| 1:C:36:PHE:HB3   | 3:C:142:HEC:CMC  | 0.89     | 1.96        | 12     | 1     |
| 2:B:40:ARG:HD3   | 1:C:92:ARG:HD3   | 0.89     | 1.39        | 18     | 1     |
| 2:B:38:THR:HG21  | 3:B:147:HEC:HBC1 | 0.89     | 1.44        | 20     | 2     |
| 2:D:42:PHE:CB    | 3:D:147:HEC:HHB  | 0.88     | 1.96        | 12     | 1     |
| 2:B:106:LEU:HD13 | 3:B:147:HEC:HHC  | 0.88     | 1.44        | 5      | 9     |
| 1:A:92:ARG:NH1   | 2:D:40:ARG:HB2   | 0.88     | 1.82        | 18     | 1     |
| 2:B:106:LEU:HD13 | 3:B:147:HEC:C4B  | 0.88     | 1.98        | 9      | 13    |
| 2:B:132:LYS:CD   | 2:D:146:HIS:O    | 0.88     | 2.21        | 15     | 1     |
| 1:A:92:ARG:NE    | 2:D:40:ARG:HG2   | 0.88     | 1.84        | 8      | 1     |
| 2:D:106:LEU:HD13 | 3:D:147:HEC:C4B  | 0.88     | 1.98        | 9      | 12    |
| 2:B:146:HIS:O    | 2:D:132:LYS:CD   | 0.88     | 2.20        | 15     | 1     |
| 2:B:139:ASN:OD1  | 2:D:146:HIS:CD2  | 0.88     | 2.26        | 8      | 2     |
| 1:A:65:ALA:HB2   | 3:A:142:HEC:HMA1 | 0.88     | 1.45        | 9      | 5     |
| 1:A:92:ARG:CD    | 2:D:40:ARG:CB    | 0.88     | 2.51        | 19     | 1     |
| 2:B:146:HIS:HE2  | 2:D:135:ALA:C    | 0.88     | 1.71        | 17     | 1     |
| 3:B:147:HEC:HAB  | 2:D:106:LEU:HD22 | 0.88     | 1.45        | 15     | 1     |
| 2:B:139:ASN:ND2  | 2:D:146:HIS:CE1  | 0.87     | 2.41        | 20     | 1     |
| 2:B:40:ARG:NE    | 1:C:92:ARG:HB2   | 0.87     | 1.83        | 17     | 1     |
| 2:D:106:LEU:HD22 | 3:D:147:HEC:CAB  | 0.87     | 1.98        | 10     | 1     |
| 2:B:97:HIS:ND1   | 1:C:38:THR:CG2   | 0.87     | 2.37        | 7      | 1     |
| 2:B:106:LEU:HD22 | 3:B:147:HEC:CAB  | 0.87     | 1.98        | 10     | 1     |
| 1:C:101:LEU:HD12 | 3:C:142:HEC:HMC3 | 0.87     | 1.47        | 7      | 1     |
| 2:B:40:ARG:NE    | 1:C:92:ARG:HD3   | 0.86     | 1.83        | 18     | 1     |
| 1:C:97:ASN:HB3   | 3:C:142:HEC:HMC1 | 0.86     | 1.46        | 17     | 1     |
| 1:C:65:ALA:HB2   | 3:C:142:HEC:HMA1 | 0.86     | 1.45        | 9      | 5     |
| 2:B:63:HIS:CE1   | 3:B:147:HEC:C4D  | 0.86     | 2.58        | 19     | 7     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:106:LEU:HD12 | 3:B:147:HEC:HHC  | 0.86     | 1.45        | 9      | 5     |
| 2:D:63:HIS:CE1   | 3:D:147:HEC:C4D  | 0.86     | 2.58        | 19     | 7     |
| 2:B:82:LYS:HZ3   | 2:D:82:LYS:NZ    | 0.86     | 1.65        | 15     | 1     |
| 1:A:97:ASN:HB3   | 3:A:142:HEC:HMC1 | 0.86     | 1.46        | 17     | 1     |
| 2:D:106:LEU:HD13 | 3:D:147:HEC:HHC  | 0.86     | 1.44        | 5      | 8     |
| 2:B:146:HIS:NE2  | 2:D:139:ASN:CG   | 0.86     | 2.28        | 8      | 1     |
| 1:C:117:PHE:HD1  | 2:D:30:ARG:NH2   | 0.86     | 1.69        | 13     | 3     |
| 2:B:135:ALA:C    | 2:D:146:HIS:NE2  | 0.86     | 2.28        | 17     | 1     |
| 2:B:67:VAL:HG22  | 3:B:147:HEC:C4A  | 0.85     | 2.01        | 9      | 13    |
| 1:A:96:VAL:HG21  | 2:D:99:ASP:HB2   | 0.85     | 1.48        | 18     | 1     |
| 2:D:32:LEU:C     | 3:D:147:HEC:HMB1 | 0.85     | 1.91        | 15     | 1     |
| 2:B:3:LEU:N      | 2:B:3:LEU:HD12   | 0.85     | 1.87        | 17     | 7     |
| 1:A:92:ARG:CD    | 2:D:40:ARG:HE    | 0.85     | 1.80        | 16     | 1     |
| 1:C:32:MET:HE2   | 3:C:142:HEC:HAB  | 0.85     | 0.88        | 12     | 1     |
| 2:B:146:HIS:NE2  | 2:D:139:ASN:OD1  | 0.85     | 2.08        | 8      | 1     |
| 2:D:67:VAL:HG22  | 3:D:147:HEC:C4A  | 0.85     | 2.02        | 9      | 12    |
| 2:D:106:LEU:HD12 | 3:D:147:HEC:HHC  | 0.85     | 1.45        | 9      | 3     |
| 1:A:117:PHE:HD1  | 2:B:30:ARG:HH21  | 0.85     | 1.14        | 17     | 2     |
| 2:B:63:HIS:HE1   | 3:B:147:HEC:C1A  | 0.85     | 1.84        | 13     | 6     |
| 2:D:42:PHE:HE1   | 3:D:147:HEC:HBC1 | 0.85     | 1.18        | 17     | 2     |
| 2:D:63:HIS:NE2   | 3:D:147:HEC:CAD  | 0.85     | 2.40        | 19     | 4     |
| 2:D:67:VAL:CG1   | 3:D:147:HEC:C2B  | 0.85     | 2.54        | 19     | 3     |
| 2:B:42:PHE:HE2   | 3:B:147:HEC:CMD  | 0.85     | 1.85        | 2      | 1     |
| 2:D:38:THR:HG21  | 3:D:147:HEC:HBC1 | 0.85     | 1.44        | 20     | 2     |
| 1:A:101:LEU:HD12 | 3:A:142:HEC:HMC3 | 0.85     | 1.47        | 7      | 1     |
| 1:C:36:PHE:O     | 3:C:142:HEC:CMC  | 0.85     | 2.25        | 12     | 1     |
| 2:D:42:PHE:HE2   | 3:D:147:HEC:CMD  | 0.85     | 1.85        | 2      | 1     |
| 2:B:63:HIS:NE2   | 3:B:147:HEC:CAD  | 0.85     | 2.40        | 19     | 4     |
| 2:B:40:ARG:HG2   | 1:C:92:ARG:HD2   | 0.85     | 1.46        | 3      | 2     |
| 1:A:117:PHE:HD1  | 2:B:30:ARG:NH2   | 0.84     | 1.69        | 17     | 3     |
| 2:B:3:LEU:HD12   | 2:B:3:LEU:N      | 0.84     | 1.87        | 5      | 8     |
| 2:B:135:ALA:CB   | 2:D:146:HIS:O    | 0.84     | 2.24        | 4      | 1     |
| 1:A:92:ARG:NH1   | 2:D:40:ARG:O     | 0.84     | 2.10        | 17     | 1     |
| 2:D:3:LEU:N      | 2:D:3:LEU:HD12   | 0.84     | 1.87        | 17     | 8     |
| 2:B:40:ARG:CB    | 1:C:92:ARG:CD    | 0.84     | 2.55        | 19     | 1     |
| 1:A:101:LEU:HD23 | 3:A:142:HEC:HHC  | 0.84     | 1.46        | 4      | 1     |
| 1:A:101:LEU:HD22 | 3:A:142:HEC:HBB1 | 0.84     | 1.44        | 15     | 1     |
| 1:A:117:PHE:CE1  | 2:B:116:HIS:HD2  | 0.84     | 1.87        | 13     | 1     |
| 2:B:40:ARG:HG2   | 1:C:92:ARG:NE    | 0.84     | 1.88        | 8      | 1     |
| 2:D:67:VAL:HG22  | 3:D:147:HEC:NA   | 0.84     | 1.88        | 19     | 3     |
| 2:B:146:HIS:CE1  | 2:D:139:ASN:ND2  | 0.84     | 2.46        | 20     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:D:3:LEU:HD12   | 2:D:3:LEU:N      | 0.84     | 1.87        | 5      | 7     |
| 1:C:101:LEU:HD23 | 3:C:142:HEC:HHC  | 0.84     | 1.46        | 4      | 1     |
| 1:C:117:PHE:CE1  | 2:D:116:HIS:HD2  | 0.84     | 1.87        | 13     | 1     |
| 2:B:139:ASN:CG   | 2:D:146:HIS:CE1  | 0.83     | 2.52        | 8      | 1     |
| 2:D:63:HIS:HE1   | 3:D:147:HEC:C1A  | 0.83     | 1.84        | 13     | 6     |
| 1:A:66:LEU:O     | 1:A:66:LEU:HD12  | 0.83     | 1.73        | 17     | 1     |
| 1:C:40:LYS:O     | 3:C:142:HEC:C2D  | 0.83     | 2.09        | 12     | 1     |
| 1:C:31:ARG:HH12  | 2:D:127:GLN:CB   | 0.83     | 1.87        | 16     | 1     |
| 2:B:67:VAL:HG22  | 3:B:147:HEC:NA   | 0.83     | 1.88        | 19     | 4     |
| 1:C:39:THR:HB    | 3:C:142:HEC:CHC  | 0.83     | 2.02        | 12     | 1     |
| 1:C:66:LEU:HD12  | 1:C:66:LEU:O     | 0.83     | 1.73        | 17     | 2     |
| 2:B:146:HIS:NE2  | 2:D:135:ALA:C    | 0.83     | 2.31        | 17     | 1     |
| 2:B:42:PHE:HZ    | 3:B:147:HEC:HBC3 | 0.83     | 1.28        | 2      | 2     |
| 1:A:31:ARG:HH12  | 2:B:127:GLN:CB   | 0.83     | 1.87        | 16     | 1     |
| 1:A:113:LEU:O    | 1:A:113:LEU:HD23 | 0.83     | 1.74        | 16     | 2     |
| 2:B:42:PHE:CE1   | 3:B:147:HEC:HBC3 | 0.83     | 2.08        | 18     | 2     |
| 2:B:139:ASN:CG   | 2:D:146:HIS:NE2  | 0.83     | 2.32        | 8      | 1     |
| 2:D:42:PHE:CE1   | 3:D:147:HEC:HBC3 | 0.83     | 2.08        | 18     | 2     |
| 2:D:39:GLN:O     | 3:D:147:HEC:ND   | 0.83     | 2.09        | 12     | 1     |
| 2:D:42:PHE:CE2   | 3:D:147:HEC:HMB2 | 0.83     | 2.08        | 12     | 1     |
| 1:A:61:LYS:HB3   | 3:A:142:HEC:C3A  | 0.82     | 2.04        | 19     | 9     |
| 2:B:63:HIS:CE1   | 3:B:147:HEC:C1A  | 0.82     | 2.62        | 16     | 4     |
| 2:D:42:PHE:CG    | 3:D:147:HEC:HHB  | 0.82     | 2.08        | 12     | 1     |
| 2:B:146:HIS:CE1  | 2:D:139:ASN:CG   | 0.82     | 2.51        | 8      | 1     |
| 2:D:63:HIS:CE1   | 3:D:147:HEC:C1A  | 0.82     | 2.62        | 16     | 5     |
| 1:A:41:THR:CG2   | 2:D:97:HIS:CG    | 0.82     | 2.61        | 12     | 3     |
| 1:A:28:ALA:HB1   | 1:A:104:CYS:SG   | 0.82     | 2.14        | 5      | 1     |
| 1:C:113:LEU:O    | 1:C:113:LEU:HD23 | 0.82     | 1.74        | 16     | 3     |
| 2:B:66:LYS:HD3   | 3:B:147:HEC:O2A  | 0.82     | 1.74        | 13     | 1     |
| 2:B:67:VAL:CG1   | 3:B:147:HEC:C2B  | 0.82     | 2.54        | 19     | 3     |
| 1:C:122:HIS:HB3  | 2:D:34:VAL:HG13  | 0.82     | 1.51        | 18     | 3     |
| 2:D:106:LEU:HD12 | 3:D:147:HEC:HAB  | 0.82     | 0.82        | 18     | 1     |
| 1:C:61:LYS:HB3   | 3:C:142:HEC:C3A  | 0.82     | 2.04        | 19     | 9     |
| 1:A:101:LEU:HD12 | 3:A:142:HEC:CHC  | 0.82     | 2.03        | 19     | 2     |
| 2:D:66:LYS:HD3   | 3:D:147:HEC:O2A  | 0.82     | 1.74        | 13     | 1     |
| 2:B:97:HIS:NE2   | 1:C:41:THR:CG2   | 0.81     | 2.42        | 11     | 2     |
| 1:A:66:LEU:HD12  | 1:A:66:LEU:O     | 0.81     | 1.74        | 9      | 1     |
| 1:C:117:PHE:CE1  | 2:D:116:HIS:NE2  | 0.81     | 2.48        | 20     | 1     |
| 1:C:45:HIS:H     | 3:C:142:HEC:HMA2 | 0.81     | 1.04        | 12     | 1     |
| 2:D:38:THR:H     | 3:D:147:HEC:HHC  | 0.81     | 0.88        | 12     | 1     |
| 1:C:48:LEU:CD1   | 3:C:142:HEC:HHA  | 0.81     | 2.04        | 12     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:C:31:ARG:NH1   | 2:D:127:GLN:CD   | 0.81     | 2.33        | 16     | 1     |
| 1:A:105:LEU:O    | 1:A:105:LEU:HD12 | 0.81     | 1.76        | 13     | 2     |
| 1:A:129:LEU:O    | 1:A:129:LEU:HD12 | 0.81     | 1.76        | 7      | 3     |
| 2:D:36:PRO:O     | 3:D:147:HEC:C2C  | 0.81     | 2.29        | 12     | 1     |
| 1:C:28:ALA:HB1   | 1:C:104:CYS:SG   | 0.81     | 2.14        | 5      | 1     |
| 1:A:96:VAL:CG2   | 2:D:99:ASP:OD2   | 0.81     | 2.28        | 11     | 2     |
| 1:A:31:ARG:NH1   | 2:B:127:GLN:CD   | 0.81     | 2.33        | 16     | 1     |
| 3:C:142:HEC:HBB3 | 3:C:142:HEC:HMB1 | 0.81     | 1.50        | 11     | 3     |
| 1:A:117:PHE:CE1  | 2:B:116:HIS:NE2  | 0.81     | 2.48        | 20     | 1     |
| 2:B:40:ARG:HB2   | 1:C:92:ARG:NH1   | 0.80     | 1.90        | 18     | 1     |
| 2:D:67:VAL:HG13  | 3:D:147:HEC:CHB  | 0.80     | 2.06        | 19     | 1     |
| 1:C:117:PHE:HD1  | 2:D:30:ARG:HH21  | 0.80     | 1.14        | 17     | 2     |
| 1:A:96:VAL:CG2   | 2:D:99:ASP:CB    | 0.80     | 2.57        | 18     | 1     |
| 1:A:122:HIS:HB3  | 2:B:34:VAL:HG13  | 0.80     | 1.51        | 18     | 3     |
| 2:B:139:ASN:OD1  | 2:D:146:HIS:NE2  | 0.80     | 2.14        | 8      | 1     |
| 1:A:92:ARG:HE    | 2:D:40:ARG:CB    | 0.80     | 1.84        | 19     | 2     |
| 1:A:103:HIS:NE2  | 2:B:35:TYR:OH    | 0.80     | 2.14        | 9      | 1     |
| 2:B:146:HIS:O    | 2:D:135:ALA:CB   | 0.80     | 2.30        | 4      | 1     |
| 1:C:129:LEU:HD12 | 1:C:129:LEU:O    | 0.80     | 1.76        | 7      | 2     |
| 2:D:42:PHE:HZ    | 3:D:147:HEC:HBC3 | 0.80     | 1.28        | 2      | 2     |
| 1:C:101:LEU:HD12 | 3:C:142:HEC:CHC  | 0.80     | 2.03        | 19     | 2     |
| 1:C:105:LEU:O    | 1:C:105:LEU:HD12 | 0.80     | 1.76        | 13     | 2     |
| 2:D:133:VAL:HG13 | 2:D:134:VAL:H    | 0.80     | 1.37        | 12     | 3     |
| 3:A:142:HEC:HBB3 | 3:A:142:HEC:HMB1 | 0.80     | 1.50        | 11     | 4     |
| 1:C:36:PHE:HB3   | 3:C:142:HEC:HMC3 | 0.80     | 1.52        | 12     | 1     |
| 1:A:118:THR:O    | 1:A:120:ALA:N    | 0.80     | 2.14        | 10     | 19    |
| 2:B:67:VAL:HG13  | 3:B:147:HEC:CHB  | 0.79     | 2.06        | 19     | 1     |
| 2:D:42:PHE:CE2   | 3:D:147:HEC:CBC  | 0.79     | 2.65        | 11     | 1     |
| 1:A:38:THR:HA    | 2:D:97:HIS:HB3   | 0.79     | 1.51        | 4      | 1     |
| 2:B:106:LEU:HG   | 3:B:147:HEC:C3B  | 0.79     | 2.07        | 18     | 1     |
| 2:B:135:ALA:HB1  | 2:D:146:HIS:CG   | 0.79     | 2.13        | 3      | 1     |
| 2:B:135:ALA:O    | 2:D:146:HIS:NE2  | 0.79     | 2.15        | 17     | 1     |
| 2:B:106:LEU:HD12 | 3:B:147:HEC:HAB  | 0.79     | 0.82        | 18     | 1     |
| 1:A:92:ARG:CD    | 2:D:40:ARG:HB2   | 0.79     | 2.07        | 19     | 1     |
| 1:A:92:ARG:HH11  | 2:D:40:ARG:HD2   | 0.79     | 1.38        | 18     | 1     |
| 1:A:41:THR:HG23  | 2:D:97:HIS:CE1   | 0.79     | 2.10        | 17     | 1     |
| 3:B:147:HEC:C2B  | 2:D:67:VAL:HG13  | 0.79     | 2.07        | 15     | 1     |
| 1:A:111:ALA:HB2  | 2:B:122:PHE:CZ   | 0.79     | 2.10        | 8      | 1     |
| 1:C:103:HIS:NE2  | 2:D:35:TYR:OH    | 0.79     | 2.15        | 9      | 1     |
| 2:B:42:PHE:CE2   | 3:B:147:HEC:CBC  | 0.79     | 2.65        | 11     | 1     |
| 3:C:142:HEC:HMB1 | 3:C:142:HEC:HBB3 | 0.79     | 1.54        | 1      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:31:ARG:HG3   | 2:B:127:GLN:HE22 | 0.79     | 1.38        | 6      | 1     |
| 1:C:118:THR:O    | 1:C:120:ALA:N    | 0.78     | 2.14        | 10     | 19    |
| 1:C:31:ARG:HG3   | 2:D:127:GLN:HE22 | 0.78     | 1.38        | 6      | 1     |
| 2:D:106:LEU:HG   | 3:D:147:HEC:C3B  | 0.78     | 2.07        | 18     | 1     |
| 1:C:86:LEU:CD1   | 3:C:142:HEC:CBD  | 0.78     | 2.62        | 7      | 2     |
| 1:A:86:LEU:CD1   | 3:A:142:HEC:CBD  | 0.78     | 2.62        | 7      | 2     |
| 2:B:139:ASN:HD21 | 2:D:139:ASN:HD21 | 0.78     | 1.19        | 12     | 1     |
| 2:B:99:ASP:HB2   | 1:C:96:VAL:HG21  | 0.78     | 1.53        | 18     | 1     |
| 3:B:147:HEC:C3B  | 2:D:106:LEU:HD13 | 0.78     | 2.07        | 15     | 1     |
| 2:D:42:PHE:HB3   | 3:D:147:HEC:HMA1 | 0.78     | 0.82        | 12     | 1     |
| 1:C:46:PHE:O     | 1:C:48:LEU:N     | 0.78     | 2.16        | 19     | 8     |
| 3:B:147:HEC:HHC  | 2:D:106:LEU:HD13 | 0.78     | 1.39        | 15     | 1     |
| 2:B:133:VAL:HG13 | 2:B:134:VAL:H    | 0.78     | 1.37        | 12     | 3     |
| 2:B:135:ALA:HB3  | 2:D:146:HIS:O    | 0.77     | 1.78        | 4      | 1     |
| 2:D:106:LEU:HD23 | 3:D:147:HEC:HMC3 | 0.77     | 1.54        | 2      | 1     |
| 1:C:111:ALA:HB2  | 2:D:122:PHE:CZ   | 0.77     | 2.10        | 8      | 1     |
| 1:A:92:ARG:NH2   | 3:D:147:HEC:CBD  | 0.77     | 2.32        | 12     | 1     |
| 2:D:75:LEU:HD23  | 2:D:75:LEU:N     | 0.77     | 1.94        | 20     | 2     |
| 1:A:46:PHE:O     | 1:A:48:LEU:N     | 0.77     | 2.16        | 19     | 7     |
| 2:B:40:ARG:O     | 1:C:92:ARG:NH1   | 0.77     | 2.17        | 17     | 1     |
| 1:C:103:HIS:ND1  | 2:D:108:ASN:OD1  | 0.77     | 2.17        | 8      | 2     |
| 1:C:101:LEU:HD21 | 3:C:142:HEC:HBB3 | 0.77     | 1.56        | 2      | 4     |
| 1:C:36:PHE:CE2   | 2:D:131:GLN:NE2  | 0.77     | 2.50        | 13     | 1     |
| 1:C:31:ARG:HH21  | 2:D:127:GLN:HB2  | 0.77     | 1.40        | 15     | 1     |
| 2:D:75:LEU:N     | 2:D:75:LEU:HD23  | 0.77     | 1.95        | 4      | 1     |
| 1:C:113:LEU:HD23 | 1:C:113:LEU:O    | 0.77     | 1.79        | 3      | 1     |
| 2:B:102:ASN:OD1  | 3:B:147:HEC:CMC  | 0.77     | 2.33        | 12     | 1     |
| 1:A:65:ALA:CB    | 3:A:142:HEC:HMA1 | 0.77     | 2.10        | 9      | 1     |
| 2:D:42:PHE:CD1   | 3:D:147:HEC:HMB2 | 0.77     | 2.14        | 12     | 1     |
| 2:B:42:PHE:CZ    | 3:B:147:HEC:HBC2 | 0.77     | 2.13        | 12     | 2     |
| 2:B:106:LEU:HD23 | 3:B:147:HEC:HMC3 | 0.77     | 1.54        | 2      | 1     |
| 2:D:67:VAL:HG22  | 3:D:147:HEC:NB   | 0.77     | 1.95        | 9      | 7     |
| 1:A:101:LEU:HD21 | 3:A:142:HEC:HBB3 | 0.76     | 1.56        | 2      | 4     |
| 2:B:82:LYS:NZ    | 2:D:82:LYS:HZ3   | 0.76     | 1.76        | 15     | 1     |
| 2:B:40:ARG:HD3   | 1:C:92:ARG:NE    | 0.76     | 1.94        | 19     | 1     |
| 1:A:31:ARG:HH21  | 2:B:127:GLN:HB2  | 0.76     | 1.39        | 15     | 1     |
| 1:C:65:ALA:CB    | 3:C:142:HEC:HMA1 | 0.76     | 2.10        | 9      | 1     |
| 1:A:96:VAL:HG21  | 2:D:99:ASP:OD2   | 0.76     | 1.79        | 11     | 2     |
| 1:A:29:LEU:HD11  | 1:A:58:HIS:CG    | 0.76     | 2.16        | 4      | 3     |
| 1:A:103:HIS:ND1  | 2:B:108:ASN:OD1  | 0.76     | 2.17        | 8      | 2     |
| 2:B:97:HIS:HB3   | 1:C:38:THR:HA    | 0.76     | 1.55        | 4      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:94:ASP:CG    | 2:D:40:ARG:NH1   | 0.76     | 2.39        | 3      | 1     |
| 1:C:86:LEU:CD1   | 3:C:142:HEC:HBD2 | 0.76     | 2.06        | 7      | 1     |
| 2:D:42:PHE:HZ    | 3:D:147:HEC:HBC2 | 0.76     | 1.38        | 17     | 1     |
| 2:B:97:HIS:CG    | 1:C:41:THR:CG2   | 0.76     | 2.67        | 17     | 3     |
| 2:B:67:VAL:CG2   | 3:B:147:HEC:C1B  | 0.76     | 2.63        | 9      | 3     |
| 1:A:65:ALA:HB2   | 3:A:142:HEC:CMA  | 0.76     | 2.11        | 9      | 2     |
| 2:B:146:HIS:NE2  | 2:D:135:ALA:O    | 0.76     | 2.19        | 17     | 1     |
| 1:A:113:LEU:HD23 | 1:A:113:LEU:O    | 0.76     | 1.80        | 1      | 2     |
| 1:C:65:ALA:HB2   | 3:C:142:HEC:CMA  | 0.76     | 2.11        | 9      | 1     |
| 2:B:75:LEU:N     | 2:B:75:LEU:HD23  | 0.76     | 1.95        | 4      | 2     |
| 2:B:146:HIS:CG   | 2:D:135:ALA:HB1  | 0.76     | 2.15        | 3      | 1     |
| 2:B:42:PHE:HZ    | 3:B:147:HEC:HBC2 | 0.75     | 1.41        | 12     | 2     |
| 1:C:29:LEU:HD11  | 1:C:58:HIS:CG    | 0.75     | 2.16        | 4      | 3     |
| 1:A:92:ARG:CD    | 2:D:40:ARG:HG2   | 0.75     | 2.12        | 8      | 2     |
| 2:B:67:VAL:HG22  | 3:B:147:HEC:NB   | 0.75     | 1.96        | 9      | 7     |
| 2:B:106:LEU:CD1  | 3:B:147:HEC:C4B  | 0.75     | 2.64        | 9      | 3     |
| 1:A:92:ARG:CD    | 2:D:40:ARG:HB3   | 0.75     | 2.10        | 19     | 2     |
| 1:A:126:ASP:OD1  | 2:B:35:TYR:CD2   | 0.75     | 2.39        | 13     | 1     |
| 2:B:99:ASP:OD2   | 1:C:96:VAL:CG2   | 0.75     | 2.35        | 11     | 2     |
| 1:A:36:PHE:CE2   | 2:B:131:GLN:NE2  | 0.75     | 2.50        | 13     | 1     |
| 2:B:146:HIS:O    | 2:D:135:ALA:HB3  | 0.75     | 1.81        | 4      | 1     |
| 2:D:42:PHE:C     | 3:D:147:HEC:CMA  | 0.75     | 2.52        | 12     | 1     |
| 2:B:40:ARG:HD2   | 1:C:92:ARG:HH11  | 0.75     | 1.38        | 18     | 1     |
| 2:B:42:PHE:HE2   | 3:B:147:HEC:CBC  | 0.75     | 1.95        | 11     | 1     |
| 1:C:61:LYS:HG2   | 3:C:142:HEC:C2A  | 0.75     | 2.12        | 19     | 1     |
| 2:D:67:VAL:HA    | 3:D:147:HEC:CHB  | 0.74     | 2.12        | 19     | 5     |
| 1:A:38:THR:O     | 1:A:41:THR:HG22  | 0.74     | 1.83        | 20     | 9     |
| 2:B:40:ARG:HB3   | 1:C:92:ARG:CD    | 0.74     | 2.12        | 19     | 2     |
| 2:D:42:PHE:HE2   | 3:D:147:HEC:CBC  | 0.74     | 1.95        | 11     | 1     |
| 2:B:42:PHE:CE2   | 3:B:147:HEC:HBC3 | 0.74     | 2.16        | 11     | 1     |
| 1:A:31:ARG:HH11  | 2:B:127:GLN:HG2  | 0.74     | 1.41        | 10     | 1     |
| 3:B:147:HEC:C4A  | 2:D:67:VAL:HG22  | 0.74     | 2.12        | 15     | 1     |
| 1:C:126:ASP:OD1  | 2:D:35:TYR:CD2   | 0.74     | 2.39        | 13     | 1     |
| 1:A:115:ALA:O    | 1:A:121:VAL:HG21 | 0.74     | 1.83        | 5      | 9     |
| 1:C:31:ARG:HH11  | 2:D:127:GLN:HG2  | 0.74     | 1.41        | 10     | 1     |
| 2:B:67:VAL:HA    | 3:B:147:HEC:CHB  | 0.74     | 2.12        | 19     | 4     |
| 1:C:101:LEU:HD22 | 3:C:142:HEC:CHC  | 0.74     | 2.12        | 18     | 9     |
| 3:C:142:HEC:HMB1 | 3:C:142:HEC:HBB2 | 0.74     | 1.57        | 16     | 6     |
| 1:C:38:THR:O     | 1:C:41:THR:HG22  | 0.74     | 1.82        | 20     | 9     |
| 2:B:135:ALA:CB   | 2:D:146:HIS:HB3  | 0.74     | 2.13        | 3      | 1     |
| 1:C:93:VAL:HG22  | 1:C:94:ASP:H     | 0.74     | 1.42        | 13     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 3:A:142:HEC:HBB2 | 3:A:142:HEC:HMB1 | 0.74     | 1.57        | 16     | 5     |
| 2:B:75:LEU:H     | 2:B:75:LEU:HD23  | 0.74     | 1.43        | 20     | 2     |
| 2:D:38:THR:O     | 3:D:147:HEC:C1C  | 0.74     | 2.35        | 12     | 1     |
| 2:D:42:PHE:CB    | 3:D:147:HEC:HMA2 | 0.74     | 2.13        | 12     | 1     |
| 2:D:42:PHE:CE2   | 3:D:147:HEC:HBC3 | 0.74     | 2.16        | 11     | 1     |
| 1:C:115:ALA:O    | 1:C:121:VAL:HG21 | 0.73     | 1.83        | 5      | 9     |
| 2:D:39:GLN:O     | 3:D:147:HEC:C1D  | 0.73     | 2.36        | 12     | 1     |
| 1:C:101:LEU:HD22 | 3:C:142:HEC:HHC  | 0.73     | 1.60        | 18     | 4     |
| 1:A:101:LEU:HD22 | 3:A:142:HEC:CHC  | 0.73     | 2.12        | 18     | 9     |
| 2:B:146:HIS:CD2  | 2:D:2:HIS:CD2    | 0.73     | 2.74        | 15     | 1     |
| 2:D:75:LEU:HD23  | 2:D:75:LEU:H     | 0.73     | 1.43        | 20     | 2     |
| 2:B:132:LYS:HG2  | 2:D:146:HIS:OXT  | 0.73     | 1.84        | 3      | 1     |
| 1:A:61:LYS:HG2   | 3:A:142:HEC:C2A  | 0.73     | 2.12        | 19     | 1     |
| 2:B:99:ASP:OD2   | 1:C:96:VAL:HG21  | 0.73     | 1.83        | 11     | 2     |
| 2:D:67:VAL:CG2   | 3:D:147:HEC:C1B  | 0.73     | 2.63        | 9      | 3     |
| 1:A:101:LEU:HD22 | 3:A:142:HEC:HHC  | 0.73     | 1.60        | 18     | 4     |
| 2:B:139:ASN:OD1  | 2:D:146:HIS:O    | 0.73     | 2.06        | 6      | 1     |
| 3:C:142:HEC:HBB2 | 3:C:142:HEC:HMB1 | 0.73     | 1.60        | 9      | 5     |
| 2:B:146:HIS:HD2  | 2:D:2:HIS:CE1    | 0.73     | 1.97        | 15     | 1     |
| 2:B:106:LEU:CG   | 3:B:147:HEC:HBB3 | 0.73     | 2.13        | 19     | 1     |
| 2:D:106:LEU:CG   | 3:D:147:HEC:HBB3 | 0.73     | 2.13        | 19     | 1     |
| 1:A:93:VAL:HG22  | 1:A:94:ASP:H     | 0.73     | 1.41        | 13     | 1     |
| 2:B:40:ARG:HD2   | 1:C:92:ARG:NH1   | 0.73     | 1.98        | 18     | 1     |
| 1:A:13:ALA:O     | 1:A:17:VAL:HG23  | 0.73     | 1.84        | 2      | 17    |
| 1:C:103:HIS:CG   | 2:D:108:ASN:HD21 | 0.73     | 2.01        | 20     | 1     |
| 2:B:146:HIS:O    | 2:D:132:LYS:CG   | 0.72     | 2.36        | 9      | 2     |
| 2:D:57:ASN:N     | 2:D:58:PRO:CD    | 0.72     | 2.52        | 19     | 1     |
| 1:C:36:PHE:O     | 3:C:142:HEC:HMC1 | 0.72     | 1.83        | 12     | 1     |
| 2:B:40:ARG:NH1   | 1:C:94:ASP:CG    | 0.72     | 2.43        | 3      | 1     |
| 2:D:42:PHE:CG    | 3:D:147:HEC:CHB  | 0.72     | 2.70        | 12     | 1     |
| 2:D:63:HIS:HE1   | 3:D:147:HEC:C4D  | 0.72     | 1.94        | 19     | 1     |
| 1:A:103:HIS:CG   | 2:B:108:ASN:HD21 | 0.72     | 2.01        | 20     | 1     |
| 2:B:42:PHE:HE2   | 3:B:147:HEC:HBC1 | 0.72     | 1.44        | 11     | 1     |
| 3:B:147:HEC:C1C  | 2:D:106:LEU:HD12 | 0.72     | 2.14        | 15     | 1     |
| 2:D:106:LEU:CB   | 3:D:147:HEC:CAB  | 0.72     | 2.67        | 18     | 1     |
| 2:B:133:VAL:HG13 | 2:B:134:VAL:N    | 0.72     | 1.99        | 9      | 4     |
| 2:D:106:LEU:HD21 | 3:D:147:HEC:C4B  | 0.72     | 2.15        | 2      | 1     |
| 1:A:31:ARG:CG    | 2:B:127:GLN:HE22 | 0.72     | 1.97        | 6      | 1     |
| 2:B:106:LEU:CB   | 3:B:147:HEC:CAB  | 0.72     | 2.67        | 18     | 1     |
| 1:A:121:VAL:HG13 | 1:A:122:HIS:N    | 0.72     | 2.00        | 17     | 18    |
| 1:C:39:THR:CB    | 3:C:142:HEC:CHC  | 0.72     | 2.60        | 12     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:D:42:PHE:CE1   | 3:D:147:HEC:CMB  | 0.72     | 2.72        | 12     | 1     |
| 1:A:86:LEU:HD21  | 3:A:142:HEC:HBD2 | 0.72     | 1.59        | 12     | 2     |
| 1:A:92:ARG:NH1   | 2:D:40:ARG:HD2   | 0.71     | 1.98        | 18     | 1     |
| 1:A:84:SER:O     | 1:A:88:ALA:HB3   | 0.71     | 1.84        | 4      | 4     |
| 2:B:135:ALA:CB   | 2:D:146:HIS:NE2  | 0.71     | 2.52        | 17     | 1     |
| 1:C:31:ARG:CG    | 2:D:127:GLN:HE22 | 0.71     | 1.97        | 6      | 1     |
| 2:D:106:LEU:HD23 | 3:D:147:HEC:HHC  | 0.71     | 1.60        | 2      | 1     |
| 1:A:113:LEU:HD12 | 1:A:114:PRO:O    | 0.71     | 1.85        | 18     | 2     |
| 1:C:84:SER:O     | 1:C:88:ALA:HB3   | 0.71     | 1.84        | 4      | 4     |
| 2:B:146:HIS:O    | 2:D:139:ASN:OD1  | 0.71     | 2.07        | 6      | 1     |
| 1:C:45:HIS:H     | 3:C:142:HEC:CMA  | 0.71     | 1.89        | 12     | 1     |
| 1:C:76:MET:N     | 1:C:77:PRO:CD    | 0.71     | 2.54        | 5      | 20    |
| 2:B:14:LEU:O     | 2:B:18:VAL:HG23  | 0.71     | 1.85        | 8      | 5     |
| 1:A:48:LEU:H     | 1:A:48:LEU:CD1   | 0.71     | 1.93        | 9      | 4     |
| 1:A:96:VAL:HG11  | 2:D:99:ASP:HB3   | 0.71     | 1.62        | 9      | 1     |
| 2:D:14:LEU:O     | 2:D:18:VAL:HG23  | 0.71     | 1.85        | 8      | 5     |
| 3:A:142:HEC:HMB1 | 3:A:142:HEC:HBB3 | 0.71     | 1.62        | 8      | 1     |
| 1:C:35:SER:OG    | 2:D:131:GLN:OE1  | 0.71     | 2.09        | 16     | 1     |
| 1:A:38:THR:HB    | 2:D:97:HIS:HB3   | 0.71     | 1.61        | 19     | 1     |
| 1:C:13:ALA:O     | 1:C:17:VAL:HG23  | 0.71     | 1.84        | 2      | 17    |
| 2:B:2:HIS:CE1    | 2:D:146:HIS:HD2  | 0.71     | 2.01        | 15     | 1     |
| 3:B:147:HEC:C1B  | 2:D:67:VAL:HG13  | 0.71     | 2.15        | 15     | 1     |
| 2:B:57:ASN:N     | 2:B:58:PRO:CD    | 0.71     | 2.52        | 19     | 1     |
| 2:B:106:LEU:HD21 | 3:B:147:HEC:C4B  | 0.71     | 2.15        | 2      | 1     |
| 2:D:63:HIS:CE1   | 3:D:147:HEC:CGA  | 0.71     | 2.74        | 5      | 1     |
| 1:A:126:ASP:OD1  | 2:B:35:TYR:CE2   | 0.71     | 2.44        | 13     | 1     |
| 2:D:42:PHE:HE2   | 3:D:147:HEC:HBC1 | 0.71     | 1.44        | 11     | 1     |
| 1:C:113:LEU:HD12 | 1:C:114:PRO:O    | 0.71     | 1.85        | 18     | 2     |
| 2:D:133:VAL:HG13 | 2:D:134:VAL:N    | 0.71     | 1.99        | 9      | 4     |
| 2:B:97:HIS:CE1   | 1:C:41:THR:HG23  | 0.71     | 2.18        | 17     | 1     |
| 2:B:135:ALA:CB   | 2:D:146:HIS:CE1  | 0.71     | 2.73        | 17     | 1     |
| 2:B:135:ALA:HB1  | 2:D:146:HIS:CE1  | 0.71     | 2.21        | 17     | 1     |
| 1:C:121:VAL:HG13 | 1:C:122:HIS:N    | 0.71     | 2.00        | 13     | 18    |
| 2:B:2:HIS:CD2    | 2:D:146:HIS:CD2  | 0.71     | 2.77        | 15     | 1     |
| 2:B:40:ARG:HB2   | 1:C:92:ARG:CD    | 0.70     | 2.13        | 19     | 1     |
| 1:A:106:LEU:HD12 | 1:A:122:HIS:CE1  | 0.70     | 2.21        | 4      | 1     |
| 2:D:42:PHE:CZ    | 3:D:147:HEC:CMB  | 0.70     | 2.73        | 12     | 1     |
| 1:A:76:MET:N     | 1:A:77:PRO:CD    | 0.70     | 2.54        | 5      | 20    |
| 1:A:35:SER:OG    | 2:B:131:GLN:OE1  | 0.70     | 2.09        | 16     | 1     |
| 1:C:86:LEU:HD13  | 1:C:86:LEU:C     | 0.70     | 2.07        | 7      | 1     |
| 1:C:126:ASP:OD1  | 2:D:35:TYR:CE2   | 0.70     | 2.44        | 13     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:92:ARG:HE    | 2:D:40:ARG:CG    | 0.70     | 1.99        | 19     | 2     |
| 1:A:92:ARG:NE    | 2:D:40:ARG:HD3   | 0.70     | 1.99        | 19     | 1     |
| 2:B:63:HIS:CE1   | 3:B:147:HEC:CGA  | 0.70     | 2.74        | 5      | 1     |
| 1:A:92:ARG:CB    | 2:D:40:ARG:NE    | 0.70     | 2.55        | 18     | 2     |
| 1:A:86:LEU:HD13  | 1:A:86:LEU:C     | 0.70     | 2.07        | 7      | 1     |
| 1:A:38:THR:CB    | 2:D:97:HIS:HB3   | 0.70     | 2.17        | 19     | 2     |
| 2:B:106:LEU:CD2  | 3:B:147:HEC:HAB  | 0.69     | 2.17        | 3      | 6     |
| 2:D:32:LEU:HB3   | 3:D:147:HEC:HMB2 | 0.69     | 1.62        | 15     | 1     |
| 2:B:132:LYS:CG   | 2:D:146:HIS:O    | 0.69     | 2.38        | 9      | 2     |
| 2:D:38:THR:O     | 3:D:147:HEC:NC   | 0.69     | 2.19        | 12     | 1     |
| 1:A:101:LEU:CD2  | 3:A:142:HEC:HBB2 | 0.69     | 2.16        | 15     | 1     |
| 1:C:34:LEU:HD12  | 2:D:128:ALA:HB2  | 0.69     | 1.65        | 7      | 2     |
| 1:C:36:PHE:CE1   | 2:D:131:GLN:OE1  | 0.69     | 2.46        | 13     | 1     |
| 2:B:106:LEU:C    | 2:B:106:LEU:HD13 | 0.69     | 2.08        | 18     | 1     |
| 1:C:106:LEU:HD12 | 1:C:122:HIS:CE1  | 0.69     | 2.21        | 4      | 1     |
| 1:C:36:PHE:O     | 3:C:142:HEC:C2C  | 0.69     | 2.29        | 12     | 1     |
| 2:B:106:LEU:HD23 | 3:B:147:HEC:HHC  | 0.69     | 1.60        | 2      | 1     |
| 2:D:67:VAL:CG2   | 3:D:147:HEC:CHB  | 0.69     | 2.68        | 9      | 2     |
| 2:D:63:HIS:NE2   | 3:D:147:HEC:C1A  | 0.69     | 2.55        | 16     | 1     |
| 1:C:46:PHE:CE1   | 3:C:142:HEC:HMA3 | 0.69     | 2.22        | 12     | 1     |
| 2:B:139:ASN:HD21 | 2:D:139:ASN:ND2  | 0.69     | 1.84        | 3      | 2     |
| 1:C:117:PHE:HE1  | 2:D:116:HIS:HE2  | 0.69     | 1.29        | 20     | 1     |
| 1:A:36:PHE:CE1   | 2:B:131:GLN:OE1  | 0.69     | 2.46        | 13     | 1     |
| 2:D:106:LEU:HD13 | 2:D:106:LEU:C    | 0.68     | 2.08        | 18     | 1     |
| 1:A:6:ASP:O      | 1:A:10:VAL:HG23  | 0.68     | 1.89        | 6      | 5     |
| 1:C:97:ASN:HB3   | 3:C:142:HEC:CMC  | 0.68     | 2.19        | 17     | 1     |
| 2:B:99:ASP:CB    | 1:C:96:VAL:CG2   | 0.68     | 2.63        | 18     | 1     |
| 1:A:92:ARG:HE    | 2:D:40:ARG:HG2   | 0.68     | 1.49        | 8      | 1     |
| 2:D:106:LEU:CD1  | 3:D:147:HEC:C4B  | 0.68     | 2.64        | 9      | 3     |
| 2:B:68:LEU:O     | 2:B:68:LEU:HD23  | 0.68     | 1.89        | 20     | 6     |
| 2:B:146:HIS:OXT  | 2:D:132:LYS:HG2  | 0.68     | 1.88        | 3      | 1     |
| 2:B:63:HIS:NE2   | 3:B:147:HEC:C1A  | 0.68     | 2.55        | 16     | 1     |
| 1:C:85:ASP:O     | 1:C:89:HIS:N     | 0.68     | 2.27        | 11     | 6     |
| 2:B:96:LEU:O     | 2:B:97:HIS:ND1   | 0.68     | 2.27        | 14     | 6     |
| 1:C:61:LYS:HG2   | 3:C:142:HEC:CAA  | 0.68     | 2.19        | 19     | 3     |
| 1:C:48:LEU:H     | 1:C:48:LEU:HD23  | 0.68     | 1.49        | 3      | 1     |
| 1:C:119:PRO:HA   | 2:D:33:VAL:HG13  | 0.68     | 1.64        | 13     | 3     |
| 1:C:48:LEU:N     | 1:C:48:LEU:HD13  | 0.68     | 1.97        | 11     | 1     |
| 1:C:93:VAL:HG12  | 1:C:94:ASP:N     | 0.68     | 2.04        | 18     | 3     |
| 1:C:115:ALA:O    | 1:C:116:GLU:CB   | 0.68     | 2.42        | 1      | 17    |
| 1:A:119:PRO:HA   | 2:B:33:VAL:HG13  | 0.68     | 1.64        | 13     | 3     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:C:6:ASP:O     | 1:C:10:VAL:HG23  | 0.68     | 1.89        | 6      | 5     |
| 1:A:31:ARG:HG3  | 2:B:127:GLN:NE2  | 0.68     | 2.03        | 6      | 1     |
| 1:A:101:LEU:CD1 | 3:A:142:HEC:HBB3 | 0.68     | 2.19        | 15     | 1     |
| 2:B:40:ARG:HG2  | 1:C:92:ARG:CD    | 0.68     | 2.19        | 8      | 2     |
| 1:A:97:ASN:HB3  | 3:A:142:HEC:CMC  | 0.68     | 2.19        | 17     | 1     |
| 1:A:92:ARG:HH22 | 3:D:147:HEC:HBD2 | 0.68     | 0.63        | 12     | 1     |
| 1:A:61:LYS:CG   | 3:A:142:HEC:C2A  | 0.67     | 2.71        | 19     | 1     |
| 1:A:61:LYS:HG2  | 3:A:142:HEC:CAA  | 0.67     | 2.19        | 19     | 3     |
| 1:C:101:LEU:CD2 | 3:C:142:HEC:HBB2 | 0.67     | 2.16        | 15     | 1     |
| 1:A:111:ALA:HB1 | 2:B:122:PHE:CZ   | 0.67     | 2.23        | 8      | 1     |
| 2:B:40:ARG:CG   | 1:C:92:ARG:HE    | 0.67     | 2.02        | 19     | 2     |
| 1:C:61:LYS:CG   | 3:C:142:HEC:C2A  | 0.67     | 2.71        | 19     | 1     |
| 1:C:31:ARG:HG3  | 2:D:127:GLN:NE2  | 0.67     | 2.03        | 6      | 1     |
| 2:B:38:THR:HG21 | 3:B:147:HEC:CBC  | 0.67     | 2.19        | 20     | 1     |
| 1:A:34:LEU:HD12 | 2:B:128:ALA:HB2  | 0.67     | 1.64        | 7      | 2     |
| 1:C:101:LEU:CD1 | 3:C:142:HEC:HBB3 | 0.67     | 2.20        | 15     | 1     |
| 2:B:139:ASN:ND2 | 2:D:139:ASN:HD21 | 0.67     | 1.87        | 3      | 2     |
| 1:A:115:ALA:O   | 1:A:116:GLU:CB   | 0.67     | 2.43        | 5      | 17    |
| 3:B:147:HEC:CHA | 2:D:63:HIS:CE1   | 0.67     | 2.78        | 15     | 1     |
| 1:C:48:LEU:HD13 | 1:C:48:LEU:N     | 0.67     | 1.98        | 9      | 1     |
| 1:A:94:ASP:HB2  | 2:D:99:ASP:OD2   | 0.67     | 1.89        | 5      | 1     |
| 1:A:38:THR:CG2  | 2:D:97:HIS:HB3   | 0.67     | 2.19        | 19     | 1     |
| 2:B:82:LYS:HZ3  | 2:D:82:LYS:HZ3   | 0.67     | 1.25        | 15     | 1     |
| 2:D:38:THR:HG21 | 3:D:147:HEC:CBC  | 0.67     | 2.19        | 20     | 1     |
| 2:D:38:THR:CA   | 3:D:147:HEC:C1C  | 0.67     | 2.48        | 12     | 1     |
| 1:C:103:HIS:ND1 | 2:D:108:ASN:ND2  | 0.67     | 2.43        | 20     | 2     |
| 1:A:92:ARG:HD2  | 2:D:40:ARG:HB3   | 0.67     | 1.66        | 19     | 2     |
| 1:A:86:LEU:C    | 1:A:86:LEU:HD13  | 0.67     | 2.10        | 19     | 1     |
| 1:A:38:THR:CA   | 2:D:97:HIS:HB3   | 0.67     | 2.19        | 4      | 1     |
| 2:B:146:HIS:NE2 | 2:D:135:ALA:CB   | 0.67     | 2.57        | 17     | 1     |
| 1:A:85:ASP:O    | 1:A:89:HIS:N     | 0.67     | 2.27        | 11     | 6     |
| 2:D:106:LEU:CD2 | 3:D:147:HEC:HAB  | 0.67     | 2.19        | 5      | 5     |
| 2:D:96:LEU:O    | 2:D:97:HIS:ND1   | 0.67     | 2.27        | 14     | 7     |
| 1:A:93:VAL:HG12 | 1:A:94:ASP:N     | 0.66     | 2.04        | 18     | 3     |
| 2:D:67:VAL:HG13 | 3:D:147:HEC:CMB  | 0.66     | 2.20        | 9      | 3     |
| 1:A:103:HIS:ND1 | 2:B:108:ASN:ND2  | 0.66     | 2.43        | 20     | 2     |
| 1:A:92:ARG:HD3  | 2:D:40:ARG:HE    | 0.66     | 0.88        | 16     | 1     |
| 1:A:48:LEU:HD13 | 1:A:48:LEU:N     | 0.66     | 1.97        | 11     | 2     |
| 1:C:34:LEU:HD12 | 2:D:128:ALA:CA   | 0.66     | 2.19        | 18     | 1     |
| 2:D:68:LEU:HD23 | 2:D:68:LEU:O     | 0.66     | 1.89        | 20     | 4     |
| 2:B:146:HIS:HB3 | 2:D:135:ALA:CB   | 0.66     | 2.18        | 3      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:40:ARG:NE    | 1:C:92:ARG:CD    | 0.66     | 2.52        | 18     | 1     |
| 2:B:106:LEU:HB3  | 3:B:147:HEC:HAB  | 0.66     | 1.66        | 13     | 2     |
| 2:D:116:HIS:ND1  | 2:D:116:HIS:N    | 0.66     | 2.43        | 9      | 1     |
| 1:C:61:LYS:CG    | 3:C:142:HEC:CAA  | 0.66     | 2.74        | 19     | 2     |
| 1:C:119:PRO:HA   | 2:D:33:VAL:CG1   | 0.66     | 2.20        | 17     | 2     |
| 1:C:31:ARG:HH11  | 2:D:127:GLN:CD   | 0.66     | 1.94        | 16     | 1     |
| 1:C:86:LEU:C     | 1:C:86:LEU:HD13  | 0.66     | 2.10        | 19     | 1     |
| 1:A:48:LEU:HD23  | 1:A:48:LEU:H     | 0.66     | 1.49        | 3      | 1     |
| 1:A:31:ARG:HH11  | 2:B:127:GLN:CD   | 0.66     | 1.94        | 16     | 1     |
| 1:A:93:VAL:HG22  | 1:A:94:ASP:N     | 0.66     | 2.05        | 13     | 3     |
| 1:A:92:ARG:HD2   | 2:D:40:ARG:HD2   | 0.66     | 1.62        | 18     | 1     |
| 1:C:34:LEU:CD1   | 2:D:128:ALA:CA   | 0.66     | 2.74        | 18     | 1     |
| 1:A:119:PRO:HA   | 2:B:33:VAL:CG1   | 0.66     | 2.20        | 17     | 3     |
| 1:C:48:LEU:CD1   | 1:C:48:LEU:H     | 0.66     | 1.93        | 9      | 2     |
| 1:A:122:HIS:CD2  | 2:B:112:CYS:SG   | 0.66     | 2.89        | 17     | 1     |
| 1:C:93:VAL:HG22  | 1:C:94:ASP:N     | 0.66     | 2.05        | 13     | 3     |
| 2:D:38:THR:O     | 3:D:147:HEC:C4C  | 0.66     | 2.44        | 12     | 1     |
| 1:A:104:CYS:SG   | 1:A:105:LEU:N    | 0.66     | 2.68        | 5      | 1     |
| 1:C:104:CYS:SG   | 1:C:105:LEU:N    | 0.66     | 2.68        | 5      | 1     |
| 2:B:146:HIS:CE1  | 2:D:135:ALA:CB   | 0.66     | 2.79        | 17     | 1     |
| 2:B:106:LEU:HD23 | 3:B:147:HEC:CMC  | 0.66     | 2.21        | 2      | 1     |
| 2:B:48:LEU:HD12  | 2:B:48:LEU:N     | 0.65     | 2.07        | 16     | 3     |
| 2:B:40:ARG:HG2   | 1:C:92:ARG:HE    | 0.65     | 1.50        | 8      | 1     |
| 2:D:106:LEU:HB3  | 3:D:147:HEC:HAB  | 0.65     | 1.66        | 13     | 2     |
| 1:A:34:LEU:HD12  | 1:A:34:LEU:C     | 0.65     | 2.11        | 9      | 2     |
| 1:C:101:LEU:CB   | 3:C:142:HEC:HMC3 | 0.65     | 2.21        | 2      | 1     |
| 1:C:111:ALA:HB1  | 2:D:122:PHE:CZ   | 0.65     | 2.23        | 8      | 1     |
| 1:C:105:LEU:HD12 | 1:C:105:LEU:C    | 0.65     | 2.12        | 16     | 1     |
| 1:A:34:LEU:CD1   | 2:B:128:ALA:CA   | 0.65     | 2.74        | 18     | 1     |
| 1:A:61:LYS:CG    | 3:A:142:HEC:CAA  | 0.65     | 2.74        | 19     | 2     |
| 1:C:34:LEU:C     | 1:C:34:LEU:HD12  | 0.65     | 2.11        | 9      | 2     |
| 2:D:33:VAL:HG13  | 2:D:34:VAL:N     | 0.65     | 2.06        | 3      | 2     |
| 1:A:105:LEU:C    | 1:A:105:LEU:HD12 | 0.65     | 2.12        | 16     | 2     |
| 2:B:116:HIS:N    | 2:B:116:HIS:ND1  | 0.65     | 2.43        | 9      | 1     |
| 1:A:101:LEU:CB   | 3:A:142:HEC:HMC3 | 0.65     | 2.21        | 2      | 1     |
| 1:A:115:ALA:O    | 1:A:116:GLU:CG   | 0.65     | 2.45        | 6      | 11    |
| 3:A:142:HEC:HMB1 | 3:A:142:HEC:HBB2 | 0.65     | 1.69        | 14     | 6     |
| 1:C:45:HIS:CG    | 1:C:45:HIS:O     | 0.65     | 2.50        | 1      | 4     |
| 2:B:146:HIS:CG   | 2:D:2:HIS:NE2    | 0.65     | 2.56        | 15     | 1     |
| 2:B:63:HIS:HE1   | 3:B:147:HEC:C4D  | 0.65     | 1.94        | 19     | 1     |
| 1:C:122:HIS:CD2  | 2:D:112:CYS:SG   | 0.65     | 2.89        | 17     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:67:VAL:HG13  | 3:B:147:HEC:CMB  | 0.65     | 2.20        | 9      | 4     |
| 2:B:135:ALA:CB   | 2:D:146:HIS:OXT  | 0.65     | 2.44        | 18     | 1     |
| 3:B:147:HEC:CAB  | 2:D:106:LEU:HD13 | 0.65     | 2.22        | 15     | 1     |
| 2:B:33:VAL:HG13  | 2:B:34:VAL:N     | 0.65     | 2.06        | 3      | 2     |
| 1:C:36:PHE:HD2   | 3:C:142:HEC:CMC  | 0.65     | 2.04        | 12     | 1     |
| 2:D:81:LEU:HD23  | 2:D:81:LEU:N     | 0.65     | 2.07        | 10     | 1     |
| 2:B:130:TYR:CG   | 2:B:131:GLN:N    | 0.65     | 2.65        | 9      | 1     |
| 1:A:83:LEU:C     | 1:A:83:LEU:HD12  | 0.65     | 2.12        | 7      | 1     |
| 1:A:117:PHE:HE1  | 2:B:30:ARG:NH2   | 0.65     | 1.88        | 3      | 1     |
| 1:A:31:ARG:NH1   | 2:B:127:GLN:OE1  | 0.65     | 2.30        | 10     | 1     |
| 1:C:31:ARG:NH1   | 2:D:127:GLN:OE1  | 0.65     | 2.30        | 10     | 1     |
| 2:B:81:LEU:HD23  | 2:B:81:LEU:N     | 0.65     | 2.07        | 10     | 1     |
| 1:A:129:LEU:C    | 1:A:129:LEU:HD12 | 0.65     | 2.12        | 20     | 3     |
| 1:C:83:LEU:C     | 1:C:83:LEU:HD12  | 0.65     | 2.12        | 7      | 1     |
| 2:B:63:HIS:CE1   | 3:B:147:HEC:HHA  | 0.65     | 2.26        | 12     | 4     |
| 1:A:45:HIS:CG    | 1:A:45:HIS:O     | 0.65     | 2.50        | 1      | 2     |
| 2:B:66:LYS:HD3   | 3:B:147:HEC:CGA  | 0.65     | 2.22        | 14     | 1     |
| 2:B:63:HIS:NE2   | 3:B:147:HEC:C3D  | 0.64     | 2.60        | 13     | 9     |
| 2:D:48:LEU:HD12  | 2:D:48:LEU:N     | 0.64     | 2.07        | 16     | 4     |
| 2:D:66:LYS:HD3   | 3:D:147:HEC:CGA  | 0.64     | 2.22        | 14     | 1     |
| 2:D:130:TYR:CG   | 2:D:131:GLN:N    | 0.64     | 2.65        | 9      | 1     |
| 1:C:129:LEU:HD12 | 1:C:129:LEU:C    | 0.64     | 2.12        | 20     | 2     |
| 1:A:117:PHE:HE1  | 2:B:116:HIS:NE2  | 0.64     | 1.89        | 20     | 1     |
| 2:B:102:ASN:OD1  | 3:B:147:HEC:HMC2 | 0.64     | 1.91        | 12     | 1     |
| 2:D:106:LEU:HD23 | 3:D:147:HEC:CMC  | 0.64     | 2.21        | 2      | 1     |
| 2:D:63:HIS:NE2   | 3:D:147:HEC:C3D  | 0.64     | 2.60        | 13     | 8     |
| 2:D:42:PHE:CD2   | 3:D:147:HEC:HMB2 | 0.64     | 2.27        | 12     | 1     |
| 1:A:137:THR:HG22 | 1:A:137:THR:O    | 0.64     | 1.91        | 12     | 1     |
| 2:B:3:LEU:HD23   | 2:B:132:LYS:NZ   | 0.64     | 2.08        | 15     | 1     |
| 1:A:24:TYR:CD1   | 1:A:112:HIS:CD2  | 0.64     | 2.86        | 7      | 3     |
| 1:C:137:THR:HG22 | 1:C:137:THR:O    | 0.64     | 1.91        | 12     | 1     |
| 2:B:63:HIS:HE1   | 3:B:147:HEC:HAA1 | 0.64     | 1.52        | 16     | 1     |
| 2:B:97:HIS:O     | 2:B:97:HIS:CG    | 0.64     | 2.51        | 16     | 4     |
| 2:B:93:CYS:SG    | 2:B:94:ASP:N     | 0.64     | 2.70        | 10     | 2     |
| 1:A:24:TYR:CZ    | 1:A:112:HIS:CE1  | 0.64     | 2.85        | 16     | 1     |
| 1:C:115:ALA:O    | 1:C:116:GLU:CG   | 0.64     | 2.45        | 6      | 11    |
| 2:D:93:CYS:SG    | 2:D:94:ASP:N     | 0.64     | 2.70        | 10     | 2     |
| 1:C:24:TYR:CD1   | 1:C:112:HIS:CD2  | 0.64     | 2.86        | 7      | 3     |
| 1:A:96:VAL:CG2   | 2:D:99:ASP:HB2   | 0.64     | 2.21        | 18     | 1     |
| 2:D:3:LEU:HD23   | 2:D:132:LYS:NZ   | 0.64     | 2.08        | 15     | 1     |
| 2:D:97:HIS:O     | 2:D:97:HIS:CG    | 0.64     | 2.51        | 16     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:146:HIS:CE1  | 2:D:135:ALA:HB1  | 0.64     | 2.27        | 17     | 1     |
| 2:B:3:LEU:CD1    | 2:B:3:LEU:N      | 0.64     | 2.59        | 1      | 10    |
| 1:A:109:LEU:C    | 1:A:109:LEU:HD12 | 0.64     | 2.14        | 16     | 1     |
| 1:C:24:TYR:CZ    | 1:C:112:HIS:CE1  | 0.64     | 2.85        | 16     | 1     |
| 1:A:105:LEU:HD12 | 1:A:105:LEU:O    | 0.64     | 1.93        | 6      | 1     |
| 1:A:34:LEU:HD12  | 2:B:128:ALA:CA   | 0.63     | 2.19        | 18     | 1     |
| 1:A:109:LEU:O    | 1:A:109:LEU:HD12 | 0.63     | 1.93        | 16     | 1     |
| 2:B:99:ASP:HB3   | 1:C:96:VAL:HG11  | 0.63     | 1.68        | 9      | 1     |
| 2:B:101:GLU:OE2  | 2:D:101:GLU:OE2  | 0.63     | 2.15        | 6      | 1     |
| 1:A:101:LEU:HD12 | 3:A:142:HEC:CMC  | 0.63     | 2.22        | 7      | 1     |
| 3:B:147:HEC:HMD3 | 2:D:42:PHE:CE2   | 0.63     | 2.28        | 15     | 1     |
| 1:C:109:LEU:HD12 | 1:C:109:LEU:O    | 0.63     | 1.93        | 16     | 1     |
| 2:B:40:ARG:CG    | 1:C:92:ARG:NE    | 0.63     | 2.62        | 19     | 1     |
| 1:A:129:LEU:CD2  | 3:A:142:HEC:HBB1 | 0.63     | 2.24        | 13     | 2     |
| 2:B:38:THR:CG2   | 3:B:147:HEC:CBC  | 0.63     | 2.74        | 20     | 1     |
| 1:A:121:VAL:HG13 | 1:A:122:HIS:H    | 0.63     | 1.53        | 17     | 3     |
| 2:B:146:HIS:HB2  | 2:D:139:ASN:HD21 | 0.63     | 1.51        | 17     | 1     |
| 1:A:69:ALA:O     | 1:A:73:VAL:N     | 0.63     | 2.31        | 17     | 17    |
| 2:D:63:HIS:HE1   | 3:D:147:HEC:HAA1 | 0.63     | 1.52        | 16     | 1     |
| 1:C:109:LEU:C    | 1:C:109:LEU:HD12 | 0.63     | 2.13        | 16     | 1     |
| 2:B:97:HIS:HB3   | 1:C:38:THR:HB    | 0.63     | 1.69        | 19     | 1     |
| 3:B:147:HEC:CHB  | 2:D:67:VAL:HG22  | 0.63     | 2.23        | 15     | 1     |
| 1:C:101:LEU:HD12 | 3:C:142:HEC:CMC  | 0.63     | 2.22        | 7      | 1     |
| 2:B:135:ALA:O    | 2:D:146:HIS:HD2  | 0.63     | 1.71        | 17     | 1     |
| 2:D:38:THR:CG2   | 3:D:147:HEC:CBC  | 0.63     | 2.74        | 20     | 1     |
| 2:B:139:ASN:HD22 | 2:D:146:HIS:CE1  | 0.63     | 2.08        | 20     | 1     |
| 2:B:135:ALA:HB1  | 2:D:146:HIS:CB   | 0.63     | 2.24        | 3      | 1     |
| 2:B:40:ARG:NE    | 1:C:92:ARG:CB    | 0.63     | 2.61        | 18     | 2     |
| 1:C:129:LEU:CD2  | 3:C:142:HEC:HBB1 | 0.63     | 2.24        | 16     | 2     |
| 2:D:67:VAL:CG2   | 3:D:147:HEC:C4A  | 0.63     | 2.77        | 9      | 2     |
| 1:C:129:LEU:O    | 1:C:133:SER:N    | 0.63     | 2.31        | 18     | 14    |
| 2:B:146:HIS:CE1  | 2:D:139:ASN:HD22 | 0.63     | 2.10        | 20     | 1     |
| 1:A:113:LEU:O    | 1:A:113:LEU:HD12 | 0.63     | 1.94        | 2      | 2     |
| 2:D:68:LEU:O     | 2:D:68:LEU:HD23  | 0.62     | 1.93        | 3      | 4     |
| 2:B:42:PHE:CD2   | 2:B:45:PHE:CE1   | 0.62     | 2.88        | 15     | 2     |
| 1:A:3:SER:N      | 1:A:4:PRO:CD     | 0.62     | 2.62        | 10     | 11    |
| 1:A:92:ARG:NH2   | 2:D:40:ARG:CD    | 0.62     | 2.62        | 15     | 1     |
| 1:A:101:LEU:CD2  | 3:A:142:HEC:HAB  | 0.62     | 2.24        | 11     | 2     |
| 1:A:36:PHE:CZ    | 2:B:131:GLN:CD   | 0.62     | 2.73        | 13     | 1     |
| 1:A:129:LEU:O    | 1:A:133:SER:N    | 0.62     | 2.31        | 18     | 14    |
| 1:A:45:HIS:O     | 1:A:45:HIS:CG    | 0.62     | 2.52        | 19     | 9     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:C:101:LEU:CD2  | 3:C:142:HEC:HAB  | 0.62     | 2.24        | 11     | 2     |
| 2:B:40:ARG:HB3   | 1:C:92:ARG:HD2   | 0.62     | 1.70        | 19     | 2     |
| 2:B:97:HIS:HB3   | 1:C:38:THR:CG2   | 0.62     | 2.23        | 19     | 1     |
| 1:C:24:TYR:CE1   | 1:C:112:HIS:CD2  | 0.62     | 2.88        | 6      | 3     |
| 2:B:33:VAL:HG13  | 2:B:34:VAL:H     | 0.62     | 1.54        | 3      | 1     |
| 2:B:139:ASN:HD21 | 2:D:146:HIS:HB2  | 0.62     | 1.53        | 17     | 1     |
| 1:C:36:PHE:CZ    | 2:D:131:GLN:CD   | 0.62     | 2.73        | 13     | 1     |
| 2:B:67:VAL:CG2   | 3:B:147:HEC:C4A  | 0.62     | 2.77        | 9      | 3     |
| 1:A:46:PHE:O     | 1:A:47:ASP:C     | 0.62     | 2.37        | 17     | 11    |
| 1:C:83:LEU:HD12  | 1:C:83:LEU:O     | 0.62     | 1.95        | 7      | 1     |
| 1:C:36:PHE:CD2   | 3:C:142:HEC:CMC  | 0.62     | 2.82        | 12     | 1     |
| 1:C:72:HIS:O     | 1:C:74:ASP:N     | 0.62     | 2.33        | 15     | 20    |
| 1:C:69:ALA:O     | 1:C:73:VAL:N     | 0.62     | 2.31        | 17     | 16    |
| 2:B:146:HIS:OXT  | 2:D:135:ALA:CB   | 0.62     | 2.48        | 18     | 1     |
| 1:C:103:HIS:CB   | 2:D:108:ASN:HD21 | 0.62     | 2.08        | 10     | 2     |
| 2:D:106:LEU:HD23 | 2:D:106:LEU:C    | 0.62     | 2.15        | 3      | 2     |
| 1:C:103:HIS:CG   | 2:D:108:ASN:ND2  | 0.62     | 2.67        | 20     | 1     |
| 2:D:42:PHE:CG    | 3:D:147:HEC:HMB2 | 0.62     | 2.29        | 12     | 1     |
| 1:A:24:TYR:CD1   | 1:A:112:HIS:NE2  | 0.62     | 2.68        | 7      | 2     |
| 1:C:3:SER:N      | 1:C:4:PRO:CD     | 0.62     | 2.62        | 10     | 10    |
| 1:C:45:HIS:C     | 1:C:45:HIS:ND1   | 0.62     | 2.53        | 1      | 6     |
| 1:C:31:ARG:HH22  | 2:D:124:PRO:HA   | 0.62     | 1.55        | 15     | 1     |
| 1:A:86:LEU:CD1   | 3:A:142:HEC:HBD2 | 0.62     | 2.06        | 7      | 1     |
| 1:A:103:HIS:CG   | 2:B:108:ASN:ND2  | 0.62     | 2.67        | 20     | 1     |
| 2:B:40:ARG:NH2   | 1:C:92:ARG:CB    | 0.62     | 2.63        | 17     | 1     |
| 1:C:39:THR:N     | 3:C:142:HEC:CAC  | 0.62     | 2.63        | 12     | 1     |
| 1:A:24:TYR:CE1   | 1:A:112:HIS:CD2  | 0.62     | 2.88        | 6      | 3     |
| 1:C:46:PHE:CE1   | 3:C:142:HEC:CMA  | 0.62     | 2.83        | 12     | 1     |
| 2:B:67:VAL:CG2   | 3:B:147:HEC:CHB  | 0.62     | 2.68        | 9      | 2     |
| 1:A:72:HIS:O     | 1:A:74:ASP:N     | 0.62     | 2.33        | 1      | 20    |
| 2:B:31:LEU:CD2   | 3:B:147:HEC:HBC2 | 0.62     | 2.25        | 10     | 1     |
| 1:A:101:LEU:CG   | 3:A:142:HEC:HBB3 | 0.62     | 2.24        | 15     | 1     |
| 1:C:36:PHE:HB3   | 3:C:142:HEC:HMC1 | 0.62     | 1.72        | 12     | 1     |
| 2:B:75:LEU:HD23  | 2:B:75:LEU:N     | 0.62     | 2.08        | 12     | 1     |
| 1:C:93:VAL:HG12  | 1:C:94:ASP:H     | 0.61     | 1.53        | 18     | 1     |
| 2:D:63:HIS:CE1   | 3:D:147:HEC:HHA  | 0.61     | 2.26        | 18     | 3     |
| 2:D:117:HIS:ND1  | 2:D:118:PHE:CZ   | 0.61     | 2.69        | 10     | 1     |
| 2:D:96:LEU:O     | 2:D:97:HIS:CD2   | 0.61     | 2.53        | 5      | 4     |
| 1:A:101:LEU:HD23 | 3:A:142:HEC:HAB  | 0.61     | 1.71        | 8      | 2     |
| 2:D:33:VAL:HG13  | 2:D:34:VAL:H     | 0.61     | 1.54        | 3      | 1     |
| 2:B:117:HIS:ND1  | 2:B:118:PHE:CZ   | 0.61     | 2.68        | 10     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:96:LEU:O     | 2:B:97:HIS:CD2   | 0.61     | 2.53        | 5      | 4     |
| 2:B:106:LEU:HD23 | 2:B:106:LEU:C    | 0.61     | 2.15        | 3      | 3     |
| 2:B:97:HIS:HB3   | 1:C:38:THR:CB    | 0.61     | 2.24        | 19     | 2     |
| 1:A:83:LEU:O     | 1:A:83:LEU:HD12  | 0.61     | 1.95        | 7      | 1     |
| 1:A:93:VAL:HG12  | 1:A:94:ASP:H     | 0.61     | 1.53        | 18     | 1     |
| 1:C:118:THR:C    | 1:C:120:ALA:H    | 0.61     | 1.99        | 18     | 19    |
| 1:A:115:ALA:O    | 1:A:116:GLU:HB2  | 0.61     | 1.95        | 7      | 15    |
| 3:B:147:HEC:C4B  | 2:D:106:LEU:CD1  | 0.61     | 2.60        | 15     | 1     |
| 2:D:42:PHE:CD2   | 2:D:45:PHE:CE1   | 0.61     | 2.88        | 15     | 2     |
| 2:B:96:LEU:C     | 2:B:97:HIS:CG    | 0.61     | 2.73        | 17     | 6     |
| 1:C:34:LEU:HD12  | 1:C:35:SER:N     | 0.61     | 2.10        | 1      | 4     |
| 1:C:24:TYR:CD1   | 1:C:112:HIS:NE2  | 0.61     | 2.68        | 7      | 2     |
| 1:C:50:HIS:ND1   | 1:C:51:GLY:N     | 0.61     | 2.48        | 11     | 4     |
| 1:C:101:LEU:CG   | 3:C:142:HEC:HBB3 | 0.61     | 2.24        | 15     | 1     |
| 1:C:112:HIS:CG   | 1:C:113:LEU:N    | 0.61     | 2.68        | 16     | 1     |
| 2:B:135:ALA:HB1  | 2:D:146:HIS:HB3  | 0.61     | 1.71        | 3      | 1     |
| 2:B:135:ALA:HB1  | 2:D:146:HIS:NE2  | 0.61     | 2.10        | 17     | 1     |
| 1:C:39:THR:N     | 3:C:142:HEC:C3C  | 0.61     | 2.64        | 12     | 1     |
| 2:D:42:PHE:CA    | 3:D:147:HEC:HMA2 | 0.61     | 2.24        | 12     | 1     |
| 1:C:113:LEU:HD12 | 1:C:113:LEU:O    | 0.61     | 1.94        | 2      | 1     |
| 2:D:31:LEU:CD2   | 3:D:147:HEC:HBC2 | 0.61     | 2.25        | 10     | 1     |
| 1:A:31:ARG:HH22  | 2:B:124:PRO:HA   | 0.61     | 1.55        | 15     | 1     |
| 2:D:42:PHE:CE1   | 3:D:147:HEC:HMD3 | 0.61     | 2.31        | 4      | 2     |
| 2:B:97:HIS:HB3   | 1:C:38:THR:CA    | 0.61     | 2.25        | 4      | 1     |
| 1:C:121:VAL:HG13 | 1:C:122:HIS:H    | 0.61     | 1.53        | 17     | 3     |
| 1:A:69:ALA:HB1   | 1:A:76:MET:SD    | 0.61     | 2.36        | 18     | 9     |
| 1:C:46:PHE:O     | 1:C:47:ASP:C     | 0.61     | 2.37        | 17     | 10    |
| 2:D:96:LEU:O     | 2:D:97:HIS:CG    | 0.61     | 2.54        | 20     | 11    |
| 3:B:147:HEC:NA   | 2:D:67:VAL:HG22  | 0.61     | 2.10        | 15     | 1     |
| 1:A:52:SER:O     | 1:A:53:ALA:HB3   | 0.61     | 1.96        | 3      | 13    |
| 2:B:67:VAL:HG13  | 3:B:147:HEC:NB   | 0.61     | 2.05        | 19     | 1     |
| 2:B:91:LEU:HD23  | 2:B:91:LEU:C     | 0.61     | 2.16        | 12     | 2     |
| 1:C:39:THR:H     | 3:C:142:HEC:CAC  | 0.61     | 2.08        | 12     | 1     |
| 1:C:120:ALA:O    | 1:C:124:SER:N    | 0.61     | 2.33        | 2      | 16    |
| 1:A:118:THR:C    | 1:A:120:ALA:H    | 0.61     | 1.99        | 10     | 19    |
| 2:B:96:LEU:O     | 2:B:97:HIS:CG    | 0.61     | 2.54        | 6      | 11    |
| 1:A:101:LEU:HB2  | 3:A:142:HEC:HMC3 | 0.61     | 1.73        | 2      | 2     |
| 2:B:99:ASP:OD2   | 1:C:94:ASP:HB2   | 0.61     | 1.96        | 5      | 1     |
| 1:C:105:LEU:C    | 1:C:105:LEU:HD12 | 0.61     | 2.16        | 13     | 1     |
| 1:A:103:HIS:CB   | 2:B:108:ASN:HD21 | 0.61     | 2.08        | 10     | 2     |
| 2:B:3:LEU:HD13   | 2:B:8:LYS:HB3    | 0.61     | 1.73        | 6      | 6     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:D:96:LEU:C     | 2:D:97:HIS:CG    | 0.61     | 2.73        | 17     | 6     |
| 1:C:101:LEU:HD23 | 3:C:142:HEC:HAB  | 0.61     | 1.71        | 8      | 2     |
| 2:D:91:LEU:HD23  | 2:D:91:LEU:C     | 0.61     | 2.16        | 12     | 2     |
| 1:C:100:LEU:N    | 1:C:100:LEU:HD12 | 0.61     | 2.11        | 3      | 1     |
| 1:C:34:LEU:HD11  | 2:D:128:ALA:N    | 0.61     | 2.11        | 18     | 1     |
| 1:A:112:HIS:CG   | 1:A:113:LEU:H    | 0.61     | 2.14        | 16     | 1     |
| 1:C:24:TYR:CE1   | 1:C:112:HIS:CG   | 0.61     | 2.88        | 20     | 1     |
| 1:A:100:LEU:HD12 | 1:A:100:LEU:N    | 0.61     | 2.11        | 3      | 2     |
| 1:A:41:THR:CB    | 2:D:97:HIS:CE1   | 0.61     | 2.83        | 12     | 1     |
| 1:C:115:ALA:O    | 1:C:116:GLU:HB2  | 0.60     | 1.95        | 1      | 15    |
| 1:A:72:HIS:O     | 1:A:73:VAL:HG12  | 0.60     | 1.95        | 13     | 20    |
| 3:B:147:HEC:HHD  | 2:D:42:PHE:HZ    | 0.60     | 1.56        | 15     | 1     |
| 1:A:24:TYR:CE1   | 1:A:112:HIS:CG   | 0.60     | 2.88        | 20     | 1     |
| 1:A:50:HIS:ND1   | 1:A:51:GLY:N     | 0.60     | 2.48        | 11     | 4     |
| 1:C:112:HIS:CG   | 1:C:113:LEU:H    | 0.60     | 2.14        | 16     | 1     |
| 2:D:38:THR:HB    | 3:D:147:HEC:HBC1 | 0.60     | 1.73        | 6      | 1     |
| 2:B:67:VAL:CG2   | 3:B:147:HEC:NB   | 0.60     | 2.65        | 9      | 2     |
| 1:C:69:ALA:HB1   | 1:C:76:MET:SD    | 0.60     | 2.36        | 18     | 9     |
| 1:C:72:HIS:O     | 1:C:73:VAL:HG12  | 0.60     | 1.95        | 13     | 20    |
| 1:A:35:SER:HA    | 2:B:131:GLN:OE1  | 0.60     | 1.97        | 10     | 1     |
| 1:A:45:HIS:C     | 1:A:45:HIS:ND1   | 0.60     | 2.54        | 19     | 6     |
| 1:A:112:HIS:CG   | 1:A:113:LEU:N    | 0.60     | 2.68        | 16     | 1     |
| 2:B:42:PHE:CE1   | 3:B:147:HEC:HMD3 | 0.60     | 2.31        | 4      | 2     |
| 2:D:56:GLY:O     | 2:D:57:ASN:CB    | 0.60     | 2.49        | 19     | 1     |
| 2:B:40:ARG:HE    | 1:C:92:ARG:HH21  | 0.60     | 0.62        | 15     | 1     |
| 2:D:31:LEU:HD23  | 2:D:31:LEU:O     | 0.60     | 1.97        | 9      | 1     |
| 2:D:37:TRP:CZ2   | 2:D:102:ASN:ND2  | 0.60     | 2.70        | 5      | 1     |
| 1:C:80:LEU:HD12  | 1:C:80:LEU:N     | 0.60     | 2.12        | 18     | 2     |
| 1:A:34:LEU:HD12  | 1:A:35:SER:N     | 0.60     | 2.11        | 1      | 4     |
| 1:A:92:ARG:NE    | 2:D:40:ARG:CG    | 0.60     | 2.61        | 19     | 2     |
| 2:B:38:THR:HB    | 3:B:147:HEC:HBC1 | 0.60     | 1.73        | 6      | 1     |
| 2:B:139:ASN:HD22 | 2:D:139:ASN:ND2  | 0.60     | 1.94        | 3      | 1     |
| 1:A:34:LEU:HD11  | 2:B:128:ALA:N    | 0.60     | 2.11        | 18     | 1     |
| 1:A:45:HIS:ND1   | 1:A:45:HIS:C     | 0.60     | 2.53        | 1      | 1     |
| 1:A:34:LEU:CB    | 2:B:128:ALA:HB2  | 0.60     | 2.23        | 15     | 1     |
| 1:A:5:ALA:O      | 1:A:7:LYS:N      | 0.60     | 2.35        | 12     | 8     |
| 1:C:101:LEU:HD12 | 3:C:142:HEC:C1C  | 0.60     | 2.27        | 19     | 1     |
| 2:D:3:LEU:HD13   | 2:D:8:LYS:HB3    | 0.60     | 1.73        | 6      | 6     |
| 1:C:129:LEU:C    | 1:C:129:LEU:HD12 | 0.60     | 2.17        | 6      | 1     |
| 1:A:120:ALA:O    | 1:A:124:SER:N    | 0.60     | 2.35        | 4      | 17    |
| 1:A:33:PHE:O     | 1:A:36:PHE:CD2   | 0.60     | 2.55        | 3      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:C:48:LEU:CD1   | 3:C:142:HEC:C1A  | 0.60     | 2.66        | 12     | 1     |
| 1:C:5:ALA:O      | 1:C:7:LYS:N      | 0.59     | 2.34        | 12     | 7     |
| 1:C:52:SER:O     | 1:C:53:ALA:HB3   | 0.59     | 1.96        | 3      | 13    |
| 1:A:121:VAL:CG1  | 1:A:122:HIS:N    | 0.59     | 2.65        | 13     | 18    |
| 1:C:33:PHE:O     | 1:C:36:PHE:CD2   | 0.59     | 2.55        | 3      | 2     |
| 2:B:146:HIS:HD2  | 2:D:135:ALA:O    | 0.59     | 1.72        | 17     | 1     |
| 1:A:113:LEU:CD2  | 1:A:113:LEU:O    | 0.59     | 2.50        | 1      | 1     |
| 2:B:17:LYS:CD    | 2:B:17:LYS:H     | 0.59     | 2.09        | 14     | 4     |
| 2:B:31:LEU:HD23  | 2:B:31:LEU:O     | 0.59     | 1.97        | 9      | 1     |
| 1:A:46:PHE:O     | 1:A:48:LEU:CD1   | 0.59     | 2.50        | 5      | 3     |
| 3:B:147:HEC:HHC  | 2:D:106:LEU:HD12 | 0.59     | 1.49        | 15     | 1     |
| 2:B:37:TRP:CZ2   | 2:B:102:ASN:ND2  | 0.59     | 2.70        | 5      | 1     |
| 1:C:40:LYS:O     | 3:C:142:HEC:ND   | 0.59     | 2.20        | 12     | 1     |
| 1:C:101:LEU:HD13 | 3:C:142:HEC:C1C  | 0.59     | 2.27        | 2      | 1     |
| 1:A:94:ASP:O     | 1:A:96:VAL:N     | 0.59     | 2.35        | 4      | 8     |
| 1:C:117:PHE:HE1  | 2:D:30:ARG:NH2   | 0.59     | 1.88        | 3      | 1     |
| 1:C:35:SER:HA    | 2:D:131:GLN:OE1  | 0.59     | 1.97        | 10     | 1     |
| 1:C:101:LEU:HB2  | 3:C:142:HEC:HMC3 | 0.59     | 1.73        | 2      | 2     |
| 1:C:94:ASP:O     | 1:C:96:VAL:N     | 0.59     | 2.35        | 4      | 8     |
| 1:C:34:LEU:CD1   | 2:D:128:ALA:N    | 0.59     | 2.66        | 18     | 1     |
| 1:C:97:ASN:N     | 1:C:97:ASN:HD22  | 0.59     | 1.95        | 9      | 2     |
| 1:A:97:ASN:N     | 1:A:97:ASN:HD22  | 0.59     | 1.95        | 9      | 1     |
| 1:A:101:LEU:HD13 | 3:A:142:HEC:C1C  | 0.59     | 2.27        | 2      | 1     |
| 2:B:97:HIS:ND1   | 2:B:97:HIS:C     | 0.59     | 2.56        | 14     | 2     |
| 1:C:113:LEU:CD2  | 1:C:113:LEU:O    | 0.59     | 2.50        | 1      | 1     |
| 2:B:106:LEU:HD21 | 3:B:147:HEC:CAB  | 0.59     | 2.28        | 2      | 1     |
| 2:B:99:ASP:HB2   | 1:C:96:VAL:CG2   | 0.59     | 2.27        | 18     | 1     |
| 2:D:3:LEU:N      | 2:D:3:LEU:CD1    | 0.59     | 2.64        | 8      | 8     |
| 1:C:34:LEU:CB    | 2:D:128:ALA:HB2  | 0.59     | 2.23        | 15     | 1     |
| 1:A:101:LEU:HD12 | 3:A:142:HEC:C1C  | 0.59     | 2.27        | 19     | 2     |
| 2:B:56:GLY:O     | 2:B:57:ASN:CB    | 0.59     | 2.49        | 19     | 1     |
| 1:C:7:LYS:N      | 1:C:7:LYS:CD     | 0.59     | 2.66        | 20     | 1     |
| 2:D:93:CYS:SG    | 2:D:145:TYR:CD1  | 0.59     | 2.96        | 3      | 1     |
| 1:A:122:HIS:NE2  | 2:B:112:CYS:SG   | 0.59     | 2.76        | 17     | 1     |
| 2:D:106:LEU:HD21 | 3:D:147:HEC:CAB  | 0.58     | 2.28        | 2      | 1     |
| 1:A:34:LEU:CD1   | 2:B:128:ALA:N    | 0.58     | 2.66        | 18     | 1     |
| 1:A:80:LEU:N     | 1:A:80:LEU:HD12  | 0.58     | 2.12        | 18     | 2     |
| 2:D:17:LYS:H     | 2:D:17:LYS:CD    | 0.58     | 2.09        | 14     | 2     |
| 2:B:30:ARG:NH2   | 2:B:55:MET:SD    | 0.58     | 2.77        | 9      | 1     |
| 2:D:82:LYS:NZ    | 2:D:143:HIS:CD2  | 0.58     | 2.71        | 20     | 2     |
| 1:C:122:HIS:NE2  | 2:D:112:CYS:SG   | 0.58     | 2.76        | 17     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:D:75:LEU:H     | 2:D:75:LEU:HD23  | 0.58     | 1.58        | 12     | 1     |
| 1:A:24:TYR:N     | 1:A:24:TYR:CD1   | 0.58     | 2.71        | 12     | 9     |
| 2:D:92:HIS:O     | 2:D:97:HIS:N     | 0.58     | 2.37        | 11     | 14    |
| 2:B:133:VAL:CG1  | 2:B:134:VAL:N    | 0.58     | 2.66        | 19     | 6     |
| 2:D:30:ARG:NH2   | 2:D:55:MET:SD    | 0.58     | 2.77        | 9      | 1     |
| 1:C:117:PHE:HE1  | 2:D:116:HIS:NE2  | 0.58     | 1.89        | 20     | 1     |
| 2:D:67:VAL:CG2   | 3:D:147:HEC:NB   | 0.58     | 2.64        | 9      | 2     |
| 1:C:121:VAL:CG1  | 1:C:122:HIS:N    | 0.58     | 2.65        | 13     | 18    |
| 1:C:46:PHE:O     | 1:C:48:LEU:CD1   | 0.58     | 2.50        | 5      | 3     |
| 2:B:119:GLY:O    | 2:B:122:PHE:CD1  | 0.58     | 2.57        | 6      | 9     |
| 2:D:117:HIS:CE1  | 2:D:118:PHE:CZ   | 0.58     | 2.92        | 10     | 1     |
| 2:B:117:HIS:CE1  | 2:B:118:PHE:CZ   | 0.58     | 2.92        | 10     | 1     |
| 2:B:97:HIS:N     | 2:B:97:HIS:CD2   | 0.58     | 2.72        | 15     | 1     |
| 2:D:3:LEU:CD1    | 2:D:3:LEU:N      | 0.58     | 2.58        | 5      | 4     |
| 2:B:3:LEU:CD1    | 2:B:3:LEU:H      | 0.58     | 2.06        | 12     | 2     |
| 1:A:7:LYS:N      | 1:A:7:LYS:CD     | 0.58     | 2.66        | 20     | 1     |
| 2:B:75:LEU:HD23  | 2:B:75:LEU:H     | 0.58     | 1.58        | 12     | 1     |
| 1:C:48:LEU:N     | 1:C:48:LEU:CD2   | 0.58     | 2.66        | 2      | 1     |
| 2:D:88:LEU:O     | 2:D:92:HIS:N     | 0.58     | 2.37        | 18     | 2     |
| 2:B:92:HIS:O     | 2:B:97:HIS:N     | 0.58     | 2.37        | 11     | 14    |
| 1:C:31:ARG:HH12  | 2:D:127:GLN:HB2  | 0.58     | 1.57        | 16     | 1     |
| 2:D:2:HIS:O      | 2:D:2:HIS:CG     | 0.58     | 2.55        | 14     | 1     |
| 2:D:67:VAL:HG13  | 3:D:147:HEC:NB   | 0.58     | 2.06        | 19     | 1     |
| 1:C:24:TYR:CG    | 1:C:112:HIS:NE2  | 0.58     | 2.72        | 7      | 1     |
| 1:A:101:LEU:HD13 | 3:A:142:HEC:HBB3 | 0.58     | 1.76        | 15     | 1     |
| 1:A:38:THR:HB    | 2:D:97:HIS:HB2   | 0.58     | 1.74        | 5      | 1     |
| 1:A:92:ARG:HD3   | 2:D:40:ARG:HB3   | 0.58     | 1.76        | 17     | 1     |
| 1:A:96:VAL:HB    | 2:D:99:ASP:OD2   | 0.58     | 1.98        | 2      | 2     |
| 1:A:92:ARG:O     | 1:A:93:VAL:O     | 0.58     | 2.21        | 13     | 2     |
| 1:C:7:LYS:O      | 1:C:10:VAL:N     | 0.58     | 2.36        | 20     | 11    |
| 1:A:86:LEU:HD21  | 3:A:142:HEC:CBD  | 0.58     | 2.29        | 12     | 4     |
| 2:B:2:HIS:O      | 2:B:2:HIS:CG     | 0.58     | 2.55        | 14     | 2     |
| 2:B:82:LYS:NZ    | 2:B:143:HIS:CD2  | 0.58     | 2.71        | 20     | 2     |
| 1:A:48:LEU:N     | 1:A:48:LEU:CD2   | 0.58     | 2.66        | 2      | 1     |
| 2:D:106:LEU:HB3  | 3:D:147:HEC:CAB  | 0.58     | 2.29        | 18     | 3     |
| 1:A:7:LYS:O      | 1:A:10:VAL:N     | 0.58     | 2.36        | 20     | 11    |
| 2:B:45:PHE:CZ    | 3:B:147:HEC:HMD3 | 0.58     | 2.34        | 16     | 1     |
| 1:C:92:ARG:O     | 1:C:93:VAL:O     | 0.58     | 2.21        | 13     | 2     |
| 1:C:113:LEU:O    | 1:C:113:LEU:HD12 | 0.58     | 1.99        | 20     | 2     |
| 1:C:58:HIS:ND1   | 1:C:58:HIS:O     | 0.58     | 2.36        | 10     | 4     |
| 2:D:45:PHE:CZ    | 3:D:147:HEC:HMD3 | 0.58     | 2.34        | 16     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:40:ARG:CD    | 1:C:92:ARG:NE    | 0.58     | 2.50        | 19     | 1     |
| 2:D:92:HIS:NE2   | 2:D:141:LEU:O    | 0.58     | 2.37        | 5      | 3     |
| 2:D:75:LEU:N     | 2:D:75:LEU:CD2   | 0.58     | 2.67        | 20     | 3     |
| 2:D:39:GLN:HG2   | 3:D:147:HEC:CHC  | 0.58     | 2.06        | 12     | 1     |
| 2:B:41:PHE:CE2   | 3:B:147:HEC:CMD  | 0.58     | 2.86        | 12     | 1     |
| 1:C:101:LEU:CD1  | 3:C:142:HEC:C1C  | 0.58     | 2.82        | 15     | 1     |
| 2:B:3:LEU:N      | 2:B:3:LEU:CD1    | 0.58     | 2.64        | 8      | 4     |
| 2:B:92:HIS:NE2   | 2:B:141:LEU:O    | 0.58     | 2.37        | 5      | 3     |
| 1:A:24:TYR:CG    | 1:A:112:HIS:NE2  | 0.58     | 2.72        | 7      | 1     |
| 2:B:145:TYR:CG   | 2:B:145:TYR:O    | 0.58     | 2.57        | 12     | 3     |
| 1:C:93:VAL:CG2   | 1:C:97:ASN:ND2   | 0.58     | 2.67        | 12     | 1     |
| 1:A:92:ARG:O     | 2:D:40:ARG:NH1   | 0.57     | 2.36        | 14     | 1     |
| 2:B:40:ARG:NH2   | 1:C:93:VAL:O     | 0.57     | 2.37        | 14     | 1     |
| 2:D:133:VAL:CG1  | 2:D:134:VAL:N    | 0.57     | 2.66        | 19     | 5     |
| 2:D:146:HIS:HD1  | 2:D:146:HIS:H    | 0.57     | 1.41        | 17     | 1     |
| 1:A:31:ARG:NH1   | 1:A:104:CYS:SG   | 0.57     | 2.77        | 2      | 1     |
| 2:D:97:HIS:O     | 2:D:97:HIS:ND1   | 0.57     | 2.38        | 6      | 3     |
| 1:A:45:HIS:O     | 1:A:45:HIS:ND1   | 0.57     | 2.37        | 20     | 10    |
| 1:A:36:PHE:CZ    | 2:B:104:ARG:NH2  | 0.57     | 2.73        | 5      | 1     |
| 2:B:139:ASN:ND2  | 2:D:139:ASN:HD22 | 0.57     | 1.93        | 3      | 1     |
| 1:C:45:HIS:ND1   | 1:C:45:HIS:O     | 0.57     | 2.37        | 20     | 4     |
| 1:C:45:HIS:O     | 1:C:45:HIS:CG    | 0.57     | 2.55        | 6      | 6     |
| 1:A:17:VAL:O     | 1:A:18:GLY:C     | 0.57     | 2.42        | 11     | 3     |
| 2:D:97:HIS:ND1   | 2:D:97:HIS:C     | 0.57     | 2.56        | 14     | 1     |
| 1:C:35:SER:O     | 1:C:36:PHE:C     | 0.57     | 2.43        | 1      | 2     |
| 2:B:88:LEU:O     | 2:B:92:HIS:N     | 0.57     | 2.37        | 18     | 3     |
| 1:C:52:SER:O     | 1:C:53:ALA:HB2   | 0.57     | 1.99        | 14     | 3     |
| 2:D:30:ARG:NH2   | 2:D:55:MET:CE    | 0.57     | 2.67        | 9      | 1     |
| 2:D:114:LEU:HD12 | 2:D:114:LEU:N    | 0.57     | 2.14        | 9      | 1     |
| 1:A:61:LYS:HB3   | 3:A:142:HEC:C2A  | 0.57     | 2.30        | 14     | 9     |
| 1:C:45:HIS:O     | 1:C:45:HIS:ND1   | 0.57     | 2.37        | 13     | 9     |
| 2:D:97:HIS:CD2   | 2:D:97:HIS:C     | 0.57     | 2.78        | 5      | 1     |
| 2:B:93:CYS:SG    | 2:B:145:TYR:CD1  | 0.57     | 2.96        | 3      | 1     |
| 2:B:135:ALA:HB1  | 2:D:146:HIS:OXT  | 0.57     | 1.98        | 18     | 1     |
| 1:A:29:LEU:HD11  | 1:A:58:HIS:ND1   | 0.57     | 2.15        | 18     | 9     |
| 2:D:119:GLY:O    | 2:D:122:PHE:CD1  | 0.57     | 2.57        | 6      | 10    |
| 1:A:92:ARG:NH2   | 2:D:37:TRP:O     | 0.57     | 2.38        | 19     | 1     |
| 2:D:57:ASN:N     | 2:D:58:PRO:HD3   | 0.57     | 2.13        | 19     | 1     |
| 2:D:97:HIS:CG    | 2:D:97:HIS:O     | 0.57     | 2.57        | 5      | 2     |
| 2:D:145:TYR:O    | 2:D:145:TYR:CG   | 0.57     | 2.57        | 12     | 2     |
| 2:B:106:LEU:HB3  | 3:B:147:HEC:CAB  | 0.57     | 2.29        | 18     | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:52:SER:O     | 1:A:53:ALA:HB2   | 0.57     | 1.99        | 14     | 3     |
| 1:A:45:HIS:ND1   | 1:A:45:HIS:O     | 0.57     | 2.38        | 13     | 3     |
| 1:A:106:LEU:N    | 1:A:106:LEU:HD22 | 0.57     | 2.14        | 4      | 3     |
| 1:A:94:ASP:OD2   | 2:D:40:ARG:NH1   | 0.57     | 2.38        | 3      | 1     |
| 2:B:41:PHE:CE2   | 3:B:147:HEC:HMD1 | 0.57     | 2.35        | 12     | 1     |
| 2:D:37:TRP:CD1   | 2:D:38:THR:N     | 0.57     | 2.73        | 4      | 6     |
| 1:C:24:TYR:N     | 1:C:24:TYR:CD1   | 0.57     | 2.71        | 12     | 8     |
| 1:A:18:GLY:O     | 1:A:19:ALA:HB3   | 0.57     | 2.00        | 11     | 3     |
| 2:B:114:LEU:N    | 2:B:114:LEU:HD12 | 0.57     | 2.14        | 9      | 1     |
| 1:C:50:HIS:ND1   | 1:C:50:HIS:N     | 0.57     | 2.53        | 1      | 3     |
| 1:C:36:PHE:CZ    | 2:D:104:ARG:NH2  | 0.57     | 2.73        | 5      | 1     |
| 1:C:7:LYS:H      | 1:C:7:LYS:CD     | 0.57     | 2.11        | 20     | 1     |
| 1:C:45:HIS:O     | 1:C:45:HIS:CD2   | 0.57     | 2.58        | 2      | 1     |
| 1:C:29:LEU:HD11  | 1:C:58:HIS:ND1   | 0.57     | 2.15        | 18     | 9     |
| 1:C:106:LEU:HD22 | 1:C:106:LEU:N    | 0.57     | 2.14        | 4      | 2     |
| 1:A:7:LYS:H      | 1:A:7:LYS:CD     | 0.57     | 2.12        | 20     | 1     |
| 1:C:31:ARG:NH1   | 1:C:104:CYS:SG   | 0.57     | 2.77        | 2      | 1     |
| 2:B:97:HIS:O     | 2:B:97:HIS:ND1   | 0.57     | 2.38        | 6      | 3     |
| 1:A:101:LEU:CD1  | 3:A:142:HEC:C1C  | 0.57     | 2.82        | 15     | 1     |
| 1:C:17:VAL:O     | 1:C:18:GLY:C     | 0.57     | 2.43        | 11     | 3     |
| 1:A:41:THR:HG21  | 2:D:94:ASP:O     | 0.57     | 1.99        | 6      | 1     |
| 2:B:106:LEU:HG   | 3:B:147:HEC:CHC  | 0.56     | 2.30        | 18     | 1     |
| 1:C:61:LYS:HB3   | 3:C:142:HEC:C2A  | 0.56     | 2.29        | 20     | 9     |
| 1:A:58:HIS:O     | 1:A:58:HIS:ND1   | 0.56     | 2.36        | 10     | 5     |
| 2:B:96:LEU:O     | 2:B:97:HIS:CB    | 0.56     | 2.53        | 5      | 6     |
| 1:A:97:ASN:HD22  | 1:A:97:ASN:N     | 0.56     | 1.98        | 15     | 1     |
| 2:D:96:LEU:O     | 2:D:97:HIS:CB    | 0.56     | 2.53        | 5      | 6     |
| 2:B:30:ARG:NH2   | 2:B:55:MET:CE    | 0.56     | 2.68        | 9      | 1     |
| 1:A:31:ARG:NH2   | 1:A:104:CYS:SG   | 0.56     | 2.79        | 7      | 1     |
| 1:A:93:VAL:CG2   | 1:A:97:ASN:ND2   | 0.56     | 2.67        | 12     | 1     |
| 2:B:28:LEU:HD12  | 2:B:28:LEU:N     | 0.56     | 2.15        | 18     | 1     |
| 2:B:111:VAL:CG2  | 2:B:130:TYR:CE1  | 0.56     | 2.88        | 6      | 2     |
| 1:A:4:PRO:O      | 1:A:6:ASP:N      | 0.56     | 2.38        | 7      | 5     |
| 2:B:38:THR:C     | 2:B:40:ARG:H     | 0.56     | 2.04        | 15     | 2     |
| 1:A:50:HIS:ND1   | 1:A:50:HIS:N     | 0.56     | 2.53        | 1      | 2     |
| 1:A:35:SER:O     | 1:A:36:PHE:C     | 0.56     | 2.43        | 1      | 2     |
| 1:C:34:LEU:O     | 1:C:36:PHE:CZ    | 0.56     | 2.58        | 1      | 1     |
| 2:D:42:PHE:CA    | 3:D:147:HEC:CMA  | 0.56     | 2.79        | 12     | 1     |
| 2:B:84:THR:CG2   | 2:B:85:PHE:N     | 0.56     | 2.68        | 20     | 18    |
| 2:D:45:PHE:O     | 2:D:47:ASP:N     | 0.56     | 2.39        | 14     | 7     |
| 1:C:4:PRO:O      | 1:C:6:ASP:N      | 0.56     | 2.38        | 7      | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:C:101:LEU:HD13 | 3:C:142:HEC:HBB3 | 0.56     | 1.76        | 15     | 1     |
| 2:D:96:LEU:HD12  | 2:D:96:LEU:N     | 0.56     | 2.15        | 15     | 1     |
| 2:D:97:HIS:CD2   | 2:D:97:HIS:N     | 0.56     | 2.72        | 15     | 1     |
| 1:A:48:LEU:HD12  | 1:A:48:LEU:H     | 0.56     | 1.60        | 8      | 2     |
| 1:A:92:ARG:HG2   | 2:D:40:ARG:NH1   | 0.56     | 2.16        | 14     | 1     |
| 1:A:93:VAL:O     | 2:D:40:ARG:NH2   | 0.56     | 2.38        | 14     | 1     |
| 2:B:57:ASN:N     | 2:B:58:PRO:HD3   | 0.56     | 2.13        | 19     | 1     |
| 2:D:133:VAL:CG1  | 2:D:134:VAL:H    | 0.56     | 2.13        | 9      | 3     |
| 2:B:97:HIS:C     | 2:B:97:HIS:CD2   | 0.56     | 2.78        | 5      | 1     |
| 2:B:146:HIS:CB   | 2:D:135:ALA:HB1  | 0.56     | 2.29        | 3      | 1     |
| 2:B:146:HIS:NE2  | 2:D:135:ALA:HB1  | 0.56     | 2.15        | 17     | 1     |
| 1:A:107:VAL:CG1  | 2:B:127:GLN:NE2  | 0.56     | 2.68        | 17     | 1     |
| 1:A:34:LEU:O     | 1:A:36:PHE:CZ    | 0.56     | 2.58        | 1      | 1     |
| 1:A:50:HIS:CG    | 1:A:51:GLY:N     | 0.56     | 2.73        | 11     | 1     |
| 2:B:42:PHE:CD2   | 3:B:147:HEC:HMD3 | 0.56     | 2.32        | 2      | 1     |
| 1:A:45:HIS:O     | 1:A:45:HIS:CD2   | 0.56     | 2.58        | 2      | 1     |
| 1:C:37:PRO:O     | 1:C:39:THR:N     | 0.56     | 2.39        | 10     | 9     |
| 2:B:68:LEU:HD23  | 2:B:68:LEU:O     | 0.56     | 2.00        | 1      | 2     |
| 2:B:94:ASP:O     | 2:B:97:HIS:NE2   | 0.56     | 2.39        | 4      | 6     |
| 2:B:75:LEU:N     | 2:B:75:LEU:CD2   | 0.56     | 2.66        | 20     | 1     |
| 1:C:105:LEU:HD12 | 1:C:105:LEU:O    | 0.56     | 2.01        | 16     | 1     |
| 1:C:106:LEU:N    | 1:C:106:LEU:HD22 | 0.56     | 2.16        | 20     | 3     |
| 1:C:34:LEU:O     | 1:C:36:PHE:CE2   | 0.56     | 2.59        | 1      | 1     |
| 1:C:35:SER:O     | 1:C:36:PHE:CG    | 0.56     | 2.59        | 4      | 11    |
| 2:D:122:PHE:O    | 2:D:122:PHE:CG   | 0.56     | 2.58        | 18     | 9     |
| 2:D:76:ALA:O     | 2:D:77:HIS:CG    | 0.56     | 2.59        | 6      | 8     |
| 2:B:80:ASN:ND2   | 2:B:80:ASN:N     | 0.56     | 2.52        | 14     | 1     |
| 2:B:133:VAL:CG1  | 2:B:134:VAL:H    | 0.56     | 2.13        | 12     | 3     |
| 2:B:139:ASN:HD22 | 2:D:146:HIS:HE1  | 0.56     | 1.41        | 20     | 1     |
| 1:A:38:THR:HG22  | 2:D:97:HIS:O     | 0.56     | 2.01        | 3      | 1     |
| 1:C:20:HIS:O     | 1:C:24:TYR:CD2   | 0.56     | 2.59        | 1      | 1     |
| 1:C:58:HIS:O     | 1:C:58:HIS:ND1   | 0.56     | 2.39        | 19     | 4     |
| 2:D:38:THR:C     | 2:D:40:ARG:H     | 0.56     | 2.04        | 15     | 2     |
| 2:D:122:PHE:CG   | 2:D:122:PHE:O    | 0.56     | 2.59        | 13     | 6     |
| 1:C:48:LEU:HD12  | 1:C:48:LEU:H     | 0.56     | 1.60        | 8      | 2     |
| 2:B:40:ARG:NH1   | 1:C:92:ARG:O     | 0.56     | 2.38        | 14     | 1     |
| 1:C:31:ARG:NH2   | 1:C:104:CYS:SG   | 0.56     | 2.79        | 7      | 1     |
| 1:A:46:PHE:O     | 1:A:48:LEU:HD12  | 0.56     | 2.01        | 18     | 3     |
| 2:D:111:VAL:CG2  | 2:D:130:TYR:CE1  | 0.56     | 2.89        | 18     | 2     |
| 2:D:28:LEU:N     | 2:D:28:LEU:HD12  | 0.56     | 2.15        | 18     | 1     |
| 2:B:122:PHE:CG   | 2:B:122:PHE:O    | 0.56     | 2.58        | 16     | 10    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:D:84:THR:CG2   | 2:D:85:PHE:N     | 0.56     | 2.69        | 12     | 18    |
| 2:D:80:ASN:ND2   | 2:D:80:ASN:N     | 0.56     | 2.52        | 14     | 1     |
| 1:A:20:HIS:O     | 1:A:24:TYR:CD2   | 0.56     | 2.59        | 1      | 1     |
| 2:D:48:LEU:HD21  | 3:D:147:HEC:HMA3 | 0.56     | 1.77        | 12     | 1     |
| 1:A:101:LEU:HD23 | 3:A:142:HEC:CAB  | 0.56     | 2.31        | 20     | 2     |
| 2:B:45:PHE:O     | 2:B:47:ASP:N     | 0.56     | 2.39        | 14     | 7     |
| 1:A:92:ARG:CZ    | 2:D:40:ARG:HG3   | 0.56     | 2.31        | 15     | 1     |
| 2:B:42:PHE:CE1   | 2:B:45:PHE:CE1   | 0.56     | 2.94        | 16     | 1     |
| 1:C:129:LEU:HD22 | 3:C:142:HEC:HBB1 | 0.56     | 1.78        | 16     | 2     |
| 1:A:34:LEU:O     | 1:A:36:PHE:CE2   | 0.56     | 2.59        | 1      | 1     |
| 1:A:95:PRO:O     | 1:A:98:PHE:CD2   | 0.56     | 2.58        | 13     | 1     |
| 1:C:95:PRO:O     | 1:C:98:PHE:CD2   | 0.56     | 2.59        | 13     | 1     |
| 2:B:106:LEU:HG   | 3:B:147:HEC:C4B  | 0.55     | 2.30        | 18     | 1     |
| 1:C:52:SER:O     | 1:C:54:GLN:N     | 0.55     | 2.39        | 18     | 7     |
| 2:B:37:TRP:CD1   | 2:B:38:THR:N     | 0.55     | 2.73        | 4      | 6     |
| 1:A:37:PRO:O     | 1:A:39:THR:N     | 0.55     | 2.39        | 10     | 9     |
| 1:C:107:VAL:CG1  | 2:D:127:GLN:NE2  | 0.55     | 2.68        | 17     | 1     |
| 1:C:50:HIS:CG    | 1:C:51:GLY:N     | 0.55     | 2.73        | 11     | 1     |
| 2:D:106:LEU:HG   | 3:D:147:HEC:C4B  | 0.55     | 2.30        | 18     | 1     |
| 1:C:91:LEU:HD12  | 1:C:91:LEU:N     | 0.55     | 2.16        | 7      | 4     |
| 2:D:19:ASN:O     | 2:D:21:ASP:N     | 0.55     | 2.40        | 16     | 15    |
| 2:D:103:PHE:HA   | 3:D:147:HEC:HBB2 | 0.55     | 1.77        | 16     | 1     |
| 2:D:94:ASP:O     | 2:D:97:HIS:NE2   | 0.55     | 2.38        | 4      | 6     |
| 2:D:38:THR:OG1   | 2:D:39:GLN:N     | 0.55     | 2.40        | 20     | 4     |
| 2:D:146:HIS:HD1  | 2:D:146:HIS:N    | 0.55     | 1.98        | 17     | 1     |
| 2:B:19:ASN:O     | 2:B:21:ASP:N     | 0.55     | 2.40        | 16     | 15    |
| 2:D:45:PHE:HZ    | 3:D:147:HEC:CMD  | 0.55     | 2.15        | 16     | 1     |
| 2:B:132:LYS:HG3  | 2:D:146:HIS:HB3  | 0.55     | 1.77        | 19     | 1     |
| 1:A:35:SER:O     | 1:A:36:PHE:CG    | 0.55     | 2.59        | 4      | 12    |
| 1:C:101:LEU:HD23 | 3:C:142:HEC:CAB  | 0.55     | 2.31        | 20     | 2     |
| 1:C:97:ASN:OD1   | 1:C:97:ASN:N     | 0.55     | 2.40        | 12     | 1     |
| 1:A:94:ASP:CG    | 2:D:99:ASP:OD1   | 0.55     | 2.45        | 2      | 1     |
| 1:C:113:LEU:O    | 1:C:114:PRO:O    | 0.55     | 2.25        | 18     | 12    |
| 3:B:147:HEC:CHA  | 2:D:63:HIS:HE1   | 0.55     | 2.13        | 15     | 1     |
| 2:B:96:LEU:HD12  | 2:B:96:LEU:N     | 0.55     | 2.15        | 15     | 2     |
| 2:B:103:PHE:HA   | 3:B:147:HEC:HBB2 | 0.55     | 1.77        | 16     | 1     |
| 1:C:108:THR:CG2  | 1:C:109:LEU:N    | 0.55     | 2.69        | 16     | 2     |
| 1:A:91:LEU:N     | 1:A:91:LEU:HD12  | 0.55     | 2.16        | 7      | 1     |
| 2:B:146:HIS:OXT  | 2:D:135:ALA:HB1  | 0.55     | 2.02        | 18     | 1     |
| 1:C:46:PHE:O     | 1:C:48:LEU:HD12  | 0.55     | 2.01        | 18     | 3     |
| 2:B:76:ALA:O     | 2:B:77:HIS:CG    | 0.55     | 2.59        | 6      | 8     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:105:LEU:HD12 | 2:B:105:LEU:N    | 0.55     | 2.16        | 13     | 3     |
| 1:C:111:ALA:HB2  | 2:D:122:PHE:CD2  | 0.55     | 2.30        | 8      | 2     |
| 1:A:31:ARG:NH2   | 2:B:124:PRO:HA   | 0.55     | 2.17        | 15     | 1     |
| 2:B:40:ARG:CB    | 1:C:92:ARG:HE    | 0.55     | 1.89        | 19     | 2     |
| 2:D:63:HIS:HE1   | 3:D:147:HEC:CAA  | 0.55     | 2.14        | 16     | 1     |
| 3:C:142:HEC:CBB  | 3:C:142:HEC:HMB1 | 0.55     | 2.31        | 11     | 3     |
| 2:B:66:LYS:HB3   | 3:B:147:HEC:HBA2 | 0.55     | 1.78        | 14     | 1     |
| 1:A:113:LEU:C    | 1:A:113:LEU:HD13 | 0.55     | 2.21        | 12     | 3     |
| 2:B:75:LEU:CD2   | 2:B:75:LEU:N     | 0.55     | 2.67        | 4      | 2     |
| 2:D:106:LEU:HG   | 3:D:147:HEC:CHC  | 0.55     | 2.31        | 18     | 1     |
| 1:A:52:SER:O     | 1:A:54:GLN:N     | 0.55     | 2.39        | 1      | 7     |
| 1:A:111:ALA:HB2  | 2:B:122:PHE:CD2  | 0.55     | 2.30        | 8      | 2     |
| 2:B:63:HIS:HE1   | 3:B:147:HEC:CAA  | 0.55     | 2.14        | 16     | 1     |
| 2:D:55:MET:SD    | 2:D:55:MET:N     | 0.55     | 2.80        | 6      | 2     |
| 1:C:113:LEU:C    | 1:C:113:LEU:HD13 | 0.55     | 2.21        | 12     | 2     |
| 2:B:40:ARG:NH1   | 1:C:94:ASP:OD2   | 0.55     | 2.40        | 3      | 1     |
| 1:C:61:LYS:O     | 1:C:65:ALA:N     | 0.55     | 2.40        | 17     | 2     |
| 1:A:61:LYS:HG2   | 3:A:142:HEC:HAA1 | 0.55     | 1.78        | 11     | 2     |
| 1:C:36:PHE:CB    | 3:C:142:HEC:CMC  | 0.55     | 2.82        | 12     | 1     |
| 2:B:53:ALA:O     | 2:B:57:ASN:ND2   | 0.55     | 2.40        | 3      | 2     |
| 2:D:63:HIS:CE1   | 3:D:147:HEC:C2A  | 0.55     | 2.90        | 16     | 1     |
| 1:A:31:ARG:HH12  | 2:B:127:GLN:HB2  | 0.55     | 1.57        | 16     | 1     |
| 1:C:18:GLY:O     | 1:C:19:ALA:HB3   | 0.55     | 2.00        | 11     | 3     |
| 2:D:106:LEU:HD12 | 3:D:147:HEC:HMC3 | 0.55     | 1.79        | 17     | 3     |
| 2:B:97:HIS:HB2   | 1:C:38:THR:HB    | 0.55     | 1.79        | 5      | 1     |
| 2:D:103:PHE:CD1  | 2:D:103:PHE:N    | 0.55     | 2.73        | 11     | 2     |
| 1:C:101:LEU:CD2  | 3:C:142:HEC:CAB  | 0.55     | 2.85        | 20     | 5     |
| 2:D:37:TRP:NE1   | 2:D:38:THR:OG1   | 0.55     | 2.40        | 18     | 4     |
| 1:A:106:LEU:N    | 1:A:106:LEU:CD2  | 0.55     | 2.70        | 20     | 4     |
| 2:D:59:LYS:O     | 2:D:63:HIS:N     | 0.55     | 2.39        | 7      | 2     |
| 1:C:48:LEU:H     | 1:C:48:LEU:CD1   | 0.55     | 2.13        | 8      | 3     |
| 1:A:61:LYS:O     | 1:A:65:ALA:N     | 0.55     | 2.40        | 17     | 3     |
| 2:D:105:LEU:N    | 2:D:105:LEU:HD12 | 0.55     | 2.16        | 13     | 4     |
| 1:C:100:LEU:N    | 1:C:100:LEU:HD22 | 0.55     | 2.17        | 9      | 1     |
| 1:A:100:LEU:HD22 | 1:A:100:LEU:N    | 0.55     | 2.17        | 9      | 1     |
| 2:D:3:LEU:CD1    | 2:D:3:LEU:H      | 0.55     | 2.12        | 20     | 3     |
| 2:B:81:LEU:O     | 2:B:85:PHE:CZ    | 0.55     | 2.60        | 6      | 1     |
| 1:C:106:LEU:N    | 1:C:106:LEU:CD2  | 0.55     | 2.70        | 5      | 2     |
| 1:C:85:ASP:OD1   | 1:C:89:HIS:CE1   | 0.55     | 2.60        | 20     | 1     |
| 2:D:93:CYS:O     | 2:D:97:HIS:CD2   | 0.55     | 2.60        | 12     | 1     |
| 2:B:93:CYS:O     | 2:B:97:HIS:CD2   | 0.55     | 2.60        | 12     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:101:LEU:CD2  | 3:A:142:HEC:CAB  | 0.55     | 2.85        | 20     | 5     |
| 1:A:47:ASP:O     | 1:A:49:SER:N     | 0.55     | 2.40        | 19     | 10    |
| 2:B:73:ASP:CG    | 2:B:84:THR:HG1   | 0.55     | 2.05        | 15     | 1     |
| 2:D:13:ALA:O     | 2:D:15:TRP:N     | 0.55     | 2.40        | 15     | 3     |
| 1:A:48:LEU:CD1   | 1:A:48:LEU:H     | 0.55     | 2.13        | 8      | 1     |
| 2:D:45:PHE:CZ    | 3:D:147:HEC:CMD  | 0.55     | 2.90        | 16     | 1     |
| 1:A:3:SER:O      | 1:A:4:PRO:O      | 0.55     | 2.25        | 3      | 3     |
| 1:C:3:SER:O      | 1:C:4:PRO:O      | 0.55     | 2.25        | 3      | 2     |
| 1:C:34:LEU:CD1   | 2:D:128:ALA:H    | 0.54     | 2.15        | 18     | 1     |
| 2:B:123:THR:OG1  | 2:B:126:VAL:HG23 | 0.54     | 2.03        | 18     | 8     |
| 2:D:81:LEU:N     | 2:D:81:LEU:CD2   | 0.54     | 2.71        | 10     | 1     |
| 2:B:45:PHE:CZ    | 3:B:147:HEC:CMD  | 0.54     | 2.90        | 16     | 1     |
| 1:A:129:LEU:HD22 | 3:A:142:HEC:HBB1 | 0.54     | 1.78        | 16     | 2     |
| 2:B:42:PHE:O     | 2:B:44:SER:N     | 0.54     | 2.40        | 7      | 2     |
| 2:D:42:PHE:CD1   | 3:D:147:HEC:CHB  | 0.54     | 2.90        | 12     | 1     |
| 1:A:35:SER:O     | 1:A:36:PHE:CD2   | 0.54     | 2.61        | 19     | 6     |
| 2:B:122:PHE:O    | 2:B:122:PHE:CG   | 0.54     | 2.59        | 14     | 5     |
| 1:A:92:ARG:CB    | 2:D:40:ARG:NH2   | 0.54     | 2.67        | 17     | 2     |
| 2:B:105:LEU:N    | 2:B:105:LEU:HD12 | 0.54     | 2.17        | 3      | 2     |
| 2:D:42:PHE:O     | 2:D:44:SER:N     | 0.54     | 2.40        | 7      | 2     |
| 2:B:42:PHE:CD1   | 2:B:43:GLU:N     | 0.54     | 2.76        | 5      | 1     |
| 1:C:36:PHE:CD2   | 3:C:142:HEC:HMC1 | 0.54     | 2.36        | 12     | 1     |
| 1:C:36:PHE:CB    | 3:C:142:HEC:HMC1 | 0.54     | 2.33        | 12     | 1     |
| 2:D:105:LEU:HD12 | 2:D:105:LEU:N    | 0.54     | 2.17        | 18     | 1     |
| 1:A:95:PRO:O     | 1:A:97:ASN:N     | 0.54     | 2.41        | 6      | 10    |
| 1:C:31:ARG:NH2   | 2:D:124:PRO:HA   | 0.54     | 2.17        | 15     | 1     |
| 2:D:81:LEU:HD22  | 2:D:81:LEU:N     | 0.54     | 2.17        | 15     | 1     |
| 1:A:116:GLU:O    | 1:A:117:PHE:CG   | 0.54     | 2.60        | 14     | 2     |
| 2:B:142:ALA:O    | 2:B:145:TYR:CD1  | 0.54     | 2.61        | 16     | 2     |
| 2:B:55:MET:SD    | 2:B:55:MET:N     | 0.54     | 2.80        | 6      | 3     |
| 1:C:61:LYS:HG2   | 3:C:142:HEC:HAA1 | 0.54     | 1.78        | 11     | 3     |
| 1:C:32:MET:O     | 1:C:36:PHE:N     | 0.54     | 2.40        | 7      | 1     |
| 2:B:106:LEU:HD12 | 3:B:147:HEC:HMC3 | 0.54     | 1.79        | 17     | 3     |
| 1:C:48:LEU:H     | 1:C:48:LEU:HD12  | 0.54     | 1.63        | 4      | 1     |
| 1:C:123:ALA:HB2  | 2:D:34:VAL:HA    | 0.54     | 1.79        | 20     | 1     |
| 2:B:146:HIS:HB3  | 2:D:135:ALA:HB1  | 0.54     | 1.77        | 3      | 1     |
| 1:A:34:LEU:CD1   | 2:B:128:ALA:H    | 0.54     | 2.15        | 18     | 1     |
| 1:A:65:ALA:O     | 1:A:69:ALA:N     | 0.54     | 2.40        | 12     | 5     |
| 2:D:42:PHE:CE1   | 2:D:45:PHE:CE1   | 0.54     | 2.95        | 16     | 1     |
| 1:A:109:LEU:O    | 1:A:112:HIS:NE2  | 0.54     | 2.41        | 16     | 1     |
| 1:C:98:PHE:CG    | 1:C:99:LYS:N     | 0.54     | 2.75        | 19     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:C:100:LEU:N    | 1:C:100:LEU:CD2  | 0.54     | 2.71        | 9      | 1     |
| 1:A:86:LEU:CG    | 3:A:142:HEC:HBD1 | 0.54     | 2.32        | 7      | 1     |
| 1:A:113:LEU:O    | 1:A:114:PRO:O    | 0.54     | 2.25        | 18     | 12    |
| 2:B:116:HIS:ND1  | 2:B:116:HIS:C    | 0.54     | 2.61        | 18     | 7     |
| 2:B:37:TRP:NE1   | 2:B:38:THR:OG1   | 0.54     | 2.41        | 9      | 4     |
| 2:D:53:ALA:O     | 2:D:57:ASN:ND2   | 0.54     | 2.40        | 3      | 2     |
| 2:D:73:ASP:CG    | 2:D:84:THR:HG1   | 0.54     | 2.05        | 15     | 1     |
| 2:B:81:LEU:N     | 2:B:81:LEU:HD22  | 0.54     | 2.17        | 15     | 1     |
| 2:B:45:PHE:HZ    | 3:B:147:HEC:CMD  | 0.54     | 2.15        | 16     | 1     |
| 2:B:40:ARG:NH1   | 1:C:92:ARG:HG2   | 0.54     | 2.17        | 14     | 1     |
| 2:D:94:ASP:O     | 2:D:97:HIS:CD2   | 0.54     | 2.61        | 9      | 2     |
| 1:C:86:LEU:CG    | 3:C:142:HEC:HBD1 | 0.54     | 2.32        | 7      | 1     |
| 2:D:42:PHE:CD1   | 2:D:43:GLU:N     | 0.54     | 2.76        | 5      | 1     |
| 1:C:101:LEU:HD23 | 1:C:101:LEU:O    | 0.54     | 2.02        | 13     | 1     |
| 1:A:101:LEU:HD23 | 1:A:101:LEU:O    | 0.54     | 2.02        | 13     | 1     |
| 1:C:127:LYS:O    | 1:C:130:ALA:N    | 0.54     | 2.39        | 17     | 12    |
| 2:B:11:VAL:HG23  | 2:B:130:TYR:CD2  | 0.54     | 2.38        | 15     | 4     |
| 2:B:2:HIS:NE2    | 2:D:146:HIS:CG   | 0.54     | 2.62        | 15     | 1     |
| 1:A:92:ARG:CZ    | 2:D:40:ARG:CG    | 0.54     | 2.85        | 15     | 1     |
| 1:C:100:LEU:HD12 | 1:C:100:LEU:N    | 0.54     | 2.18        | 1      | 2     |
| 2:B:63:HIS:CE1   | 3:B:147:HEC:C2A  | 0.54     | 2.90        | 16     | 1     |
| 1:A:108:THR:CG2  | 1:A:109:LEU:N    | 0.54     | 2.69        | 16     | 2     |
| 1:A:124:SER:OG   | 1:A:125:LEU:N    | 0.54     | 2.41        | 3      | 8     |
| 1:A:97:ASN:ND2   | 1:A:97:ASN:N     | 0.54     | 2.55        | 9      | 2     |
| 2:B:47:ASP:O     | 2:B:48:LEU:CB    | 0.54     | 2.54        | 20     | 1     |
| 1:A:89:HIS:O     | 1:A:89:HIS:ND1   | 0.54     | 2.41        | 17     | 1     |
| 2:D:94:ASP:O     | 2:D:97:HIS:CE1   | 0.54     | 2.61        | 12     | 2     |
| 2:B:97:HIS:CE1   | 1:C:41:THR:CB    | 0.54     | 2.91        | 12     | 1     |
| 1:C:72:HIS:C     | 1:C:74:ASP:N     | 0.54     | 2.61        | 19     | 20    |
| 2:D:143:HIS:O    | 2:D:146:HIS:CG   | 0.54     | 2.60        | 18     | 1     |
| 2:B:143:HIS:O    | 2:B:146:HIS:CG   | 0.54     | 2.60        | 18     | 1     |
| 1:C:47:ASP:O     | 1:C:49:SER:N     | 0.54     | 2.40        | 19     | 10    |
| 1:A:97:ASN:N     | 1:A:97:ASN:OD1   | 0.54     | 2.40        | 12     | 2     |
| 1:C:95:PRO:O     | 1:C:97:ASN:N     | 0.54     | 2.41        | 6      | 9     |
| 1:A:100:LEU:CD1  | 1:A:100:LEU:N    | 0.54     | 2.71        | 15     | 2     |
| 2:B:59:LYS:O     | 2:B:63:HIS:N     | 0.54     | 2.39        | 7      | 2     |
| 1:A:101:LEU:HD11 | 3:A:142:HEC:CHC  | 0.54     | 2.32        | 7      | 1     |
| 1:A:85:ASP:OD1   | 1:A:89:HIS:CE1   | 0.54     | 2.60        | 20     | 1     |
| 1:A:92:ARG:HD3   | 2:D:40:ARG:CB    | 0.54     | 2.32        | 17     | 1     |
| 2:B:94:ASP:O     | 2:B:97:HIS:CE1   | 0.54     | 2.61        | 12     | 2     |
| 1:A:72:HIS:C     | 1:A:74:ASP:N     | 0.54     | 2.61        | 16     | 20    |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:C:46:PHE:O    | 1:C:48:LEU:HG    | 0.54     | 2.03        | 14     | 4     |
| 1:A:100:LEU:N   | 1:A:100:LEU:HD12 | 0.54     | 2.18        | 15     | 1     |
| 2:B:13:ALA:O    | 2:B:15:TRP:N     | 0.54     | 2.41        | 14     | 3     |
| 1:C:11:LYS:O    | 1:C:15:GLY:N     | 0.54     | 2.41        | 20     | 2     |
| 2:D:97:HIS:C    | 2:D:97:HIS:ND1   | 0.54     | 2.61        | 16     | 1     |
| 2:D:66:LYS:HB3  | 3:D:147:HEC:HBA2 | 0.54     | 1.78        | 14     | 1     |
| 1:A:37:PRO:O    | 1:A:40:LYS:N     | 0.54     | 2.39        | 14     | 4     |
| 1:C:61:LYS:CB   | 3:C:142:HEC:C3A  | 0.54     | 2.83        | 19     | 1     |
| 1:A:38:THR:HB   | 2:D:97:HIS:CB    | 0.54     | 2.31        | 19     | 1     |
| 1:C:34:LEU:HD11 | 2:D:127:GLN:NE2  | 0.54     | 2.18        | 9      | 1     |
| 2:D:115:ALA:O   | 2:D:119:GLY:N    | 0.54     | 2.41        | 9      | 2     |
| 2:D:81:LEU:O    | 2:D:85:PHE:CZ    | 0.54     | 2.60        | 6      | 1     |
| 2:D:37:TRP:CH2  | 2:D:102:ASN:ND2  | 0.54     | 2.76        | 5      | 1     |
| 1:A:87:HIS:NE2  | 3:A:142:HEC:ND   | 0.54     | 2.55        | 12     | 1     |
| 2:D:123:THR:OG1 | 2:D:126:VAL:HG23 | 0.54     | 2.03        | 18     | 7     |
| 1:A:91:LEU:HD12 | 1:A:91:LEU:N     | 0.54     | 2.17        | 9      | 3     |
| 1:C:106:LEU:CD2 | 1:C:106:LEU:N    | 0.54     | 2.71        | 4      | 4     |
| 2:B:81:LEU:CD2  | 2:B:81:LEU:N     | 0.54     | 2.71        | 10     | 2     |
| 1:C:109:LEU:O   | 1:C:112:HIS:NE2  | 0.54     | 2.41        | 16     | 1     |
| 2:B:37:TRP:O    | 1:C:92:ARG:NH2   | 0.54     | 2.41        | 19     | 1     |
| 1:C:97:ASN:H    | 1:C:97:ASN:HD22  | 0.54     | 1.45        | 9      | 1     |
| 2:B:115:ALA:O   | 2:B:119:GLY:N    | 0.54     | 2.41        | 9      | 2     |
| 1:A:86:LEU:CD1  | 3:A:142:HEC:HBD1 | 0.54     | 2.32        | 7      | 1     |
| 1:A:32:MET:O    | 1:A:36:PHE:N     | 0.54     | 2.40        | 7      | 1     |
| 1:A:123:ALA:HB2 | 2:B:34:VAL:HA    | 0.54     | 1.79        | 20     | 1     |
| 1:C:48:LEU:H    | 1:C:48:LEU:CD2   | 0.54     | 2.13        | 3      | 1     |
| 1:C:31:ARG:NE   | 1:C:31:ARG:O     | 0.54     | 2.41        | 1      | 1     |
| 2:D:89:SER:O    | 2:D:93:CYS:N     | 0.54     | 2.41        | 2      | 1     |
| 1:A:46:PHE:O    | 1:A:48:LEU:HG    | 0.54     | 2.03        | 14     | 5     |
| 2:D:116:HIS:C   | 2:D:116:HIS:ND1  | 0.54     | 2.61        | 18     | 9     |
| 1:C:124:SER:OG  | 1:C:125:LEU:N    | 0.54     | 2.41        | 3      | 8     |
| 1:A:134:THR:O   | 1:A:138:SER:N    | 0.54     | 2.41        | 9      | 2     |
| 1:C:91:LEU:O    | 1:C:93:VAL:N     | 0.54     | 2.41        | 3      | 7     |
| 1:A:91:LEU:O    | 1:A:93:VAL:N     | 0.54     | 2.41        | 12     | 7     |
| 2:B:37:TRP:CH2  | 2:B:102:ASN:ND2  | 0.54     | 2.76        | 5      | 1     |
| 1:C:68:ASN:O    | 1:C:72:HIS:CD2   | 0.54     | 2.61        | 11     | 2     |
| 1:A:33:PHE:O    | 1:A:33:PHE:CD1   | 0.53     | 2.62        | 15     | 2     |
| 1:A:11:LYS:O    | 1:A:15:GLY:N     | 0.53     | 2.41        | 20     | 2     |
| 1:A:83:LEU:HD22 | 3:A:142:HEC:HBA1 | 0.53     | 1.79        | 9      | 2     |
| 2:D:142:ALA:O   | 2:D:145:TYR:CD1  | 0.53     | 2.61        | 16     | 2     |
| 1:C:91:LEU:C    | 1:C:93:VAL:H     | 0.53     | 2.06        | 17     | 4     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:98:PHE:CG    | 1:A:99:LYS:N    | 0.53     | 2.75        | 19     | 1     |
| 2:D:46:GLY:O     | 2:D:48:LEU:N    | 0.53     | 2.41        | 19     | 1     |
| 2:B:38:THR:OG1   | 2:B:39:GLN:N    | 0.53     | 2.41        | 3      | 4     |
| 1:A:92:ARG:HD3   | 2:D:40:ARG:CG   | 0.53     | 2.32        | 17     | 1     |
| 1:A:68:ASN:O     | 1:A:72:HIS:CD2  | 0.53     | 2.61        | 11     | 2     |
| 1:A:21:ALA:O     | 1:A:23:GLU:N    | 0.53     | 2.42        | 5      | 16    |
| 2:B:81:LEU:N     | 2:B:81:LEU:HD12 | 0.53     | 2.18        | 11     | 3     |
| 1:A:35:SER:O     | 1:A:36:PHE:CD1  | 0.53     | 2.61        | 5      | 8     |
| 3:B:147:HEC:HAD2 | 2:D:63:HIS:NE2  | 0.53     | 2.17        | 15     | 1     |
| 2:D:81:LEU:CD2   | 2:D:81:LEU:N    | 0.53     | 2.71        | 15     | 1     |
| 1:C:100:LEU:CD1  | 1:C:100:LEU:N   | 0.53     | 2.71        | 15     | 2     |
| 1:C:35:SER:O     | 1:C:36:PHE:CD2  | 0.53     | 2.61        | 19     | 6     |
| 1:C:33:PHE:CD1   | 1:C:33:PHE:O    | 0.53     | 2.62        | 5      | 2     |
| 1:C:17:VAL:O     | 1:C:20:HIS:N    | 0.53     | 2.40        | 16     | 3     |
| 1:C:35:SER:O     | 1:C:36:PHE:CD1  | 0.53     | 2.62        | 5      | 7     |
| 1:A:97:ASN:H     | 1:A:97:ASN:HD22 | 0.53     | 1.45        | 9      | 1     |
| 2:B:94:ASP:O     | 2:B:97:HIS:CD2  | 0.53     | 2.61        | 9      | 2     |
| 1:C:123:ALA:HB2  | 2:D:33:VAL:O    | 0.53     | 2.04        | 17     | 1     |
| 1:A:36:PHE:CE2   | 1:A:38:THR:OG1  | 0.53     | 2.61        | 12     | 1     |
| 2:B:39:GLN:O     | 2:B:42:PHE:CD1  | 0.53     | 2.62        | 14     | 3     |
| 2:B:7:GLU:OE1    | 2:B:7:GLU:N     | 0.53     | 2.42        | 15     | 2     |
| 1:C:116:GLU:O    | 1:C:117:PHE:CG  | 0.53     | 2.61        | 15     | 2     |
| 2:D:11:VAL:HG23  | 2:D:130:TYR:CD2 | 0.53     | 2.38        | 15     | 2     |
| 1:A:27:GLU:N     | 1:A:27:GLU:OE1  | 0.53     | 2.41        | 15     | 1     |
| 1:A:97:ASN:OD1   | 1:A:98:PHE:N    | 0.53     | 2.41        | 8      | 1     |
| 2:D:101:GLU:OE1  | 2:D:101:GLU:N   | 0.53     | 2.42        | 8      | 1     |
| 1:C:58:HIS:C     | 1:C:58:HIS:ND1  | 0.53     | 2.62        | 8      | 8     |
| 2:B:42:PHE:CE2   | 2:B:45:PHE:CG   | 0.53     | 2.97        | 16     | 1     |
| 2:B:2:HIS:O      | 2:B:2:HIS:CD2   | 0.53     | 2.61        | 14     | 1     |
| 2:B:105:LEU:CD1  | 2:B:105:LEU:N   | 0.53     | 2.72        | 13     | 3     |
| 2:D:92:HIS:CE1   | 2:D:141:LEU:O   | 0.53     | 2.62        | 5      | 2     |
| 2:B:92:HIS:ND1   | 2:B:93:CYS:N    | 0.53     | 2.56        | 20     | 2     |
| 2:B:127:GLN:OE1  | 2:B:127:GLN:N   | 0.53     | 2.42        | 20     | 1     |
| 1:C:89:HIS:O     | 1:C:89:HIS:ND1  | 0.53     | 2.41        | 17     | 1     |
| 2:B:139:ASN:OD1  | 2:D:139:ASN:OD1 | 0.53     | 2.25        | 13     | 1     |
| 1:A:30:GLU:OE1   | 1:A:50:HIS:ND1  | 0.53     | 2.41        | 2      | 1     |
| 2:B:106:LEU:HB3  | 3:B:147:HEC:CBB | 0.53     | 2.34        | 18     | 1     |
| 1:C:21:ALA:O     | 1:C:23:GLU:N    | 0.53     | 2.42        | 7      | 16    |
| 2:D:100:PRO:O    | 2:D:102:ASN:N   | 0.53     | 2.41        | 10     | 1     |
| 1:A:27:GLU:OE2   | 1:A:112:HIS:NE2 | 0.53     | 2.41        | 10     | 2     |
| 1:C:90:LYS:O     | 1:C:92:ARG:N    | 0.53     | 2.42        | 16     | 3     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 2:D:95:LYS:O    | 2:D:97:HIS:CE1   | 0.53     | 2.61        | 9      | 1     |
| 1:C:35:SER:OG   | 1:C:36:PHE:CD2   | 0.53     | 2.62        | 7      | 1     |
| 2:D:47:ASP:O    | 2:D:48:LEU:CB    | 0.53     | 2.54        | 20     | 1     |
| 2:D:81:LEU:HD12 | 2:D:81:LEU:N     | 0.53     | 2.18        | 11     | 4     |
| 2:B:48:LEU:N    | 2:B:48:LEU:HD12  | 0.53     | 2.19        | 14     | 2     |
| 1:C:2:LEU:HD22  | 1:C:2:LEU:N      | 0.53     | 2.18        | 19     | 1     |
| 1:A:100:LEU:CD2 | 1:A:100:LEU:N    | 0.53     | 2.71        | 9      | 1     |
| 2:B:95:LYS:O    | 2:B:97:HIS:CE1   | 0.53     | 2.61        | 9      | 1     |
| 1:C:134:THR:O   | 1:C:138:SER:N    | 0.53     | 2.41        | 9      | 2     |
| 2:B:131:GLN:H   | 2:B:131:GLN:NE2  | 0.53     | 2.02        | 5      | 1     |
| 1:C:36:PHE:CE2  | 1:C:38:THR:OG1   | 0.53     | 2.61        | 12     | 1     |
| 2:B:122:PHE:O   | 2:B:127:GLN:NE2  | 0.53     | 2.42        | 11     | 1     |
| 2:B:105:LEU:N   | 2:B:105:LEU:CD1  | 0.53     | 2.72        | 18     | 2     |
| 2:D:81:LEU:CD1  | 2:D:81:LEU:N     | 0.53     | 2.72        | 11     | 4     |
| 2:D:117:HIS:O   | 2:D:118:PHE:CD1  | 0.53     | 2.62        | 3      | 6     |
| 1:C:37:PRO:O    | 1:C:40:LYS:N     | 0.53     | 2.39        | 14     | 4     |
| 1:A:2:LEU:N     | 1:A:2:LEU:HD22   | 0.53     | 2.18        | 19     | 1     |
| 1:A:34:LEU:HD11 | 2:B:127:GLN:NE2  | 0.53     | 2.18        | 9      | 1     |
| 2:D:133:VAL:O   | 2:D:135:ALA:N    | 0.53     | 2.42        | 12     | 1     |
| 2:D:106:LEU:HB3 | 3:D:147:HEC:CBB  | 0.53     | 2.34        | 18     | 1     |
| 2:D:15:TRP:HE1  | 2:D:72:SER:CB    | 0.53     | 2.17        | 9      | 5     |
| 2:B:40:ARG:CD   | 1:C:92:ARG:NH2   | 0.53     | 2.69        | 15     | 1     |
| 1:C:27:GLU:N    | 1:C:27:GLU:OE1   | 0.53     | 2.41        | 15     | 1     |
| 2:D:97:HIS:ND1  | 2:D:97:HIS:O     | 0.53     | 2.42        | 8      | 1     |
| 1:C:26:ALA:HB1  | 1:C:55:VAL:O     | 0.53     | 2.04        | 8      | 2     |
| 2:D:2:HIS:O     | 2:D:2:HIS:CD2    | 0.53     | 2.62        | 14     | 1     |
| 2:B:46:GLY:O    | 2:B:48:LEU:N     | 0.53     | 2.41        | 19     | 1     |
| 2:B:92:HIS:CE1  | 2:B:141:LEU:O    | 0.53     | 2.62        | 5      | 2     |
| 1:A:33:PHE:CE2  | 1:A:48:LEU:O     | 0.53     | 2.62        | 13     | 1     |
| 2:B:99:ASP:OD2  | 1:C:96:VAL:HB    | 0.53     | 2.04        | 2      | 2     |
| 2:B:81:LEU:N    | 2:B:81:LEU:CD1   | 0.53     | 2.72        | 11     | 1     |
| 2:D:105:LEU:CD1 | 2:D:105:LEU:N    | 0.53     | 2.72        | 18     | 3     |
| 2:D:77:HIS:CE1  | 2:D:80:ASN:OD1   | 0.53     | 2.62        | 10     | 1     |
| 2:D:80:ASN:OD1  | 2:D:80:ASN:N     | 0.53     | 2.42        | 6      | 2     |
| 2:D:22:GLU:O    | 2:D:25:GLY:N     | 0.53     | 2.42        | 20     | 3     |
| 2:D:139:ASN:O   | 2:D:143:HIS:N    | 0.53     | 2.42        | 16     | 3     |
| 1:C:83:LEU:HD22 | 3:C:142:HEC:HBA1 | 0.53     | 1.79        | 9      | 2     |
| 1:A:2:LEU:CD2   | 1:A:2:LEU:N      | 0.53     | 2.72        | 19     | 1     |
| 1:A:94:ASP:OD1  | 1:A:94:ASP:N     | 0.53     | 2.42        | 9      | 4     |
| 1:A:52:SER:OG   | 1:A:53:ALA:N     | 0.53     | 2.42        | 9      | 2     |
| 1:A:38:THR:HA   | 2:D:97:HIS:CB    | 0.53     | 2.29        | 4      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:31:ARG:O    | 1:A:31:ARG:NE    | 0.53     | 2.41        | 1      | 1     |
| 2:D:57:ASN:OD1  | 2:D:59:LYS:N     | 0.53     | 2.42        | 1      | 1     |
| 2:B:88:LEU:O    | 2:B:92:HIS:ND1   | 0.53     | 2.42        | 19     | 6     |
| 2:D:96:LEU:N    | 2:D:96:LEU:CD1   | 0.53     | 2.71        | 15     | 3     |
| 1:C:24:TYR:CD1  | 1:C:112:HIS:ND1  | 0.53     | 2.77        | 18     | 1     |
| 1:A:24:TYR:CD1  | 1:A:112:HIS:ND1  | 0.53     | 2.77        | 18     | 1     |
| 2:D:50:THR:O    | 2:D:53:ALA:N     | 0.53     | 2.41        | 11     | 8     |
| 2:B:117:HIS:O   | 2:B:118:PHE:CG   | 0.53     | 2.62        | 9      | 4     |
| 2:D:117:HIS:O   | 2:D:118:PHE:CG   | 0.53     | 2.62        | 9      | 4     |
| 1:C:73:VAL:HG22 | 1:C:73:VAL:O     | 0.53     | 2.04        | 15     | 9     |
| 1:A:58:HIS:C    | 1:A:58:HIS:ND1   | 0.53     | 2.62        | 8      | 11    |
| 1:A:27:GLU:OE1  | 1:A:112:HIS:NE2  | 0.53     | 2.42        | 3      | 3     |
| 1:C:27:GLU:OE1  | 1:C:112:HIS:NE2  | 0.53     | 2.42        | 3      | 3     |
| 2:B:15:TRP:HE1  | 2:B:72:SER:CB    | 0.53     | 2.17        | 9      | 5     |
| 2:D:39:GLN:O    | 2:D:42:PHE:CD1   | 0.53     | 2.62        | 14     | 3     |
| 2:B:139:ASN:O   | 2:B:143:HIS:N    | 0.53     | 2.42        | 8      | 3     |
| 1:A:83:LEU:O    | 1:A:87:HIS:ND1   | 0.53     | 2.42        | 14     | 3     |
| 1:C:122:HIS:CD2 | 2:D:34:VAL:HG22  | 0.53     | 2.39        | 14     | 1     |
| 1:A:35:SER:OG   | 2:B:131:GLN:NE2  | 0.53     | 2.38        | 14     | 1     |
| 2:D:95:LYS:O    | 2:D:97:HIS:NE2   | 0.53     | 2.42        | 19     | 1     |
| 1:C:97:ASN:ND2  | 1:C:97:ASN:N     | 0.53     | 2.56        | 9      | 2     |
| 1:C:83:LEU:O    | 1:C:86:LEU:N     | 0.53     | 2.42        | 4      | 2     |
| 2:D:92:HIS:ND1  | 2:D:93:CYS:N     | 0.53     | 2.56        | 20     | 2     |
| 1:A:92:ARG:CB   | 2:D:40:ARG:NH1   | 0.53     | 2.37        | 17     | 1     |
| 2:B:71:PHE:O    | 2:B:71:PHE:CD1   | 0.53     | 2.62        | 17     | 1     |
| 2:B:146:HIS:OXT | 2:B:146:HIS:CG   | 0.53     | 2.62        | 11     | 1     |
| 2:D:146:HIS:OXT | 2:D:146:HIS:CG   | 0.53     | 2.62        | 11     | 1     |
| 2:B:103:PHE:CD1 | 2:B:103:PHE:N    | 0.53     | 2.73        | 11     | 1     |
| 2:D:144:LYS:O   | 2:D:146:HIS:N    | 0.53     | 2.43        | 16     | 6     |
| 1:C:27:GLU:OE2  | 1:C:112:HIS:NE2  | 0.53     | 2.41        | 10     | 2     |
| 2:B:127:GLN:O   | 2:B:131:GLN:NE2  | 0.53     | 2.42        | 5      | 2     |
| 1:A:67:THR:O    | 1:A:71:ALA:N     | 0.53     | 2.42        | 6      | 6     |
| 2:D:105:LEU:N   | 2:D:105:LEU:CD1  | 0.53     | 2.72        | 13     | 2     |
| 1:C:86:LEU:CD1  | 3:C:142:HEC:HBD1 | 0.53     | 2.32        | 7      | 1     |
| 2:B:112:CYS:O   | 2:B:116:HIS:ND1  | 0.53     | 2.41        | 3      | 2     |
| 2:D:146:HIS:ND1 | 2:D:146:HIS:N    | 0.53     | 2.56        | 17     | 2     |
| 2:D:71:PHE:CD1  | 2:D:71:PHE:O     | 0.53     | 2.62        | 17     | 1     |
| 1:C:33:PHE:CE2  | 1:C:48:LEU:O     | 0.53     | 2.62        | 13     | 1     |
| 2:D:42:PHE:CD2  | 3:D:147:HEC:HMD3 | 0.53     | 2.32        | 2      | 1     |
| 1:C:82:ALA:O    | 1:C:85:ASP:N     | 0.52     | 2.42        | 11     | 19    |
| 1:C:6:ASP:OD2   | 1:C:127:LYS:NZ   | 0.52     | 2.42        | 10     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:127:LYS:O   | 1:A:130:ALA:N    | 0.52     | 2.39        | 17     | 11    |
| 2:B:116:HIS:C   | 2:B:116:HIS:ND1  | 0.52     | 2.60        | 7      | 8     |
| 2:D:7:GLU:OE1   | 2:D:7:GLU:N      | 0.52     | 2.42        | 15     | 2     |
| 1:C:107:VAL:O   | 1:C:110:ALA:HB3  | 0.52     | 2.04        | 5      | 5     |
| 1:A:61:LYS:CB   | 3:A:142:HEC:C3A  | 0.52     | 2.83        | 19     | 1     |
| 1:C:52:SER:OG   | 1:C:53:ALA:N     | 0.52     | 2.42        | 9      | 2     |
| 2:D:77:HIS:NE2  | 2:D:80:ASN:OD1   | 0.52     | 2.42        | 7      | 1     |
| 2:D:68:LEU:HD23 | 2:D:68:LEU:C     | 0.52     | 2.24        | 4      | 2     |
| 2:D:131:GLN:NE2 | 2:D:131:GLN:H    | 0.52     | 2.02        | 5      | 1     |
| 2:B:133:VAL:O   | 2:B:135:ALA:N    | 0.52     | 2.41        | 12     | 1     |
| 1:C:84:SER:O    | 1:C:88:ALA:N     | 0.52     | 2.42        | 13     | 1     |
| 2:D:19:ASN:O    | 2:D:22:GLU:N     | 0.52     | 2.42        | 9      | 8     |
| 2:B:80:ASN:OD1  | 2:B:83:GLY:N     | 0.52     | 2.42        | 11     | 6     |
| 2:B:50:THR:O    | 2:B:53:ALA:N     | 0.52     | 2.41        | 11     | 7     |
| 1:A:71:ALA:O    | 1:A:72:HIS:CD2   | 0.52     | 2.62        | 17     | 4     |
| 2:D:89:SER:O    | 2:D:93:CYS:SG    | 0.52     | 2.67        | 10     | 3     |
| 2:B:77:HIS:CE1  | 2:B:80:ASN:OD1   | 0.52     | 2.62        | 10     | 1     |
| 1:A:6:ASP:OD2   | 1:A:127:LYS:NZ   | 0.52     | 2.42        | 10     | 1     |
| 1:C:61:LYS:O    | 3:C:142:HEC:HMA3 | 0.52     | 2.05        | 9      | 3     |
| 1:C:97:ASN:OD1  | 1:C:98:PHE:N     | 0.52     | 2.41        | 8      | 1     |
| 2:D:42:PHE:CE2  | 2:D:45:PHE:CG    | 0.52     | 2.97        | 16     | 1     |
| 1:C:115:ALA:CB  | 1:C:122:HIS:CE1  | 0.52     | 2.93        | 16     | 1     |
| 2:D:28:LEU:N    | 2:D:28:LEU:CD2   | 0.52     | 2.73        | 13     | 2     |
| 2:D:61:LYS:O    | 2:D:65:LYS:NZ    | 0.52     | 2.42        | 9      | 3     |
| 1:A:32:MET:HE1  | 3:A:142:HEC:HBC2 | 0.52     | 1.81        | 19     | 1     |
| 2:B:95:LYS:O    | 2:B:97:HIS:NE2   | 0.52     | 2.42        | 19     | 1     |
| 1:C:2:LEU:CD2   | 1:C:2:LEU:N      | 0.52     | 2.72        | 19     | 1     |
| 1:C:94:ASP:N    | 1:C:94:ASP:OD1   | 0.52     | 2.42        | 9      | 1     |
| 2:B:114:LEU:CD1 | 2:B:130:TYR:CZ   | 0.52     | 2.92        | 12     | 2     |
| 1:C:106:LEU:CD1 | 1:C:106:LEU:N    | 0.52     | 2.73        | 3      | 2     |
| 1:A:123:ALA:HB2 | 2:B:33:VAL:O     | 0.52     | 2.04        | 17     | 1     |
| 2:B:145:TYR:CD2 | 2:B:145:TYR:O    | 0.52     | 2.62        | 17     | 1     |
| 1:A:92:ARG:HB2  | 2:D:40:ARG:NH2   | 0.52     | 2.20        | 18     | 1     |
| 2:B:144:LYS:O   | 2:B:146:HIS:N    | 0.52     | 2.42        | 19     | 6     |
| 2:D:88:LEU:O    | 2:D:92:HIS:ND1   | 0.52     | 2.42        | 19     | 6     |
| 1:A:91:LEU:N    | 1:A:91:LEU:CD1   | 0.52     | 2.72        | 7      | 3     |
| 1:A:6:ASP:N     | 1:A:6:ASP:OD1    | 0.52     | 2.42        | 4      | 2     |
| 2:B:61:LYS:CB   | 2:B:61:LYS:NZ    | 0.52     | 2.72        | 6      | 1     |
| 2:D:61:LYS:CB   | 2:D:61:LYS:NZ    | 0.52     | 2.72        | 6      | 2     |
| 2:B:77:HIS:NE2  | 2:B:80:ASN:OD1   | 0.52     | 2.42        | 7      | 1     |
| 1:C:2:LEU:HD13  | 1:C:131:SER:OG   | 0.52     | 2.05        | 5      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:C:39:THR:CA   | 3:C:142:HEC:C3C  | 0.52     | 2.79        | 12     | 1     |
| 1:A:93:VAL:CG1  | 1:A:94:ASP:N     | 0.52     | 2.73        | 18     | 2     |
| 2:B:122:PHE:C   | 2:B:122:PHE:CD1  | 0.52     | 2.82        | 8      | 7     |
| 1:C:91:LEU:CD1  | 1:C:91:LEU:N     | 0.52     | 2.72        | 7      | 3     |
| 1:A:18:GLY:O    | 1:A:20:HIS:N     | 0.52     | 2.41        | 17     | 14    |
| 1:C:71:ALA:O    | 1:C:72:HIS:CD2   | 0.52     | 2.62        | 17     | 4     |
| 2:B:97:HIS:ND1  | 2:B:97:HIS:O     | 0.52     | 2.42        | 10     | 1     |
| 2:D:145:TYR:CE1 | 2:D:146:HIS:OXT  | 0.52     | 2.63        | 10     | 1     |
| 1:C:6:ASP:N     | 1:C:6:ASP:OD1    | 0.52     | 2.42        | 4      | 2     |
| 2:B:61:LYS:O    | 2:B:65:LYS:NZ    | 0.52     | 2.42        | 9      | 3     |
| 1:A:53:ALA:O    | 1:A:55:VAL:N     | 0.52     | 2.42        | 2      | 5     |
| 2:B:68:LEU:HD23 | 2:B:68:LEU:C     | 0.52     | 2.24        | 4      | 1     |
| 2:B:40:ARG:NH1  | 1:C:92:ARG:CB    | 0.52     | 2.35        | 17     | 1     |
| 1:A:92:ARG:NH1  | 2:D:40:ARG:C     | 0.52     | 2.62        | 17     | 1     |
| 1:C:30:GLU:OE1  | 1:C:50:HIS:ND1   | 0.52     | 2.41        | 2      | 1     |
| 1:C:121:VAL:CG1 | 1:C:122:HIS:H    | 0.52     | 2.18        | 13     | 3     |
| 1:A:95:PRO:O    | 1:A:98:PHE:N     | 0.52     | 2.41        | 4      | 7     |
| 1:C:87:HIS:NE2  | 1:C:136:LEU:O    | 0.52     | 2.42        | 10     | 1     |
| 1:C:65:ALA:O    | 1:C:69:ALA:N     | 0.52     | 2.40        | 12     | 6     |
| 1:C:35:SER:OG   | 2:D:131:GLN:NE2  | 0.52     | 2.38        | 14     | 1     |
| 1:A:91:LEU:C    | 1:A:93:VAL:H     | 0.52     | 2.06        | 17     | 4     |
| 2:D:30:ARG:O    | 2:D:33:VAL:N     | 0.52     | 2.43        | 9      | 2     |
| 1:C:130:ALA:O   | 1:C:134:THR:N    | 0.52     | 2.43        | 7      | 2     |
| 1:A:37:PRO:O    | 2:D:97:HIS:ND1   | 0.52     | 2.43        | 3      | 1     |
| 2:D:91:LEU:HD23 | 2:D:92:HIS:N     | 0.52     | 2.20        | 12     | 1     |
| 1:A:82:ALA:O    | 1:A:85:ASP:N     | 0.52     | 2.42        | 11     | 17    |
| 2:B:3:LEU:HD21  | 2:B:133:VAL:HG22 | 0.52     | 1.81        | 15     | 3     |
| 2:B:96:LEU:CD1  | 2:B:96:LEU:N     | 0.52     | 2.72        | 15     | 2     |
| 2:B:28:LEU:CD2  | 2:B:28:LEU:N     | 0.52     | 2.73        | 13     | 2     |
| 2:B:39:GLN:O    | 2:B:42:PHE:CE1   | 0.52     | 2.63        | 14     | 1     |
| 2:B:100:PRO:O   | 2:B:102:ASN:ND2  | 0.52     | 2.43        | 9      | 1     |
| 1:A:86:LEU:HG   | 3:A:142:HEC:HBD1 | 0.52     | 1.82        | 7      | 1     |
| 1:A:5:ALA:O     | 1:A:8:THR:N      | 0.52     | 2.42        | 7      | 4     |
| 1:C:31:ARG:CZ   | 1:C:104:CYS:SG   | 0.52     | 2.98        | 7      | 1     |
| 2:D:114:LEU:CD1 | 2:D:130:TYR:CZ   | 0.52     | 2.92        | 12     | 2     |
| 2:D:127:GLN:OE1 | 2:D:127:GLN:N    | 0.52     | 2.41        | 20     | 2     |
| 1:A:48:LEU:CD2  | 1:A:48:LEU:H     | 0.52     | 2.12        | 3      | 1     |
| 2:B:146:HIS:ND1 | 2:B:146:HIS:N    | 0.52     | 2.56        | 17     | 2     |
| 2:D:42:PHE:CD1  | 3:D:147:HEC:CMB  | 0.52     | 2.91        | 12     | 1     |
| 2:D:122:PHE:O   | 2:D:127:GLN:NE2  | 0.52     | 2.42        | 11     | 1     |
| 1:C:103:HIS:HB3 | 2:D:108:ASN:HD21 | 0.52     | 1.65        | 10     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:117:HIS:O   | 2:B:118:PHE:CD1 | 0.52     | 2.62        | 3      | 6     |
| 2:B:42:PHE:CZ   | 2:B:45:PHE:CE2  | 0.52     | 2.98        | 16     | 1     |
| 2:D:145:TYR:CD1 | 2:D:146:HIS:N   | 0.52     | 2.77        | 16     | 2     |
| 1:A:122:HIS:CD2 | 2:B:34:VAL:HG22 | 0.52     | 2.39        | 14     | 1     |
| 1:A:92:ARG:NE   | 2:D:40:ARG:CD   | 0.52     | 2.54        | 19     | 1     |
| 1:C:68:ASN:OD1  | 1:C:69:ALA:N    | 0.52     | 2.43        | 9      | 1     |
| 1:C:5:ALA:O     | 1:C:8:THR:N     | 0.52     | 2.42        | 7      | 4     |
| 1:A:130:ALA:O   | 1:A:134:THR:N   | 0.52     | 2.43        | 7      | 2     |
| 1:A:31:ARG:NH2  | 2:B:127:GLN:CB  | 0.52     | 2.73        | 4      | 1     |
| 1:A:92:ARG:NH1  | 2:D:43:GLU:OE2  | 0.52     | 2.42        | 20     | 1     |
| 2:D:128:ALA:O   | 2:D:132:LYS:NZ  | 0.52     | 2.43        | 3      | 1     |
| 2:D:145:TYR:O   | 2:D:145:TYR:CD2 | 0.52     | 2.62        | 17     | 1     |
| 1:A:84:SER:O    | 1:A:88:ALA:N    | 0.52     | 2.42        | 13     | 1     |
| 1:A:127:LYS:CD  | 1:A:128:PHE:N   | 0.52     | 2.73        | 6      | 6     |
| 2:D:127:GLN:O   | 2:D:131:GLN:NE2 | 0.52     | 2.42        | 5      | 2     |
| 1:C:76:MET:N    | 1:C:77:PRO:HD2  | 0.52     | 2.20        | 13     | 4     |
| 1:A:73:VAL:HG22 | 1:A:73:VAL:O    | 0.52     | 2.04        | 15     | 10    |
| 2:D:32:LEU:O    | 2:D:36:PRO:N    | 0.52     | 2.43        | 1      | 4     |
| 1:A:90:LYS:O    | 1:A:92:ARG:N    | 0.52     | 2.42        | 16     | 4     |
| 1:A:115:ALA:CB  | 1:A:122:HIS:CE1 | 0.52     | 2.93        | 16     | 1     |
| 2:D:39:GLN:O    | 2:D:42:PHE:CE1  | 0.52     | 2.63        | 14     | 1     |
| 1:A:98:PHE:CE1  | 1:A:102:SER:OG  | 0.52     | 2.63        | 7      | 1     |
| 1:C:90:LYS:C    | 1:C:92:ARG:H    | 0.52     | 2.08        | 3      | 3     |
| 2:D:41:PHE:O    | 2:D:43:GLU:N    | 0.52     | 2.43        | 3      | 1     |
| 2:D:21:ASP:OD1  | 2:D:22:GLU:N    | 0.52     | 2.42        | 3      | 2     |
| 1:A:97:ASN:O    | 1:A:100:LEU:N   | 0.52     | 2.41        | 1      | 1     |
| 2:B:77:HIS:CE1  | 2:B:79:ASP:OD2  | 0.52     | 2.63        | 1      | 1     |
| 1:C:39:THR:C    | 3:C:142:HEC:C1C | 0.52     | 2.76        | 12     | 1     |
| 2:D:122:PHE:CD1 | 2:D:122:PHE:C   | 0.52     | 2.83        | 7      | 8     |
| 3:B:147:HEC:HAB | 2:D:106:LEU:CD2 | 0.52     | 2.29        | 15     | 1     |
| 2:B:101:GLU:N   | 2:B:101:GLU:OE1 | 0.52     | 2.42        | 8      | 1     |
| 1:A:106:LEU:CD1 | 1:A:106:LEU:N   | 0.52     | 2.73        | 3      | 2     |
| 1:A:2:LEU:HD21  | 1:A:131:SER:OG  | 0.52     | 2.05        | 6      | 2     |
| 2:B:61:LYS:NZ   | 2:B:61:LYS:CB   | 0.52     | 2.73        | 4      | 1     |
| 2:D:112:CYS:O   | 2:D:116:HIS:ND1 | 0.52     | 2.41        | 3      | 2     |
| 2:B:41:PHE:O    | 2:B:43:GLU:N    | 0.52     | 2.43        | 3      | 1     |
| 2:D:77:HIS:CE1  | 2:D:79:ASP:OD2  | 0.52     | 2.63        | 1      | 1     |
| 2:D:117:HIS:HD1 | 2:D:117:HIS:N   | 0.52     | 2.03        | 12     | 1     |
| 2:B:89:SER:O    | 2:B:93:CYS:N    | 0.52     | 2.41        | 2      | 1     |
| 1:A:121:VAL:CG1 | 1:A:122:HIS:H   | 0.52     | 2.18        | 17     | 3     |
| 1:C:127:LYS:CD  | 1:C:128:PHE:N   | 0.52     | 2.73        | 6      | 6     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:D:111:VAL:CG2  | 2:D:130:TYR:CD1  | 0.52     | 2.93        | 18     | 1     |
| 1:C:18:GLY:O     | 1:C:20:HIS:N     | 0.52     | 2.41        | 17     | 13    |
| 1:C:10:VAL:HG21  | 1:C:128:PHE:CD2  | 0.52     | 2.40        | 10     | 3     |
| 1:C:32:MET:CE    | 3:C:142:HEC:CBC  | 0.52     | 2.88        | 5      | 4     |
| 2:B:143:HIS:O    | 2:B:143:HIS:CG   | 0.52     | 2.63        | 10     | 1     |
| 2:D:143:HIS:O    | 2:D:143:HIS:CG   | 0.52     | 2.63        | 10     | 1     |
| 2:D:42:PHE:CE1   | 2:D:45:PHE:CD2   | 0.52     | 2.98        | 8      | 1     |
| 2:B:81:LEU:HD12  | 2:B:81:LEU:N     | 0.52     | 2.19        | 8      | 3     |
| 1:C:53:ALA:O     | 1:C:55:VAL:N     | 0.52     | 2.43        | 2      | 5     |
| 1:C:2:LEU:HD21   | 1:C:131:SER:OG   | 0.52     | 2.05        | 6      | 2     |
| 2:D:80:ASN:N     | 2:D:80:ASN:OD1   | 0.52     | 2.42        | 19     | 1     |
| 1:A:38:THR:HG22  | 2:D:97:HIS:CG    | 0.52     | 2.35        | 7      | 1     |
| 2:B:57:ASN:OD1   | 2:B:59:LYS:N     | 0.52     | 2.42        | 1      | 1     |
| 1:A:41:THR:HG22  | 2:D:97:HIS:CE1   | 0.52     | 2.40        | 11     | 1     |
| 1:A:92:ARG:HB3   | 2:D:40:ARG:NE    | 0.51     | 2.19        | 18     | 1     |
| 1:A:113:LEU:HD12 | 1:A:113:LEU:O    | 0.51     | 2.04        | 18     | 1     |
| 2:B:89:SER:O     | 2:B:93:CYS:SG    | 0.51     | 2.67        | 10     | 3     |
| 1:C:67:THR:O     | 1:C:71:ALA:N     | 0.51     | 2.42        | 6      | 6     |
| 1:A:61:LYS:HB3   | 3:A:142:HEC:C4A  | 0.51     | 2.35        | 19     | 1     |
| 1:A:68:ASN:OD1   | 1:A:69:ALA:N     | 0.51     | 2.43        | 9      | 1     |
| 1:C:103:HIS:CD2  | 2:D:108:ASN:OD1  | 0.51     | 2.63        | 5      | 2     |
| 2:B:146:HIS:HE1  | 2:D:139:ASN:HD22 | 0.51     | 1.45        | 20     | 1     |
| 2:B:139:ASN:N    | 2:B:139:ASN:OD1  | 0.51     | 2.42        | 17     | 1     |
| 2:D:122:PHE:C    | 2:D:122:PHE:CD1  | 0.51     | 2.80        | 6      | 7     |
| 1:A:32:MET:CE    | 3:A:142:HEC:CBC  | 0.51     | 2.88        | 5      | 4     |
| 2:B:145:TYR:CE1  | 2:B:146:HIS:OXT  | 0.51     | 2.63        | 10     | 1     |
| 2:D:63:HIS:CE1   | 3:D:147:HEC:C3D  | 0.51     | 2.93        | 19     | 1     |
| 1:A:31:ARG:CZ    | 1:A:104:CYS:SG   | 0.51     | 2.98        | 7      | 1     |
| 1:A:2:LEU:HD13   | 1:A:131:SER:OG   | 0.51     | 2.05        | 5      | 1     |
| 1:C:20:HIS:O     | 1:C:24:TYR:CE2   | 0.51     | 2.64        | 1      | 2     |
| 1:A:34:LEU:HD11  | 2:B:128:ALA:H    | 0.51     | 1.64        | 18     | 1     |
| 1:A:32:MET:O     | 1:A:34:LEU:N     | 0.51     | 2.43        | 16     | 2     |
| 1:C:57:GLY:O     | 1:C:61:LYS:NZ    | 0.51     | 2.41        | 3      | 2     |
| 2:D:144:LYS:O    | 2:D:146:HIS:ND1  | 0.51     | 2.44        | 11     | 5     |
| 2:D:80:ASN:OD1   | 2:D:83:GLY:N     | 0.51     | 2.42        | 11     | 6     |
| 1:A:10:VAL:HG21  | 1:A:128:PHE:CD2  | 0.51     | 2.40        | 10     | 3     |
| 2:B:122:PHE:CD1  | 2:B:122:PHE:C    | 0.51     | 2.84        | 10     | 8     |
| 1:A:106:LEU:HD12 | 1:A:106:LEU:N    | 0.51     | 2.19        | 3      | 3     |
| 1:C:106:LEU:N    | 1:C:106:LEU:HD12 | 0.51     | 2.19        | 3      | 4     |
| 1:A:48:LEU:N     | 1:A:48:LEU:HD12  | 0.51     | 2.20        | 8      | 2     |
| 1:A:17:VAL:O     | 1:A:20:HIS:N     | 0.51     | 2.40        | 16     | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:D:99:ASP:O     | 2:D:102:ASN:ND2  | 0.51     | 2.43        | 16     | 2     |
| 2:D:80:ASN:HD22  | 2:D:80:ASN:N     | 0.51     | 2.02        | 14     | 1     |
| 1:A:48:LEU:N     | 1:A:48:LEU:HD22  | 0.51     | 2.19        | 2      | 3     |
| 1:C:48:LEU:HD22  | 1:C:48:LEU:N     | 0.51     | 2.19        | 2      | 2     |
| 2:B:63:HIS:CE1   | 3:B:147:HEC:O2A  | 0.51     | 2.63        | 5      | 1     |
| 1:A:57:GLY:O     | 1:A:61:LYS:NZ    | 0.51     | 2.41        | 3      | 1     |
| 1:A:27:GLU:OE1   | 1:A:112:HIS:CE1  | 0.51     | 2.64        | 3      | 1     |
| 2:B:21:ASP:OD1   | 2:B:22:GLU:N     | 0.51     | 2.42        | 3      | 2     |
| 2:D:142:ALA:O    | 2:D:146:HIS:N    | 0.51     | 2.44        | 17     | 1     |
| 2:D:36:PRO:O     | 3:D:147:HEC:CMC  | 0.51     | 2.55        | 12     | 1     |
| 2:B:102:ASN:OD1  | 3:B:147:HEC:HMC1 | 0.51     | 2.03        | 12     | 1     |
| 1:C:24:TYR:CD1   | 1:C:24:TYR:N     | 0.51     | 2.78        | 16     | 9     |
| 1:A:87:HIS:NE2   | 1:A:136:LEU:O    | 0.51     | 2.42        | 10     | 1     |
| 2:B:48:LEU:N     | 2:B:48:LEU:CD1   | 0.51     | 2.74        | 16     | 2     |
| 1:A:24:TYR:CD1   | 1:A:24:TYR:N     | 0.51     | 2.77        | 11     | 9     |
| 2:B:22:GLU:O     | 2:B:25:GLY:N     | 0.51     | 2.42        | 20     | 4     |
| 1:A:61:LYS:O     | 3:A:142:HEC:HMA3 | 0.51     | 2.05        | 9      | 3     |
| 1:A:26:ALA:HB1   | 1:A:55:VAL:O     | 0.51     | 2.04        | 8      | 2     |
| 1:A:107:VAL:O    | 1:A:110:ALA:HB3  | 0.51     | 2.04        | 5      | 5     |
| 1:A:92:ARG:C     | 2:D:40:ARG:HH12  | 0.51     | 2.07        | 14     | 1     |
| 2:B:146:HIS:HB3  | 2:D:132:LYS:HG3  | 0.51     | 1.81        | 19     | 1     |
| 1:A:117:PHE:HZ   | 2:B:116:HIS:CE1  | 0.51     | 2.18        | 4      | 1     |
| 1:A:90:LYS:C     | 1:A:92:ARG:H     | 0.51     | 2.08        | 3      | 3     |
| 1:C:27:GLU:OE1   | 1:C:112:HIS:CE1  | 0.51     | 2.64        | 3      | 1     |
| 1:C:105:LEU:HD11 | 1:C:125:LEU:HD13 | 0.51     | 1.82        | 13     | 1     |
| 1:A:96:VAL:HG11  | 2:D:99:ASP:CB    | 0.51     | 2.34        | 11     | 1     |
| 1:C:93:VAL:CG1   | 1:C:94:ASP:N     | 0.51     | 2.73        | 18     | 2     |
| 1:C:86:LEU:HD21  | 3:C:142:HEC:CBD  | 0.51     | 2.35        | 13     | 4     |
| 2:D:42:PHE:CZ    | 2:D:45:PHE:CE2   | 0.51     | 2.98        | 16     | 1     |
| 1:A:3:SER:N      | 1:A:6:ASP:OD2    | 0.51     | 2.39        | 20     | 2     |
| 2:B:23:VAL:O     | 2:B:27:ALA:N     | 0.51     | 2.42        | 5      | 1     |
| 2:B:128:ALA:O    | 2:B:132:LYS:NZ   | 0.51     | 2.43        | 3      | 1     |
| 2:B:40:ARG:CG    | 1:C:92:ARG:HD3   | 0.51     | 2.36        | 17     | 1     |
| 2:D:39:GLN:O     | 3:D:147:HEC:C4D  | 0.51     | 2.58        | 12     | 1     |
| 1:A:72:HIS:C     | 1:A:74:ASP:H     | 0.51     | 2.09        | 11     | 20    |
| 2:B:111:VAL:CG2  | 2:B:130:TYR:CD1  | 0.51     | 2.93        | 18     | 1     |
| 1:A:2:LEU:O      | 1:A:3:SER:CB     | 0.51     | 2.59        | 10     | 1     |
| 1:C:117:PHE:O    | 1:C:117:PHE:CD2  | 0.51     | 2.64        | 7      | 2     |
| 2:B:146:HIS:CD2  | 2:D:2:HIS:CE1    | 0.51     | 2.78        | 15     | 1     |
| 3:B:147:HEC:HBC2 | 2:D:31:LEU:CD2   | 0.51     | 2.36        | 15     | 1     |
| 1:A:76:MET:N     | 1:A:77:PRO:HD2   | 0.51     | 2.20        | 13     | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:99:ASP:O     | 2:B:102:ASN:ND2  | 0.51     | 2.43        | 16     | 2     |
| 1:A:36:PHE:CZ    | 1:A:100:LEU:HD22 | 0.51     | 2.41        | 16     | 1     |
| 2:B:3:LEU:HD13   | 2:B:8:LYS:HB2    | 0.51     | 1.82        | 1      | 4     |
| 1:C:83:LEU:O     | 1:C:87:HIS:ND1   | 0.51     | 2.42        | 14     | 3     |
| 2:B:63:HIS:CE1   | 3:B:147:HEC:C3D  | 0.51     | 2.93        | 19     | 1     |
| 2:D:81:LEU:N     | 2:D:81:LEU:HD12  | 0.51     | 2.19        | 6      | 2     |
| 1:A:103:HIS:CD2  | 2:B:108:ASN:OD1  | 0.51     | 2.63        | 5      | 2     |
| 2:B:91:LEU:HD23  | 2:B:92:HIS:N     | 0.51     | 2.20        | 12     | 1     |
| 1:A:86:LEU:HD11  | 3:A:142:HEC:CGD  | 0.51     | 2.36        | 12     | 1     |
| 2:D:21:ASP:OD1   | 2:D:65:LYS:NZ    | 0.51     | 2.43        | 12     | 1     |
| 2:B:81:LEU:CD1   | 2:B:81:LEU:N     | 0.51     | 2.74        | 8      | 3     |
| 2:D:14:LEU:O     | 2:D:16:GLY:N     | 0.51     | 2.44        | 19     | 6     |
| 2:B:145:TYR:C    | 2:B:145:TYR:CD1  | 0.51     | 2.83        | 19     | 3     |
| 3:B:147:HEC:C1B  | 2:D:67:VAL:HG22  | 0.51     | 2.35        | 15     | 1     |
| 3:B:147:HEC:HMD3 | 2:D:42:PHE:CZ    | 0.51     | 2.40        | 15     | 1     |
| 2:D:108:ASN:ND2  | 2:D:108:ASN:O    | 0.51     | 2.44        | 8      | 2     |
| 2:B:103:PHE:O    | 3:B:147:HEC:HBB1 | 0.51     | 2.05        | 16     | 1     |
| 2:B:145:TYR:CD1  | 2:B:146:HIS:N    | 0.51     | 2.77        | 16     | 2     |
| 2:D:3:LEU:HD13   | 2:D:8:LYS:HB2    | 0.51     | 1.83        | 17     | 4     |
| 2:D:114:LEU:O    | 2:D:118:PHE:N    | 0.51     | 2.44        | 7      | 5     |
| 2:D:100:PRO:O    | 2:D:102:ASN:ND2  | 0.51     | 2.43        | 9      | 1     |
| 1:C:31:ARG:NH2   | 2:D:127:GLN:CB   | 0.51     | 2.73        | 4      | 1     |
| 2:D:14:LEU:HD12  | 2:D:14:LEU:N     | 0.51     | 2.20        | 20     | 1     |
| 2:B:28:LEU:N     | 2:B:28:LEU:HD12  | 0.51     | 2.20        | 17     | 1     |
| 1:A:109:LEU:O    | 1:A:113:LEU:O    | 0.51     | 2.29        | 14     | 8     |
| 1:A:113:LEU:O    | 1:A:113:LEU:CD1  | 0.51     | 2.58        | 2      | 2     |
| 2:B:145:TYR:CD1  | 2:B:145:TYR:C    | 0.51     | 2.83        | 18     | 3     |
| 2:B:15:TRP:NE1   | 2:B:72:SER:OG    | 0.51     | 2.43        | 15     | 1     |
| 2:B:42:PHE:CE1   | 2:B:45:PHE:CD2   | 0.51     | 2.98        | 8      | 1     |
| 2:B:80:ASN:N     | 2:B:80:ASN:HD22  | 0.51     | 2.03        | 14     | 1     |
| 1:C:103:HIS:N    | 1:C:103:HIS:ND1  | 0.51     | 2.58        | 7      | 1     |
| 1:C:98:PHE:CE1   | 1:C:102:SER:OG   | 0.51     | 2.63        | 7      | 1     |
| 1:A:83:LEU:O     | 1:A:86:LEU:N     | 0.51     | 2.42        | 4      | 2     |
| 2:D:139:ASN:N    | 2:D:139:ASN:OD1  | 0.51     | 2.42        | 17     | 2     |
| 1:A:103:HIS:HB3  | 2:B:108:ASN:HD21 | 0.51     | 1.65        | 10     | 1     |
| 1:A:117:PHE:CD2  | 1:A:117:PHE:O    | 0.51     | 2.64        | 7      | 2     |
| 2:D:3:LEU:HD21   | 2:D:133:VAL:HG22 | 0.51     | 1.81        | 15     | 4     |
| 2:B:38:THR:O     | 2:B:40:ARG:N     | 0.51     | 2.44        | 2      | 2     |
| 1:A:107:VAL:CG1  | 2:B:127:GLN:HE22 | 0.51     | 2.19        | 8      | 1     |
| 1:C:46:PHE:O     | 1:C:46:PHE:CG    | 0.51     | 2.64        | 11     | 3     |
| 2:D:103:PHE:O    | 3:D:147:HEC:HBB1 | 0.51     | 2.05        | 16     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:C:61:LYS:HB3   | 3:C:142:HEC:C4A  | 0.51     | 2.35        | 19     | 1     |
| 1:A:103:HIS:ND1  | 1:A:103:HIS:N    | 0.51     | 2.58        | 7      | 1     |
| 2:D:102:ASN:O    | 3:D:147:HEC:HMC2 | 0.51     | 2.06        | 2      | 1     |
| 2:B:99:ASP:OD1   | 1:C:94:ASP:CG    | 0.51     | 2.49        | 2      | 1     |
| 2:B:80:ASN:N     | 2:B:80:ASN:OD1   | 0.51     | 2.44        | 10     | 2     |
| 2:D:38:THR:O     | 2:D:40:ARG:N     | 0.51     | 2.44        | 2      | 2     |
| 1:C:36:PHE:CZ    | 1:C:100:LEU:HD22 | 0.51     | 2.41        | 16     | 1     |
| 2:B:107:GLY:O    | 2:B:109:VAL:N    | 0.51     | 2.44        | 19     | 1     |
| 2:D:17:LYS:O     | 2:D:118:PHE:CZ   | 0.51     | 2.65        | 9      | 4     |
| 1:A:34:LEU:O     | 1:A:36:PHE:N     | 0.51     | 2.44        | 6      | 1     |
| 1:A:38:THR:HA    | 2:D:97:HIS:ND1   | 0.51     | 2.21        | 7      | 1     |
| 1:C:113:LEU:CD1  | 1:C:113:LEU:O    | 0.51     | 2.59        | 2      | 2     |
| 1:A:105:LEU:HD11 | 1:A:125:LEU:HD13 | 0.51     | 1.82        | 13     | 1     |
| 1:A:58:HIS:ND1   | 1:A:58:HIS:C     | 0.50     | 2.65        | 18     | 4     |
| 1:C:95:PRO:O     | 1:C:98:PHE:N     | 0.50     | 2.41        | 4      | 8     |
| 2:D:116:HIS:ND1  | 2:D:116:HIS:C    | 0.50     | 2.62        | 20     | 6     |
| 1:C:99:LYS:O     | 1:C:103:HIS:ND1  | 0.50     | 2.44        | 15     | 1     |
| 1:C:48:LEU:HD12  | 1:C:48:LEU:N     | 0.50     | 2.20        | 8      | 1     |
| 2:D:145:TYR:C    | 2:D:145:TYR:CD1  | 0.50     | 2.83        | 19     | 2     |
| 1:A:66:LEU:HD12  | 1:A:66:LEU:C     | 0.50     | 2.25        | 17     | 2     |
| 1:C:117:PHE:HZ   | 2:D:116:HIS:CE1  | 0.50     | 2.18        | 4      | 1     |
| 1:A:124:SER:O    | 1:A:128:PHE:N    | 0.50     | 2.44        | 17     | 2     |
| 2:D:28:LEU:HD12  | 2:D:28:LEU:N     | 0.50     | 2.20        | 17     | 1     |
| 2:B:102:ASN:O    | 3:B:147:HEC:HMC2 | 0.50     | 2.06        | 2      | 1     |
| 1:C:109:LEU:O    | 1:C:113:LEU:O    | 0.50     | 2.29        | 14     | 8     |
| 2:B:144:LYS:O    | 2:B:146:HIS:ND1  | 0.50     | 2.44        | 11     | 5     |
| 1:C:100:LEU:O    | 1:C:104:CYS:SG   | 0.50     | 2.70        | 10     | 15    |
| 2:B:32:LEU:O     | 2:B:36:PRO:N     | 0.50     | 2.43        | 1      | 4     |
| 2:B:96:LEU:N     | 2:B:96:LEU:CD2   | 0.50     | 2.74        | 3      | 2     |
| 1:C:116:GLU:O    | 1:C:117:PHE:CB   | 0.50     | 2.60        | 5      | 5     |
| 1:A:106:LEU:CD2  | 1:A:106:LEU:N    | 0.50     | 2.74        | 19     | 2     |
| 1:A:101:LEU:HD22 | 3:A:142:HEC:CAB  | 0.50     | 2.36        | 9      | 2     |
| 1:A:87:HIS:O     | 1:A:93:VAL:N     | 0.50     | 2.44        | 9      | 1     |
| 2:B:14:LEU:HD12  | 2:B:14:LEU:N     | 0.50     | 2.20        | 20     | 1     |
| 2:B:117:HIS:HD1  | 2:B:117:HIS:N    | 0.50     | 2.03        | 12     | 1     |
| 1:C:32:MET:O     | 1:C:34:LEU:N     | 0.50     | 2.43        | 16     | 2     |
| 1:C:58:HIS:ND1   | 1:C:58:HIS:C     | 0.50     | 2.65        | 10     | 7     |
| 2:B:84:THR:HG23  | 2:B:85:PHE:N     | 0.50     | 2.22        | 8      | 13    |
| 1:C:2:LEU:O      | 1:C:3:SER:CB     | 0.50     | 2.59        | 10     | 1     |
| 1:C:86:LEU:HG    | 3:C:142:HEC:HBD1 | 0.50     | 1.82        | 7      | 1     |
| 2:D:63:HIS:CE1   | 3:D:147:HEC:O2A  | 0.50     | 2.63        | 5      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 2:B:142:ALA:O   | 2:B:146:HIS:N    | 0.50     | 2.44        | 17     | 1     |
| 1:C:66:LEU:HD12 | 1:C:66:LEU:C     | 0.50     | 2.25        | 17     | 1     |
| 1:A:119:PRO:HA  | 2:B:33:VAL:HG11  | 0.50     | 1.82        | 17     | 1     |
| 1:A:20:HIS:O    | 1:A:24:TYR:CE2   | 0.50     | 2.63        | 1      | 2     |
| 1:C:34:LEU:HD11 | 2:D:128:ALA:H    | 0.50     | 1.65        | 18     | 1     |
| 1:C:72:HIS:C    | 1:C:74:ASP:H     | 0.50     | 2.10        | 15     | 20    |
| 1:C:72:HIS:O    | 1:C:73:VAL:CG1   | 0.50     | 2.60        | 5      | 20    |
| 1:A:72:HIS:O    | 1:A:73:VAL:CG1   | 0.50     | 2.60        | 5      | 20    |
| 2:D:71:PHE:CE2  | 3:D:147:HEC:HMB1 | 0.50     | 2.42        | 5      | 2     |
| 1:C:76:MET:CE   | 1:C:131:SER:OG   | 0.50     | 2.60        | 4      | 5     |
| 2:D:115:ALA:O   | 2:D:119:GLY:CA   | 0.50     | 2.60        | 10     | 16    |
| 1:C:107:VAL:CG1 | 2:D:127:GLN:HE22 | 0.50     | 2.19        | 8      | 1     |
| 2:D:107:GLY:O   | 2:D:109:VAL:N    | 0.50     | 2.45        | 19     | 1     |
| 2:B:30:ARG:O    | 2:B:33:VAL:N     | 0.50     | 2.43        | 9      | 2     |
| 1:C:86:LEU:C    | 1:C:86:LEU:CD1   | 0.50     | 2.79        | 7      | 1     |
| 2:D:96:LEU:C    | 2:D:97:HIS:ND1   | 0.50     | 2.65        | 12     | 3     |
| 2:D:50:THR:HG1  | 2:D:52:ASP:CG    | 0.50     | 2.09        | 5      | 1     |
| 1:A:85:ASP:OD1  | 1:A:85:ASP:N     | 0.50     | 2.44        | 11     | 2     |
| 1:A:86:LEU:CD2  | 3:A:142:HEC:CBD  | 0.50     | 2.89        | 12     | 1     |
| 2:D:28:LEU:N    | 2:D:28:LEU:HD22  | 0.50     | 2.21        | 13     | 1     |
| 2:D:63:HIS:ND1  | 2:D:63:HIS:O     | 0.50     | 2.43        | 14     | 4     |
| 1:A:47:ASP:C    | 1:A:49:SER:H     | 0.50     | 2.10        | 14     | 9     |
| 1:A:21:ALA:C    | 1:A:23:GLU:N     | 0.50     | 2.65        | 5      | 16    |
| 2:B:71:PHE:CE2  | 3:B:147:HEC:HMB1 | 0.50     | 2.42        | 5      | 2     |
| 1:A:100:LEU:O   | 1:A:104:CYS:SG   | 0.50     | 2.68        | 6      | 13    |
| 1:C:32:MET:HE1  | 3:C:142:HEC:HBC2 | 0.50     | 1.82        | 19     | 1     |
| 1:C:34:LEU:O    | 1:C:36:PHE:N     | 0.50     | 2.44        | 6      | 1     |
| 2:B:127:GLN:CD  | 2:B:127:GLN:H    | 0.50     | 2.09        | 20     | 1     |
| 2:D:96:LEU:N    | 2:D:96:LEU:CD2   | 0.50     | 2.74        | 3      | 1     |
| 1:A:126:ASP:OD2 | 2:B:35:TYR:OH    | 0.50     | 2.25        | 17     | 1     |
| 2:B:21:ASP:OD1  | 2:B:65:LYS:NZ    | 0.50     | 2.43        | 12     | 1     |
| 1:A:128:PHE:O   | 1:A:128:PHE:CD1  | 0.50     | 2.65        | 10     | 5     |
| 2:D:41:PHE:HE1  | 3:D:147:HEC:NB   | 0.50     | 2.02        | 15     | 1     |
| 1:A:46:PHE:O    | 1:A:46:PHE:CG    | 0.50     | 2.64        | 11     | 3     |
| 1:C:99:LYS:N    | 1:C:99:LYS:CD    | 0.50     | 2.75        | 7      | 1     |
| 1:A:53:ALA:O    | 1:A:56:LYS:N     | 0.50     | 2.42        | 13     | 3     |
| 1:C:53:ALA:O    | 1:C:56:LYS:N     | 0.50     | 2.42        | 13     | 2     |
| 2:B:33:VAL:CG1  | 2:B:34:VAL:N     | 0.50     | 2.75        | 3      | 2     |
| 2:B:97:HIS:O    | 1:C:38:THR:HG22  | 0.50     | 2.07        | 3      | 1     |
| 1:C:33:PHE:HE1  | 3:C:142:HEC:ND   | 0.50     | 2.04        | 12     | 1     |
| 1:C:1:VAL:CG1   | 1:C:131:SER:OG   | 0.50     | 2.60        | 12     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:C:93:VAL:CG2  | 1:C:94:ASP:N    | 0.50     | 2.75        | 13     | 1     |
| 1:C:52:SER:C    | 1:C:54:GLN:N    | 0.50     | 2.65        | 1      | 2     |
| 2:B:14:LEU:O    | 2:B:16:GLY:N    | 0.50     | 2.45        | 2      | 6     |
| 2:D:4:THR:O     | 2:D:6:GLU:N     | 0.50     | 2.45        | 14     | 7     |
| 2:B:4:THR:O     | 2:B:6:GLU:N     | 0.50     | 2.45        | 14     | 6     |
| 1:A:99:LYS:O    | 1:A:103:HIS:ND1 | 0.50     | 2.44        | 15     | 1     |
| 2:B:99:ASP:O    | 2:B:100:PRO:O   | 0.50     | 2.30        | 17     | 5     |
| 2:B:108:ASN:O   | 2:B:108:ASN:ND2 | 0.50     | 2.44        | 8      | 2     |
| 1:C:87:HIS:O    | 1:C:93:VAL:N    | 0.50     | 2.44        | 9      | 1     |
| 2:B:96:LEU:C    | 2:B:97:HIS:ND1  | 0.50     | 2.65        | 12     | 3     |
| 1:A:56:LYS:H    | 1:A:56:LYS:CD   | 0.50     | 2.20        | 5      | 1     |
| 1:A:1:VAL:CG1   | 1:A:131:SER:OG  | 0.50     | 2.60        | 12     | 1     |
| 1:A:93:VAL:CG2  | 1:A:94:ASP:N    | 0.50     | 2.75        | 13     | 1     |
| 1:C:119:PRO:HB3 | 2:D:51:PRO:HB3  | 0.50     | 1.83        | 11     | 1     |
| 1:C:34:LEU:HD12 | 1:C:34:LEU:C    | 0.50     | 2.27        | 2      | 1     |
| 2:B:143:HIS:O   | 2:B:146:HIS:CD2 | 0.50     | 2.65        | 18     | 1     |
| 1:A:58:HIS:ND1  | 1:A:58:HIS:O    | 0.50     | 2.45        | 18     | 3     |
| 2:B:8:LYS:O     | 2:B:12:THR:OG1  | 0.50     | 2.29        | 8      | 14    |
| 1:A:18:GLY:C    | 1:A:20:HIS:H    | 0.50     | 2.10        | 16     | 18    |
| 2:D:55:MET:N    | 2:D:55:MET:SD   | 0.50     | 2.85        | 8      | 4     |
| 2:D:96:LEU:HD22 | 2:D:96:LEU:N    | 0.50     | 2.22        | 16     | 1     |
| 1:A:116:GLU:O   | 1:A:117:PHE:CB  | 0.50     | 2.60        | 5      | 5     |
| 2:B:134:VAL:O   | 2:B:137:VAL:N   | 0.50     | 2.45        | 9      | 7     |
| 2:B:114:LEU:O   | 2:B:118:PHE:N   | 0.50     | 2.44        | 7      | 6     |
| 1:A:118:THR:OG1 | 1:A:121:VAL:HB  | 0.50     | 2.07        | 20     | 6     |
| 2:B:97:HIS:CB   | 1:C:38:THR:HA   | 0.50     | 2.34        | 4      | 1     |
| 1:A:119:PRO:HB3 | 2:B:51:PRO:HB3  | 0.50     | 1.83        | 11     | 1     |
| 1:C:2:LEU:CD1   | 1:C:2:LEU:N     | 0.50     | 2.75        | 2      | 1     |
| 2:D:67:VAL:HG13 | 3:D:147:HEC:C3B | 0.50     | 2.34        | 18     | 1     |
| 1:A:73:VAL:O    | 1:A:73:VAL:HG22 | 0.50     | 2.07        | 6      | 9     |
| 2:D:145:TYR:CD1 | 2:D:145:TYR:C   | 0.50     | 2.84        | 16     | 4     |
| 1:C:18:GLY:C    | 1:C:20:HIS:H    | 0.50     | 2.10        | 16     | 17    |
| 1:C:11:LYS:N    | 1:C:11:LYS:CD   | 0.50     | 2.75        | 15     | 3     |
| 2:D:63:HIS:HE1  | 3:D:147:HEC:C2A | 0.50     | 2.19        | 16     | 1     |
| 2:B:28:LEU:HD22 | 2:B:28:LEU:N    | 0.50     | 2.21        | 13     | 2     |
| 2:B:94:ASP:O    | 1:C:41:THR:HG21 | 0.50     | 2.07        | 6      | 1     |
| 1:A:35:SER:OG   | 1:A:36:PHE:CD2  | 0.50     | 2.62        | 7      | 1     |
| 1:C:3:SER:N     | 1:C:6:ASP:OD2   | 0.50     | 2.40        | 20     | 2     |
| 2:D:106:LEU:CB  | 3:D:147:HEC:HAB | 0.50     | 2.37        | 13     | 1     |
| 1:A:96:VAL:CG1  | 2:D:99:ASP:CG   | 0.50     | 2.53        | 11     | 1     |
| 2:B:106:LEU:CD1 | 2:B:106:LEU:C   | 0.49     | 2.81        | 18     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:C:47:ASP:C     | 1:C:49:SER:H     | 0.49     | 2.10        | 14     | 8     |
| 2:D:84:THR:HG23  | 2:D:85:PHE:N     | 0.49     | 2.22        | 8      | 13    |
| 2:B:115:ALA:O    | 2:B:119:GLY:CA   | 0.49     | 2.60        | 6      | 15    |
| 2:B:55:MET:N     | 2:B:55:MET:SD    | 0.49     | 2.85        | 8      | 3     |
| 2:D:48:LEU:CD1   | 2:D:48:LEU:N     | 0.49     | 2.74        | 16     | 1     |
| 1:A:98:PHE:C     | 1:A:98:PHE:CD1   | 0.49     | 2.85        | 6      | 2     |
| 2:B:80:ASN:OD1   | 2:B:80:ASN:N     | 0.49     | 2.42        | 19     | 1     |
| 1:C:17:VAL:CG1   | 1:C:21:ALA:HB2   | 0.49     | 2.37        | 1      | 1     |
| 2:D:42:PHE:C     | 3:D:147:HEC:C3A  | 0.49     | 2.81        | 12     | 1     |
| 2:B:106:LEU:CB   | 3:B:147:HEC:HAB  | 0.49     | 2.37        | 13     | 1     |
| 1:C:73:VAL:O     | 1:C:73:VAL:HG22  | 0.49     | 2.07        | 6      | 10    |
| 2:D:143:HIS:O    | 2:D:146:HIS:CD2  | 0.49     | 2.65        | 18     | 1     |
| 2:B:19:ASN:O     | 2:B:22:GLU:N     | 0.49     | 2.42        | 9      | 7     |
| 2:D:131:GLN:H    | 2:D:131:GLN:CD   | 0.49     | 2.10        | 15     | 1     |
| 2:B:97:HIS:CD2   | 1:C:38:THR:CG2   | 0.49     | 2.96        | 1      | 1     |
| 1:A:17:VAL:CG1   | 1:A:21:ALA:HB2   | 0.49     | 2.37        | 1      | 1     |
| 2:D:120:LYS:CD   | 2:D:120:LYS:N    | 0.49     | 2.75        | 11     | 1     |
| 1:C:21:ALA:C     | 1:C:23:GLU:N     | 0.49     | 2.65        | 18     | 16    |
| 1:C:128:PHE:O    | 1:C:128:PHE:CD1  | 0.49     | 2.65        | 10     | 9     |
| 1:A:76:MET:CE    | 1:A:131:SER:OG   | 0.49     | 2.61        | 12     | 5     |
| 2:B:40:ARG:HG3   | 1:C:92:ARG:CZ    | 0.49     | 2.37        | 15     | 1     |
| 2:B:131:GLN:O    | 2:B:135:ALA:HB2  | 0.49     | 2.07        | 15     | 4     |
| 1:A:49:SER:C     | 1:A:50:HIS:CG    | 0.49     | 2.85        | 19     | 1     |
| 1:C:118:THR:OG1  | 1:C:121:VAL:HB   | 0.49     | 2.07        | 20     | 6     |
| 2:B:37:TRP:N     | 2:B:37:TRP:CD1   | 0.49     | 2.79        | 20     | 2     |
| 2:B:95:LYS:CA    | 2:B:97:HIS:NE2   | 0.49     | 2.75        | 15     | 1     |
| 1:C:101:LEU:HD22 | 3:C:142:HEC:CAB  | 0.49     | 2.36        | 9      | 2     |
| 1:A:50:HIS:N     | 1:A:50:HIS:ND1   | 0.49     | 2.60        | 5      | 2     |
| 1:C:101:LEU:HD11 | 3:C:142:HEC:CHC  | 0.49     | 2.32        | 7      | 1     |
| 1:A:99:LYS:N     | 1:A:99:LYS:CD    | 0.49     | 2.75        | 7      | 1     |
| 1:C:108:THR:OG1  | 1:C:109:LEU:N    | 0.49     | 2.45        | 20     | 1     |
| 1:C:33:PHE:HE1   | 3:C:142:HEC:C4D  | 0.49     | 2.20        | 12     | 1     |
| 2:D:39:GLN:HG2   | 3:D:147:HEC:C4B  | 0.49     | 2.32        | 12     | 1     |
| 1:A:93:VAL:CG1   | 1:A:94:ASP:H     | 0.49     | 2.21        | 18     | 1     |
| 1:A:92:ARG:CZ    | 2:D:40:ARG:HD2   | 0.49     | 2.38        | 18     | 1     |
| 1:C:118:THR:C    | 1:C:120:ALA:N    | 0.49     | 2.64        | 18     | 12    |
| 1:A:118:THR:C    | 1:A:120:ALA:N    | 0.49     | 2.64        | 18     | 18    |
| 2:B:131:GLN:CD   | 2:B:131:GLN:H    | 0.49     | 2.10        | 15     | 1     |
| 1:A:106:LEU:N    | 1:A:106:LEU:HD12 | 0.49     | 2.21        | 17     | 1     |
| 1:A:56:LYS:CD    | 1:A:56:LYS:H     | 0.49     | 2.21        | 1      | 1     |
| 2:B:63:HIS:O     | 2:B:63:HIS:ND1   | 0.49     | 2.43        | 10     | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:50:HIS:CD2   | 1:A:50:HIS:N     | 0.49     | 2.81        | 19     | 2     |
| 1:C:50:HIS:N     | 1:C:50:HIS:CD2   | 0.49     | 2.81        | 19     | 2     |
| 2:D:8:LYS:O      | 2:D:12:THR:OG1   | 0.49     | 2.30        | 16     | 15    |
| 1:C:1:VAL:O      | 1:C:2:LEU:CB     | 0.49     | 2.60        | 10     | 2     |
| 1:C:27:GLU:OE1   | 1:C:112:HIS:CD2  | 0.49     | 2.66        | 10     | 1     |
| 2:D:131:GLN:O    | 2:D:135:ALA:HB2  | 0.49     | 2.07        | 15     | 4     |
| 1:A:115:ALA:C    | 1:A:117:PHE:N    | 0.49     | 2.64        | 15     | 2     |
| 1:A:99:LYS:CB    | 1:A:99:LYS:NZ    | 0.49     | 2.76        | 16     | 2     |
| 1:A:46:PHE:O     | 1:A:48:LEU:CD2   | 0.49     | 2.61        | 14     | 1     |
| 1:C:49:SER:C     | 1:C:50:HIS:CG    | 0.49     | 2.85        | 19     | 1     |
| 1:A:129:LEU:C    | 1:A:129:LEU:CD1  | 0.49     | 2.80        | 20     | 1     |
| 2:D:96:LEU:N     | 2:D:96:LEU:HD22  | 0.49     | 2.22        | 3      | 1     |
| 1:C:33:PHE:CE1   | 3:C:142:HEC:ND   | 0.49     | 2.81        | 12     | 1     |
| 1:A:106:LEU:N    | 1:A:106:LEU:CD1  | 0.49     | 2.76        | 17     | 2     |
| 1:C:10:VAL:HG21  | 1:C:128:PHE:CG   | 0.49     | 2.43        | 9      | 2     |
| 2:D:23:VAL:O     | 2:D:27:ALA:N     | 0.49     | 2.41        | 5      | 1     |
| 2:D:127:GLN:CD   | 2:D:127:GLN:H    | 0.49     | 2.09        | 20     | 1     |
| 2:B:43:GLU:OE2   | 1:C:92:ARG:NH1   | 0.49     | 2.46        | 20     | 1     |
| 1:C:119:PRO:HA   | 2:D:33:VAL:HG11  | 0.49     | 1.82        | 17     | 1     |
| 2:D:106:LEU:HD21 | 3:D:147:HEC:C3B  | 0.49     | 2.37        | 2      | 1     |
| 1:A:32:MET:CE    | 3:A:142:HEC:HBC2 | 0.49     | 2.38        | 2      | 3     |
| 1:C:61:LYS:O     | 3:C:142:HEC:CMA  | 0.49     | 2.61        | 9      | 4     |
| 2:B:96:LEU:HD22  | 2:B:96:LEU:N     | 0.49     | 2.22        | 16     | 2     |
| 1:C:46:PHE:O     | 1:C:48:LEU:CD2   | 0.49     | 2.61        | 14     | 1     |
| 2:D:134:VAL:O    | 2:D:137:VAL:N    | 0.49     | 2.45        | 9      | 7     |
| 2:B:17:LYS:O     | 2:B:118:PHE:CZ   | 0.49     | 2.64        | 9      | 4     |
| 2:D:95:LYS:N     | 2:D:95:LYS:CD    | 0.49     | 2.76        | 6      | 2     |
| 2:B:120:LYS:CD   | 2:B:120:LYS:N    | 0.49     | 2.75        | 11     | 1     |
| 2:B:106:LEU:HD21 | 3:B:147:HEC:C3B  | 0.49     | 2.37        | 2      | 1     |
| 1:A:34:LEU:C     | 1:A:34:LEU:HD12  | 0.49     | 2.27        | 2      | 1     |
| 1:A:86:LEU:O     | 1:A:90:LYS:O     | 0.49     | 2.31        | 8      | 7     |
| 2:D:95:LYS:CA    | 2:D:97:HIS:NE2   | 0.49     | 2.76        | 15     | 1     |
| 1:A:116:GLU:C    | 1:A:117:PHE:CG   | 0.49     | 2.86        | 14     | 3     |
| 2:D:99:ASP:O     | 2:D:100:PRO:O    | 0.49     | 2.31        | 15     | 5     |
| 1:C:98:PHE:CD1   | 1:C:98:PHE:C     | 0.49     | 2.85        | 19     | 2     |
| 1:A:10:VAL:HG21  | 1:A:128:PHE:CG   | 0.49     | 2.43        | 9      | 1     |
| 2:B:42:PHE:C     | 2:B:44:SER:N     | 0.49     | 2.66        | 7      | 2     |
| 1:C:105:LEU:CD1  | 1:C:105:LEU:C    | 0.49     | 2.80        | 13     | 1     |
| 1:A:2:LEU:CD1    | 1:A:2:LEU:N      | 0.49     | 2.75        | 2      | 2     |
| 1:A:92:ARG:NH1   | 2:D:40:ARG:CB    | 0.49     | 2.69        | 18     | 1     |
| 2:D:93:CYS:SG    | 2:D:94:ASP:OD2   | 0.49     | 2.71        | 10     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:D:95:LYS:C     | 2:D:97:HIS:NE2   | 0.49     | 2.66        | 15     | 1     |
| 1:A:116:GLU:C    | 1:A:117:PHE:CD2  | 0.49     | 2.87        | 14     | 2     |
| 1:A:93:VAL:O     | 2:D:40:ARG:CZ    | 0.49     | 2.61        | 14     | 1     |
| 1:C:113:LEU:HD13 | 1:C:113:LEU:C    | 0.49     | 2.28        | 7      | 2     |
| 1:C:36:PHE:CD1   | 1:C:100:LEU:HD13 | 0.49     | 2.43        | 5      | 1     |
| 1:A:108:THR:OG1  | 1:A:109:LEU:N    | 0.49     | 2.45        | 20     | 1     |
| 2:D:94:ASP:N     | 2:D:94:ASP:OD1   | 0.49     | 2.46        | 3      | 1     |
| 1:C:118:THR:OG1  | 1:C:121:VAL:N    | 0.48     | 2.43        | 12     | 4     |
| 1:C:86:LEU:O     | 1:C:90:LYS:O     | 0.48     | 2.31        | 8      | 7     |
| 1:A:1:VAL:O      | 1:A:2:LEU:CB     | 0.48     | 2.60        | 10     | 2     |
| 1:A:27:GLU:OE1   | 1:A:112:HIS:CD2  | 0.48     | 2.66        | 10     | 1     |
| 2:B:36:PRO:O     | 2:B:38:THR:N     | 0.48     | 2.46        | 15     | 2     |
| 2:B:95:LYS:C     | 2:B:97:HIS:NE2   | 0.48     | 2.67        | 15     | 1     |
| 1:C:115:ALA:C    | 1:C:117:PHE:N    | 0.48     | 2.63        | 15     | 2     |
| 1:A:2:LEU:CD1    | 1:A:128:PHE:CD2  | 0.48     | 2.96        | 16     | 2     |
| 1:A:95:PRO:C     | 1:A:97:ASN:H     | 0.48     | 2.12        | 13     | 4     |
| 1:A:61:LYS:HB3   | 3:A:142:HEC:HMA3 | 0.48     | 1.84        | 2      | 1     |
| 2:B:144:LYS:C    | 2:B:146:HIS:N    | 0.48     | 2.67        | 19     | 7     |
| 2:D:28:LEU:N     | 2:D:28:LEU:CD1   | 0.48     | 2.76        | 18     | 1     |
| 1:C:5:ALA:O      | 1:C:6:ASP:C      | 0.48     | 2.51        | 10     | 19    |
| 1:A:94:ASP:OD2   | 2:D:97:HIS:CE1   | 0.48     | 2.67        | 10     | 1     |
| 1:C:116:GLU:C    | 1:C:117:PHE:CG   | 0.48     | 2.86        | 14     | 3     |
| 2:B:48:LEU:CD1   | 2:B:48:LEU:N     | 0.48     | 2.77        | 14     | 2     |
| 2:B:63:HIS:HE1   | 3:B:147:HEC:C2A  | 0.48     | 2.19        | 16     | 1     |
| 2:B:95:LYS:N     | 2:B:95:LYS:CD    | 0.48     | 2.76        | 6      | 1     |
| 2:B:146:HIS:OXT  | 2:B:146:HIS:ND1  | 0.48     | 2.46        | 4      | 2     |
| 1:C:95:PRO:C     | 1:C:97:ASN:H     | 0.48     | 2.11        | 13     | 4     |
| 2:D:66:LYS:CB    | 3:D:147:HEC:HBA2 | 0.48     | 2.38        | 17     | 1     |
| 2:B:40:ARG:HB3   | 1:C:92:ARG:HD3   | 0.48     | 1.84        | 17     | 1     |
| 2:B:146:HIS:HE2  | 2:D:136:GLY:N    | 0.48     | 2.05        | 17     | 1     |
| 1:C:124:SER:O    | 1:C:128:PHE:N    | 0.48     | 2.44        | 17     | 2     |
| 1:C:56:LYS:CD    | 1:C:56:LYS:H     | 0.48     | 2.21        | 1      | 1     |
| 1:C:48:LEU:HD12  | 3:C:142:HEC:HHA  | 0.48     | 1.82        | 12     | 1     |
| 1:A:113:LEU:O    | 1:A:113:LEU:CG   | 0.48     | 2.61        | 2      | 1     |
| 1:C:40:LYS:O     | 1:C:41:THR:C     | 0.48     | 2.52        | 18     | 2     |
| 2:D:87:THR:O     | 2:D:91:LEU:N     | 0.48     | 2.47        | 12     | 3     |
| 1:A:31:ARG:HH21  | 2:B:127:GLN:CB   | 0.48     | 2.18        | 15     | 1     |
| 2:B:42:PHE:CZ    | 2:B:45:PHE:CZ    | 0.48     | 3.01        | 16     | 1     |
| 2:D:17:LYS:O     | 2:D:118:PHE:CE2  | 0.48     | 2.67        | 9      | 2     |
| 2:D:52:ASP:N     | 2:D:52:ASP:OD1   | 0.48     | 2.46        | 9      | 1     |
| 1:A:31:ARG:O     | 1:A:34:LEU:CD2   | 0.48     | 2.61        | 1      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:129:LEU:HD21 | 3:A:142:HEC:HBB1 | 0.48     | 1.85        | 13     | 1     |
| 1:C:85:ASP:N     | 1:C:85:ASP:OD1   | 0.48     | 2.44        | 11     | 1     |
| 1:C:113:LEU:CG   | 1:C:113:LEU:O    | 0.48     | 2.61        | 20     | 2     |
| 2:D:19:ASN:C     | 2:D:21:ASP:N     | 0.48     | 2.66        | 16     | 13    |
| 2:B:93:CYS:SG    | 2:B:94:ASP:OD2   | 0.48     | 2.71        | 10     | 1     |
| 2:B:40:ARG:CG    | 1:C:92:ARG:CZ    | 0.48     | 2.91        | 15     | 1     |
| 2:D:42:PHE:CZ    | 2:D:45:PHE:CZ    | 0.48     | 3.01        | 16     | 1     |
| 2:D:28:LEU:HD22  | 2:D:28:LEU:N     | 0.48     | 2.21        | 16     | 1     |
| 1:C:2:LEU:CD1    | 1:C:128:PHE:CD2  | 0.48     | 2.96        | 16     | 2     |
| 1:C:101:LEU:C    | 1:C:101:LEU:HD23 | 0.48     | 2.29        | 19     | 1     |
| 1:C:32:MET:C     | 1:C:32:MET:SD    | 0.48     | 2.92        | 6      | 1     |
| 1:A:96:VAL:HG11  | 2:D:99:ASP:OD1   | 0.48     | 2.07        | 6      | 1     |
| 1:A:11:LYS:N     | 1:A:11:LYS:CD    | 0.48     | 2.75        | 1      | 1     |
| 1:C:21:ALA:HB1   | 1:C:63:ALA:HB1   | 0.48     | 1.85        | 2      | 2     |
| 2:B:40:ARG:HD2   | 1:C:92:ARG:CZ    | 0.48     | 2.38        | 18     | 1     |
| 2:B:19:ASN:C     | 2:B:21:ASP:N     | 0.48     | 2.66        | 16     | 13    |
| 2:D:48:LEU:N     | 2:D:48:LEU:HD12  | 0.48     | 2.22        | 10     | 1     |
| 2:D:48:LEU:N     | 2:D:48:LEU:CD1   | 0.48     | 2.76        | 14     | 3     |
| 1:A:91:LEU:C     | 1:A:93:VAL:N     | 0.48     | 2.67        | 20     | 8     |
| 1:A:101:LEU:C    | 1:A:101:LEU:HD23 | 0.48     | 2.29        | 19     | 1     |
| 1:C:131:SER:O    | 1:C:135:VAL:HG23 | 0.48     | 2.09        | 19     | 2     |
| 2:B:119:GLY:O    | 2:B:122:PHE:N    | 0.48     | 2.47        | 19     | 2     |
| 2:B:8:LYS:C      | 2:B:8:LYS:CD     | 0.48     | 2.81        | 9      | 1     |
| 1:C:98:PHE:C     | 1:C:98:PHE:CD1   | 0.48     | 2.85        | 6      | 1     |
| 2:D:42:PHE:C     | 2:D:44:SER:N     | 0.48     | 2.66        | 7      | 2     |
| 2:B:72:SER:O     | 2:B:76:ALA:HB3   | 0.48     | 2.09        | 4      | 1     |
| 2:D:33:VAL:CG1   | 2:D:34:VAL:N     | 0.48     | 2.77        | 11     | 2     |
| 2:B:66:LYS:CB    | 3:B:147:HEC:HBA2 | 0.48     | 2.38        | 17     | 1     |
| 2:B:135:ALA:HB3  | 2:D:146:HIS:CE1  | 0.48     | 2.43        | 17     | 1     |
| 2:B:40:ARG:NH2   | 1:C:92:ARG:HB2   | 0.48     | 2.22        | 18     | 1     |
| 2:B:40:ARG:NE    | 1:C:92:ARG:HB3   | 0.48     | 2.23        | 18     | 1     |
| 2:D:106:LEU:C    | 2:D:106:LEU:CD1  | 0.48     | 2.81        | 18     | 1     |
| 1:A:47:ASP:C     | 1:A:49:SER:N     | 0.48     | 2.67        | 20     | 12    |
| 1:A:52:SER:C     | 1:A:54:GLN:N     | 0.48     | 2.65        | 1      | 2     |
| 1:C:32:MET:CE    | 3:C:142:HEC:HBC2 | 0.48     | 2.38        | 2      | 3     |
| 1:A:95:PRO:C     | 1:A:97:ASN:N     | 0.48     | 2.66        | 10     | 8     |
| 2:D:36:PRO:O     | 2:D:38:THR:N     | 0.48     | 2.46        | 15     | 2     |
| 1:C:99:LYS:CB    | 1:C:99:LYS:NZ    | 0.48     | 2.76        | 16     | 1     |
| 1:A:106:LEU:HD22 | 1:A:106:LEU:N    | 0.48     | 2.22        | 19     | 2     |
| 2:B:17:LYS:O     | 2:B:118:PHE:CE2  | 0.48     | 2.67        | 9      | 2     |
| 1:C:109:LEU:O    | 1:C:114:PRO:N    | 0.48     | 2.47        | 6      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:C:126:ASP:OD2  | 2:D:35:TYR:OH    | 0.48     | 2.25        | 17     | 1     |
| 1:C:31:ARG:O     | 1:C:34:LEU:CD2   | 0.48     | 2.61        | 1      | 1     |
| 1:C:32:MET:HE1   | 3:C:142:HEC:C3B  | 0.48     | 2.39        | 12     | 1     |
| 1:C:32:MET:HE1   | 3:C:142:HEC:CAB  | 0.48     | 2.30        | 12     | 1     |
| 1:A:113:LEU:CG   | 1:A:113:LEU:O    | 0.48     | 2.61        | 20     | 3     |
| 1:C:95:PRO:C     | 1:C:97:ASN:N     | 0.48     | 2.67        | 10     | 10    |
| 2:D:37:TRP:NE1   | 2:D:38:THR:HG23  | 0.48     | 2.24        | 5      | 4     |
| 3:B:147:HEC:HBA2 | 2:D:66:LYS:HB3   | 0.48     | 1.84        | 15     | 1     |
| 2:B:95:LYS:C     | 2:B:97:HIS:CD2   | 0.48     | 2.87        | 15     | 1     |
| 1:A:128:PHE:CD1  | 1:A:128:PHE:O    | 0.48     | 2.67        | 19     | 8     |
| 2:B:40:ARG:HH12  | 1:C:92:ARG:C     | 0.48     | 2.12        | 14     | 1     |
| 2:D:76:ALA:C     | 2:D:77:HIS:CG    | 0.48     | 2.86        | 14     | 1     |
| 2:D:88:LEU:N     | 2:D:88:LEU:HD12  | 0.48     | 2.24        | 14     | 1     |
| 1:A:131:SER:O    | 1:A:135:VAL:HG23 | 0.48     | 2.09        | 19     | 2     |
| 1:A:46:PHE:C     | 1:A:46:PHE:CD1   | 0.48     | 2.85        | 9      | 3     |
| 1:A:36:PHE:CD1   | 1:A:100:LEU:HD13 | 0.48     | 2.43        | 5      | 1     |
| 2:B:45:PHE:C     | 2:B:47:ASP:N     | 0.48     | 2.66        | 5      | 1     |
| 2:B:50:THR:HG1   | 2:B:52:ASP:CG    | 0.48     | 2.12        | 5      | 2     |
| 1:C:27:GLU:CD    | 1:C:112:HIS:CE1  | 0.48     | 2.87        | 3      | 1     |
| 1:C:115:ALA:O    | 1:C:121:VAL:CG2  | 0.48     | 2.60        | 1      | 1     |
| 1:A:38:THR:CG2   | 2:D:97:HIS:CD2   | 0.48     | 2.97        | 1      | 1     |
| 2:D:39:GLN:NE2   | 3:D:147:HEC:NB   | 0.48     | 2.61        | 12     | 1     |
| 2:B:63:HIS:HE1   | 3:B:147:HEC:HHA  | 0.48     | 1.64        | 12     | 1     |
| 1:C:129:LEU:HD21 | 3:C:142:HEC:HBB1 | 0.48     | 1.85        | 13     | 1     |
| 1:C:93:VAL:CG2   | 1:C:94:ASP:H     | 0.48     | 2.17        | 13     | 1     |
| 1:C:47:ASP:C     | 1:C:49:SER:N     | 0.48     | 2.67        | 9      | 13    |
| 1:C:46:PHE:C     | 1:C:48:LEU:N     | 0.48     | 2.67        | 10     | 5     |
| 2:D:96:LEU:N     | 2:D:96:LEU:HD12  | 0.48     | 2.23        | 9      | 2     |
| 2:B:31:LEU:HD21  | 3:B:147:HEC:HBC2 | 0.48     | 1.86        | 10     | 1     |
| 1:A:6:ASP:OD1    | 1:A:7:LYS:N      | 0.48     | 2.47        | 10     | 1     |
| 1:C:83:LEU:O     | 1:C:87:HIS:CE1   | 0.48     | 2.67        | 10     | 3     |
| 1:A:35:SER:C     | 1:A:36:PHE:CD2   | 0.48     | 2.87        | 15     | 1     |
| 2:D:20:VAL:O     | 2:D:22:GLU:N     | 0.48     | 2.47        | 15     | 1     |
| 2:B:20:VAL:O     | 2:B:22:GLU:N     | 0.48     | 2.47        | 15     | 1     |
| 1:A:61:LYS:O     | 3:A:142:HEC:CMA  | 0.48     | 2.61        | 9      | 4     |
| 1:A:6:ASP:OD1    | 1:A:6:ASP:N      | 0.48     | 2.46        | 16     | 1     |
| 2:D:8:LYS:CD     | 2:D:8:LYS:C      | 0.48     | 2.81        | 9      | 1     |
| 2:B:52:ASP:OD1   | 2:B:52:ASP:N     | 0.48     | 2.46        | 9      | 1     |
| 1:C:129:LEU:O    | 1:C:129:LEU:HD12 | 0.48     | 2.08        | 6      | 1     |
| 2:B:94:ASP:N     | 2:B:94:ASP:OD1   | 0.48     | 2.46        | 3      | 3     |
| 1:A:92:ARG:NH1   | 2:D:40:ARG:HA    | 0.48     | 2.24        | 12     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:120:ALA:O    | 1:A:124:SER:CB   | 0.48     | 2.62        | 18     | 1     |
| 2:D:144:LYS:C    | 2:D:146:HIS:N    | 0.48     | 2.67        | 16     | 7     |
| 1:A:5:ALA:O      | 1:A:6:ASP:C      | 0.48     | 2.51        | 10     | 19    |
| 2:D:31:LEU:HD21  | 3:D:147:HEC:HBC2 | 0.48     | 1.86        | 10     | 1     |
| 1:C:6:ASP:OD1    | 1:C:7:LYS:N      | 0.48     | 2.47        | 10     | 1     |
| 1:A:83:LEU:O     | 1:A:87:HIS:CE1   | 0.48     | 2.67        | 10     | 3     |
| 1:C:116:GLU:C    | 1:C:117:PHE:CD2  | 0.48     | 2.87        | 14     | 2     |
| 1:C:3:SER:CB     | 1:C:4:PRO:CD     | 0.48     | 2.92        | 15     | 4     |
| 1:C:52:SER:O     | 1:C:53:ALA:CB    | 0.48     | 2.61        | 3      | 7     |
| 2:B:76:ALA:C     | 2:B:77:HIS:CG    | 0.48     | 2.86        | 14     | 1     |
| 1:C:100:LEU:O    | 1:C:104:CYS:N    | 0.48     | 2.46        | 19     | 1     |
| 2:B:103:PHE:N    | 2:B:103:PHE:CD1  | 0.48     | 2.81        | 5      | 3     |
| 2:D:45:PHE:C     | 2:D:47:ASP:N     | 0.48     | 2.66        | 5      | 1     |
| 2:D:71:PHE:CZ    | 2:D:134:VAL:HG11 | 0.48     | 2.44        | 3      | 1     |
| 1:C:61:LYS:HB3   | 3:C:142:HEC:HMA3 | 0.48     | 1.84        | 2      | 1     |
| 1:C:120:ALA:O    | 1:C:124:SER:CB   | 0.48     | 2.62        | 18     | 1     |
| 2:B:124:PRO:N    | 2:B:125:PRO:CD   | 0.48     | 2.77        | 15     | 2     |
| 2:B:37:TRP:NE1   | 2:B:38:THR:HG23  | 0.48     | 2.24        | 5      | 3     |
| 1:C:109:LEU:C    | 1:C:109:LEU:CD1  | 0.48     | 2.81        | 16     | 1     |
| 2:D:82:LYS:HZ1   | 2:D:143:HIS:CD2  | 0.48     | 2.27        | 20     | 1     |
| 1:A:27:GLU:CD    | 1:A:112:HIS:CE1  | 0.48     | 2.87        | 3      | 1     |
| 2:B:88:LEU:HD12  | 2:B:88:LEU:N     | 0.47     | 2.24        | 14     | 3     |
| 2:B:28:LEU:CD1   | 2:B:28:LEU:N     | 0.47     | 2.75        | 18     | 1     |
| 2:B:117:HIS:C    | 2:B:118:PHE:CG   | 0.47     | 2.87        | 17     | 6     |
| 1:A:124:SER:O    | 1:A:128:PHE:CB   | 0.47     | 2.62        | 13     | 9     |
| 1:C:35:SER:C     | 1:C:36:PHE:CD2   | 0.47     | 2.87        | 15     | 1     |
| 1:A:127:LYS:C    | 1:A:127:LYS:CD   | 0.47     | 2.82        | 8      | 11    |
| 2:B:96:LEU:HD12  | 2:B:98:VAL:HG23  | 0.47     | 1.87        | 6      | 2     |
| 2:D:106:LEU:C    | 2:D:106:LEU:HD23 | 0.47     | 2.30        | 9      | 1     |
| 2:D:106:LEU:HD13 | 3:D:147:HEC:HAB  | 0.47     | 1.85        | 3      | 2     |
| 2:D:43:GLU:CD    | 2:D:44:SER:N     | 0.47     | 2.67        | 9      | 1     |
| 2:B:43:GLU:CD    | 2:B:44:SER:N     | 0.47     | 2.67        | 9      | 1     |
| 2:B:57:ASN:ND2   | 2:B:59:LYS:N     | 0.47     | 2.62        | 9      | 1     |
| 2:D:146:HIS:ND1  | 2:D:146:HIS:OXT  | 0.47     | 2.46        | 4      | 1     |
| 2:B:44:SER:O     | 2:B:46:GLY:N     | 0.47     | 2.47        | 3      | 6     |
| 3:D:147:HEC:HHC  | 3:D:147:HEC:HBB2 | 0.47     | 1.87        | 7      | 3     |
| 1:C:124:SER:O    | 1:C:128:PHE:CB   | 0.47     | 2.62        | 13     | 10    |
| 2:D:38:THR:C     | 2:D:40:ARG:N     | 0.47     | 2.67        | 15     | 2     |
| 1:A:3:SER:CB     | 1:A:4:PRO:CD     | 0.47     | 2.92        | 20     | 4     |
| 1:C:5:ALA:C      | 1:C:7:LYS:N      | 0.47     | 2.67        | 12     | 3     |
| 2:D:117:HIS:C    | 2:D:118:PHE:CG   | 0.47     | 2.87        | 17     | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:D:37:TRP:N     | 2:D:37:TRP:CD1   | 0.47     | 2.79        | 20     | 1     |
| 1:A:93:VAL:CG2   | 1:A:94:ASP:H     | 0.47     | 2.17        | 13     | 1     |
| 1:A:27:GLU:CD    | 1:A:112:HIS:NE2  | 0.47     | 2.68        | 10     | 1     |
| 2:B:100:PRO:O    | 2:B:102:ASN:N    | 0.47     | 2.41        | 10     | 1     |
| 1:C:137:THR:O    | 1:C:138:SER:CB   | 0.47     | 2.63        | 15     | 1     |
| 1:A:48:LEU:N     | 1:A:48:LEU:CD1   | 0.47     | 2.70        | 9      | 3     |
| 1:A:107:VAL:HG11 | 2:B:127:GLN:OE1  | 0.47     | 2.10        | 8      | 1     |
| 1:C:127:LYS:CD   | 1:C:127:LYS:C    | 0.47     | 2.83        | 11     | 6     |
| 1:C:109:LEU:O    | 1:C:112:HIS:CD2  | 0.47     | 2.68        | 16     | 1     |
| 1:A:33:PHE:CD1   | 1:A:33:PHE:C     | 0.47     | 2.87        | 14     | 2     |
| 1:C:61:LYS:HG3   | 3:C:142:HEC:HAA2 | 0.47     | 1.85        | 19     | 1     |
| 1:A:61:LYS:HG3   | 3:A:142:HEC:HAA2 | 0.47     | 1.86        | 19     | 1     |
| 1:A:38:THR:HG22  | 2:D:97:HIS:HB3   | 0.47     | 1.84        | 19     | 1     |
| 2:D:116:HIS:C    | 2:D:116:HIS:HD1  | 0.47     | 2.13        | 19     | 2     |
| 1:C:86:LEU:CG    | 3:C:142:HEC:CBD  | 0.47     | 2.93        | 7      | 1     |
| 1:A:99:LYS:O     | 1:A:103:HIS:CG   | 0.47     | 2.68        | 7      | 1     |
| 2:D:97:HIS:CD2   | 2:D:97:HIS:O     | 0.47     | 2.68        | 5      | 3     |
| 2:B:139:ASN:OD1  | 2:D:146:HIS:HD2  | 0.47     | 1.92        | 17     | 1     |
| 1:C:113:LEU:O    | 1:C:113:LEU:CG   | 0.47     | 2.61        | 2      | 2     |
| 1:C:91:LEU:O     | 1:C:92:ARG:C     | 0.47     | 2.53        | 12     | 2     |
| 2:D:63:HIS:NE2   | 3:D:147:HEC:HHA  | 0.47     | 2.24        | 2      | 1     |
| 1:C:34:LEU:HD13  | 2:D:128:ALA:CB   | 0.47     | 2.31        | 18     | 1     |
| 1:A:118:THR:OG1  | 1:A:121:VAL:N    | 0.47     | 2.43        | 2      | 5     |
| 2:B:106:LEU:CD2  | 3:B:147:HEC:CAB  | 0.47     | 2.86        | 10     | 1     |
| 2:B:123:THR:OG1  | 2:B:126:VAL:CG2  | 0.47     | 2.63        | 9      | 5     |
| 2:D:63:HIS:O     | 2:D:63:HIS:ND1   | 0.47     | 2.47        | 15     | 1     |
| 2:B:38:THR:C     | 2:B:40:ARG:N     | 0.47     | 2.67        | 15     | 2     |
| 1:A:11:LYS:CD    | 1:A:11:LYS:N     | 0.47     | 2.75        | 15     | 3     |
| 2:B:42:PHE:O     | 2:B:42:PHE:CD2   | 0.47     | 2.68        | 8      | 1     |
| 1:C:109:LEU:O    | 1:C:113:LEU:C    | 0.47     | 2.53        | 6      | 10    |
| 1:A:109:LEU:O    | 1:A:112:HIS:CD2  | 0.47     | 2.68        | 16     | 1     |
| 1:C:24:TYR:CE2   | 1:C:112:HIS:CE1  | 0.47     | 3.03        | 16     | 1     |
| 1:A:86:LEU:CD1   | 1:A:86:LEU:C     | 0.47     | 2.82        | 19     | 2     |
| 2:D:102:ASN:ND2  | 2:D:103:PHE:CD1  | 0.47     | 2.83        | 6      | 1     |
| 1:C:99:LYS:O     | 1:C:103:HIS:CG   | 0.47     | 2.68        | 7      | 1     |
| 2:D:103:PHE:N    | 2:D:103:PHE:CD1  | 0.47     | 2.81        | 5      | 1     |
| 1:C:100:LEU:N    | 1:C:100:LEU:CD1  | 0.47     | 2.77        | 3      | 1     |
| 2:D:44:SER:O     | 2:D:46:GLY:N     | 0.47     | 2.47        | 3      | 6     |
| 1:C:27:GLU:CD    | 1:C:112:HIS:NE2  | 0.47     | 2.68        | 10     | 1     |
| 2:D:95:LYS:C     | 2:D:97:HIS:CD2   | 0.47     | 2.87        | 15     | 1     |
| 1:A:109:LEU:O    | 1:A:113:LEU:C    | 0.47     | 2.53        | 6      | 10    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:C:91:LEU:C     | 1:C:93:VAL:N     | 0.47     | 2.68        | 5      | 7     |
| 1:A:52:SER:O     | 1:A:53:ALA:CB    | 0.47     | 2.61        | 3      | 7     |
| 2:D:107:GLY:C    | 2:D:109:VAL:N    | 0.47     | 2.68        | 19     | 1     |
| 2:B:81:LEU:O     | 2:B:85:PHE:CE1   | 0.47     | 2.68        | 6      | 1     |
| 2:D:72:SER:O     | 2:D:76:ALA:HB3   | 0.47     | 2.09        | 4      | 1     |
| 2:D:7:GLU:N      | 2:D:7:GLU:CD     | 0.47     | 2.68        | 20     | 1     |
| 2:B:41:PHE:C     | 2:B:43:GLU:N     | 0.47     | 2.67        | 3      | 1     |
| 1:C:32:MET:SD    | 3:C:142:HEC:HHC  | 0.47     | 2.49        | 12     | 1     |
| 1:A:41:THR:CB    | 2:D:97:HIS:NE2   | 0.47     | 2.77        | 12     | 2     |
| 1:A:92:ARG:O     | 1:A:93:VAL:HG12  | 0.47     | 2.10        | 13     | 1     |
| 2:D:123:THR:O    | 2:D:127:GLN:NE2  | 0.47     | 2.47        | 11     | 1     |
| 1:A:49:SER:O     | 1:A:50:HIS:O     | 0.47     | 2.32        | 5      | 5     |
| 1:C:2:LEU:HD21   | 1:C:6:ASP:OD2    | 0.47     | 2.09        | 8      | 1     |
| 1:A:108:THR:O    | 1:A:110:ALA:N    | 0.47     | 2.48        | 5      | 5     |
| 2:D:96:LEU:CD2   | 2:D:96:LEU:N     | 0.47     | 2.76        | 16     | 1     |
| 1:C:53:ALA:C     | 1:C:55:VAL:N     | 0.47     | 2.68        | 2      | 5     |
| 1:C:33:PHE:C     | 1:C:33:PHE:CD1   | 0.47     | 2.87        | 14     | 1     |
| 2:B:116:HIS:HD1  | 2:B:116:HIS:C    | 0.47     | 2.13        | 19     | 4     |
| 2:D:38:THR:HG22  | 3:D:147:HEC:HBC1 | 0.47     | 1.86        | 9      | 1     |
| 2:B:38:THR:HG22  | 3:B:147:HEC:HBC1 | 0.47     | 1.86        | 9      | 1     |
| 1:A:109:LEU:O    | 1:A:114:PRO:N    | 0.47     | 2.47        | 6      | 3     |
| 1:C:122:HIS:CE1  | 2:D:112:CYS:SG   | 0.47     | 3.08        | 5      | 1     |
| 2:B:7:GLU:N      | 2:B:7:GLU:CD     | 0.47     | 2.68        | 20     | 1     |
| 1:A:100:LEU:N    | 1:A:100:LEU:CD1  | 0.47     | 2.77        | 3      | 1     |
| 1:A:2:LEU:HD12   | 1:A:2:LEU:N      | 0.47     | 2.24        | 2      | 3     |
| 2:B:41:PHE:CD2   | 3:B:147:HEC:CMD  | 0.47     | 2.98        | 12     | 1     |
| 2:D:99:ASP:OD1   | 2:D:99:ASP:N     | 0.47     | 2.48        | 18     | 1     |
| 1:C:4:PRO:C      | 1:C:6:ASP:N      | 0.47     | 2.66        | 7      | 5     |
| 2:B:14:LEU:C     | 2:B:16:GLY:N     | 0.47     | 2.68        | 19     | 7     |
| 2:D:124:PRO:N    | 2:D:125:PRO:CD   | 0.47     | 2.77        | 15     | 2     |
| 2:B:87:THR:O     | 2:B:91:LEU:N     | 0.47     | 2.40        | 11     | 3     |
| 2:B:3:LEU:HD23   | 2:B:132:LYS:HZ1  | 0.47     | 1.70        | 15     | 1     |
| 1:A:101:LEU:HD21 | 3:A:142:HEC:CBB  | 0.47     | 2.30        | 15     | 2     |
| 2:B:76:ALA:O     | 2:B:77:HIS:CD2   | 0.47     | 2.68        | 6      | 4     |
| 1:A:89:HIS:O     | 1:A:90:LYS:O     | 0.47     | 2.33        | 15     | 3     |
| 1:C:127:LYS:C    | 1:C:127:LYS:CD   | 0.47     | 2.82        | 15     | 7     |
| 2:D:42:PHE:O     | 2:D:42:PHE:CD2   | 0.47     | 2.67        | 8      | 1     |
| 1:C:107:VAL:HG11 | 2:D:127:GLN:OE1  | 0.47     | 2.09        | 8      | 1     |
| 1:A:85:ASP:N     | 1:A:85:ASP:OD1   | 0.47     | 2.47        | 14     | 1     |
| 1:A:53:ALA:C     | 1:A:55:VAL:N     | 0.47     | 2.68        | 14     | 5     |
| 2:B:97:HIS:CB    | 1:C:38:THR:HB    | 0.47     | 2.39        | 19     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:C:33:PHE:O    | 1:C:33:PHE:CD1   | 0.47     | 2.68        | 19     | 1     |
| 2:D:57:ASN:ND2  | 2:D:59:LYS:N     | 0.47     | 2.63        | 9      | 1     |
| 2:B:146:HIS:C   | 2:D:139:ASN:OD1  | 0.47     | 2.53        | 6      | 1     |
| 2:D:81:LEU:O    | 2:D:85:PHE:CE1   | 0.47     | 2.68        | 6      | 1     |
| 1:A:32:MET:C    | 1:A:32:MET:SD    | 0.47     | 2.92        | 6      | 1     |
| 1:A:41:THR:HB   | 2:D:97:HIS:ND1   | 0.47     | 2.24        | 4      | 1     |
| 1:A:122:HIS:CE1 | 2:B:112:CYS:SG   | 0.47     | 3.08        | 5      | 1     |
| 2:B:142:ALA:O   | 2:B:144:LYS:N    | 0.47     | 2.48        | 20     | 1     |
| 2:B:112:CYS:SG  | 2:B:113:VAL:N    | 0.47     | 2.87        | 20     | 1     |
| 2:B:20:VAL:HG12 | 2:B:20:VAL:O     | 0.47     | 2.10        | 11     | 2     |
| 2:B:71:PHE:CZ   | 2:B:134:VAL:HG11 | 0.47     | 2.44        | 3      | 1     |
| 1:A:33:PHE:O    | 1:A:36:PHE:N     | 0.47     | 2.47        | 1      | 1     |
| 1:C:46:PHE:C    | 1:C:46:PHE:CD1   | 0.47     | 2.87        | 1      | 2     |
| 2:B:117:HIS:N   | 2:B:117:HIS:ND1  | 0.47     | 2.62        | 12     | 1     |
| 2:B:123:THR:O   | 2:B:127:GLN:NE2  | 0.47     | 2.47        | 11     | 1     |
| 2:B:95:LYS:CD   | 2:B:95:LYS:N     | 0.47     | 2.78        | 11     | 1     |
| 2:D:36:PRO:C    | 3:D:147:HEC:CHC  | 0.47     | 2.83        | 15     | 1     |
| 2:D:41:PHE:CE1  | 3:D:147:HEC:NB   | 0.47     | 2.67        | 15     | 1     |
| 1:A:2:LEU:HD21  | 1:A:6:ASP:OD2    | 0.47     | 2.10        | 8      | 1     |
| 2:B:102:ASN:ND2 | 2:B:103:PHE:CD1  | 0.47     | 2.83        | 6      | 1     |
| 1:C:83:LEU:CD1  | 1:C:83:LEU:C     | 0.47     | 2.79        | 7      | 1     |
| 2:D:145:TYR:CG  | 2:D:145:TYR:O    | 0.47     | 2.64        | 5      | 1     |
| 1:C:129:LEU:C   | 1:C:129:LEU:CD1  | 0.47     | 2.79        | 20     | 1     |
| 2:D:142:ALA:O   | 2:D:144:LYS:N    | 0.47     | 2.48        | 20     | 1     |
| 1:C:33:PHE:O    | 1:C:36:PHE:N     | 0.47     | 2.47        | 1      | 2     |
| 1:C:48:LEU:HD23 | 1:C:48:LEU:H     | 0.47     | 1.70        | 1      | 1     |
| 2:B:146:HIS:N   | 2:B:146:HIS:ND1  | 0.47     | 2.61        | 1      | 1     |
| 1:C:48:LEU:N    | 1:C:48:LEU:HD22  | 0.47     | 2.24        | 11     | 1     |
| 1:A:21:ALA:HB1  | 1:A:63:ALA:HB1   | 0.47     | 1.85        | 2      | 2     |
| 2:D:123:THR:OG1 | 2:D:126:VAL:CG2  | 0.47     | 2.63        | 9      | 6     |
| 2:D:21:ASP:C    | 2:D:65:LYS:HZ3   | 0.47     | 2.13        | 10     | 1     |
| 2:D:3:LEU:HD23  | 2:D:132:LYS:HZ1  | 0.47     | 1.67        | 15     | 1     |
| 1:C:33:PHE:CD1  | 1:C:33:PHE:C     | 0.47     | 2.87        | 15     | 3     |
| 2:D:4:THR:O     | 2:D:7:GLU:N      | 0.47     | 2.46        | 16     | 3     |
| 1:C:56:LYS:H    | 1:C:56:LYS:CD    | 0.47     | 2.20        | 5      | 1     |
| 1:C:92:ARG:O    | 1:C:93:VAL:HG12  | 0.47     | 2.10        | 13     | 1     |
| 1:A:4:PRO:C     | 1:A:6:ASP:N      | 0.47     | 2.68        | 5      | 5     |
| 1:A:37:PRO:C    | 1:A:39:THR:N     | 0.47     | 2.68        | 10     | 10    |
| 2:B:91:LEU:O    | 2:B:95:LYS:CB    | 0.47     | 2.63        | 9      | 7     |
| 1:C:31:ARG:HH21 | 2:D:127:GLN:CB   | 0.47     | 2.18        | 15     | 1     |
| 2:D:13:ALA:C    | 2:D:15:TRP:N     | 0.47     | 2.68        | 15     | 3     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:33:PHE:C     | 1:A:33:PHE:CD1  | 0.47     | 2.87        | 15     | 2     |
| 1:A:122:HIS:H    | 1:A:122:HIS:CD2 | 0.47     | 2.28        | 8      | 1     |
| 1:C:20:HIS:CB    | 1:C:24:TYR:CZ   | 0.47     | 2.98        | 16     | 1     |
| 1:A:33:PHE:CD1   | 1:A:33:PHE:O    | 0.47     | 2.68        | 19     | 1     |
| 1:C:35:SER:C     | 1:C:36:PHE:CD1  | 0.47     | 2.89        | 20     | 4     |
| 1:A:35:SER:C     | 1:A:36:PHE:CD1  | 0.47     | 2.89        | 20     | 4     |
| 1:C:47:ASP:OD1   | 1:C:47:ASP:N    | 0.47     | 2.46        | 6      | 1     |
| 2:D:3:LEU:H      | 2:D:3:LEU:CD1   | 0.47     | 2.04        | 4      | 1     |
| 1:C:31:ARG:NH2   | 2:D:127:GLN:HB3 | 0.47     | 2.25        | 4      | 1     |
| 2:B:97:HIS:O     | 2:B:97:HIS:CD2  | 0.47     | 2.68        | 5      | 2     |
| 1:C:97:ASN:O     | 1:C:100:LEU:N   | 0.47     | 2.41        | 1      | 3     |
| 2:B:142:ALA:C    | 2:B:144:LYS:N   | 0.47     | 2.69        | 20     | 1     |
| 2:B:40:ARG:CB    | 1:C:92:ARG:HD3  | 0.47     | 2.40        | 17     | 1     |
| 2:D:28:LEU:CD1   | 2:D:28:LEU:N    | 0.47     | 2.78        | 17     | 1     |
| 1:A:41:THR:OG1   | 2:D:97:HIS:CE1  | 0.47     | 2.67        | 12     | 1     |
| 2:D:117:HIS:ND1  | 2:D:117:HIS:N   | 0.47     | 2.61        | 12     | 1     |
| 1:C:122:HIS:H    | 1:C:122:HIS:CD2 | 0.46     | 2.28        | 8      | 1     |
| 1:C:108:THR:O    | 1:C:110:ALA:N   | 0.46     | 2.48        | 5      | 4     |
| 1:A:90:LYS:C     | 1:A:92:ARG:N    | 0.46     | 2.68        | 16     | 4     |
| 1:A:20:HIS:CB    | 1:A:24:TYR:CZ   | 0.46     | 2.98        | 16     | 1     |
| 1:C:90:LYS:C     | 1:C:92:ARG:N    | 0.46     | 2.68        | 16     | 4     |
| 1:C:5:ALA:O      | 1:C:9:ASN:ND2   | 0.46     | 2.48        | 16     | 3     |
| 2:B:63:HIS:ND1   | 2:B:63:HIS:O    | 0.46     | 2.43        | 14     | 2     |
| 1:A:101:LEU:HD23 | 3:A:142:HEC:CBB | 0.46     | 2.41        | 14     | 1     |
| 2:B:107:GLY:C    | 2:B:109:VAL:N   | 0.46     | 2.68        | 19     | 1     |
| 1:A:100:LEU:O    | 1:A:104:CYS:N   | 0.46     | 2.46        | 19     | 1     |
| 2:D:15:TRP:HE1   | 2:D:72:SER:HG   | 0.46     | 1.51        | 9      | 1     |
| 2:B:57:ASN:HD22  | 2:B:57:ASN:C    | 0.46     | 2.14        | 9      | 1     |
| 1:A:83:LEU:C     | 1:A:83:LEU:CD1  | 0.46     | 2.79        | 7      | 1     |
| 1:A:31:ARG:NH2   | 2:B:127:GLN:HB3 | 0.46     | 2.24        | 4      | 1     |
| 1:C:39:THR:H     | 3:C:142:HEC:C3C | 0.46     | 2.23        | 12     | 1     |
| 2:B:58:PRO:O     | 2:B:62:ALA:N    | 0.46     | 2.41        | 2      | 1     |
| 1:A:46:PHE:C     | 1:A:48:LEU:N    | 0.46     | 2.67        | 18     | 5     |
| 2:D:14:LEU:C     | 2:D:16:GLY:N    | 0.46     | 2.68        | 19     | 7     |
| 2:B:17:LYS:CD    | 2:B:17:LYS:N    | 0.46     | 2.78        | 15     | 4     |
| 1:A:3:SER:H      | 1:A:4:PRO:HD2   | 0.46     | 1.69        | 10     | 3     |
| 1:C:3:SER:H      | 1:C:4:PRO:HD2   | 0.46     | 1.70        | 10     | 3     |
| 1:C:85:ASP:OD1   | 1:C:85:ASP:N    | 0.46     | 2.47        | 14     | 2     |
| 2:D:114:LEU:H    | 2:D:114:LEU:CD1 | 0.46     | 2.24        | 9      | 1     |
| 1:A:91:LEU:CD1   | 1:A:91:LEU:H    | 0.46     | 2.23        | 9      | 1     |
| 1:A:47:ASP:N     | 1:A:47:ASP:OD1  | 0.46     | 2.46        | 6      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:113:LEU:O    | 1:A:113:LEU:CD2  | 0.46     | 2.61        | 3      | 1     |
| 2:D:58:PRO:O     | 2:D:60:VAL:N     | 0.46     | 2.48        | 11     | 1     |
| 1:A:92:ARG:HH11  | 2:D:40:ARG:CD    | 0.46     | 2.18        | 18     | 1     |
| 1:A:40:LYS:O     | 1:A:41:THR:C     | 0.46     | 2.52        | 18     | 2     |
| 1:C:45:HIS:ND1   | 1:C:45:HIS:C     | 0.46     | 2.68        | 11     | 2     |
| 1:C:101:LEU:HD21 | 3:C:142:HEC:CBB  | 0.46     | 2.30        | 15     | 2     |
| 2:D:76:ALA:O     | 2:D:77:HIS:CD2   | 0.46     | 2.68        | 6      | 4     |
| 2:B:20:VAL:C     | 2:B:22:GLU:N     | 0.46     | 2.68        | 15     | 2     |
| 1:A:24:TYR:CE2   | 1:A:112:HIS:CE1  | 0.46     | 3.03        | 16     | 1     |
| 1:C:101:LEU:HD23 | 3:C:142:HEC:CBB  | 0.46     | 2.41        | 14     | 1     |
| 1:C:128:PHE:CD1  | 1:C:128:PHE:O    | 0.46     | 2.69        | 5      | 4     |
| 2:B:99:ASP:OD1   | 1:C:96:VAL:HG11  | 0.46     | 2.10        | 6      | 1     |
| 1:A:86:LEU:CG    | 3:A:142:HEC:CBD  | 0.46     | 2.93        | 7      | 1     |
| 2:B:139:ASN:OD1  | 2:B:139:ASN:N    | 0.46     | 2.46        | 20     | 1     |
| 1:A:84:SER:CB    | 1:A:136:LEU:O    | 0.46     | 2.64        | 20     | 1     |
| 2:D:112:CYS:SG   | 2:D:113:VAL:N    | 0.46     | 2.87        | 20     | 1     |
| 2:B:28:LEU:N     | 2:B:28:LEU:CD1   | 0.46     | 2.78        | 17     | 1     |
| 1:C:3:SER:N      | 1:C:4:PRO:HD2    | 0.46     | 2.26        | 10     | 6     |
| 1:C:60:LYS:O     | 1:C:64:ASP:CB    | 0.46     | 2.63        | 11     | 9     |
| 1:A:60:LYS:O     | 1:A:64:ASP:CB    | 0.46     | 2.63        | 11     | 9     |
| 1:A:120:ALA:O    | 1:A:124:SER:OG   | 0.46     | 2.33        | 10     | 3     |
| 1:C:49:SER:O     | 1:C:50:HIS:O     | 0.46     | 2.32        | 5      | 5     |
| 2:D:95:LYS:CA    | 2:D:97:HIS:HE2   | 0.46     | 2.24        | 15     | 1     |
| 2:D:15:TRP:NE1   | 2:D:72:SER:OG    | 0.46     | 2.43        | 15     | 1     |
| 1:C:115:ALA:C    | 1:C:117:PHE:H    | 0.46     | 2.14        | 15     | 1     |
| 1:A:34:LEU:C     | 1:A:36:PHE:N     | 0.46     | 2.69        | 6      | 2     |
| 2:B:93:CYS:SG    | 2:B:145:TYR:CE1  | 0.46     | 3.09        | 9      | 1     |
| 2:D:41:PHE:C     | 2:D:43:GLU:N     | 0.46     | 2.67        | 3      | 1     |
| 1:A:137:THR:O    | 1:A:137:THR:CG2  | 0.46     | 2.63        | 12     | 1     |
| 2:D:79:ASP:O     | 2:D:80:ASN:ND2   | 0.46     | 2.49        | 13     | 1     |
| 2:B:32:LEU:CD2   | 2:B:38:THR:OG1   | 0.46     | 2.63        | 2      | 1     |
| 3:B:147:HEC:HHC  | 3:B:147:HEC:HBB2 | 0.46     | 1.87        | 7      | 3     |
| 2:D:124:PRO:N    | 2:D:125:PRO:HD2  | 0.46     | 2.25        | 10     | 15    |
| 1:A:3:SER:H      | 1:A:6:ASP:CG     | 0.46     | 2.13        | 20     | 1     |
| 1:A:27:GLU:OE2   | 1:A:112:HIS:CE1  | 0.46     | 2.69        | 17     | 1     |
| 1:C:106:LEU:O    | 1:C:110:ALA:HB2  | 0.46     | 2.10        | 12     | 1     |
| 1:A:86:LEU:CD1   | 1:A:90:LYS:NZ    | 0.46     | 2.78        | 13     | 1     |
| 2:B:79:ASP:O     | 2:B:80:ASN:ND2   | 0.46     | 2.48        | 13     | 1     |
| 1:C:2:LEU:HD12   | 1:C:2:LEU:N      | 0.46     | 2.24        | 2      | 1     |
| 2:B:40:ARG:HD2   | 1:C:92:ARG:HD2   | 0.46     | 1.70        | 18     | 1     |
| 2:D:20:VAL:C     | 2:D:22:GLU:N     | 0.46     | 2.68        | 15     | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:C:89:HIS:O    | 1:C:90:LYS:O    | 0.46     | 2.33        | 15     | 3     |
| 1:C:38:THR:O    | 1:C:40:LYS:N    | 0.46     | 2.49        | 16     | 3     |
| 1:C:105:LEU:C   | 1:C:105:LEU:CD1 | 0.46     | 2.80        | 16     | 1     |
| 1:C:101:LEU:CD1 | 3:C:142:HEC:C4B | 0.46     | 2.91        | 19     | 1     |
| 2:D:77:HIS:O    | 2:D:78:LEU:C    | 0.46     | 2.54        | 6      | 1     |
| 1:A:48:LEU:H    | 1:A:48:LEU:HD12 | 0.46     | 1.69        | 20     | 1     |
| 1:C:84:SER:CB   | 1:C:136:LEU:O   | 0.46     | 2.64        | 20     | 1     |
| 1:A:110:ALA:C   | 1:A:112:HIS:N   | 0.46     | 2.69        | 1      | 1     |
| 1:C:2:LEU:N     | 1:C:2:LEU:HD12  | 0.46     | 2.26        | 13     | 2     |
| 1:C:92:ARG:O    | 1:C:93:VAL:CG1  | 0.46     | 2.64        | 13     | 1     |
| 1:A:92:ARG:O    | 1:A:93:VAL:CG1  | 0.46     | 2.64        | 13     | 1     |
| 2:B:99:ASP:OD1  | 2:B:99:ASP:N    | 0.46     | 2.48        | 18     | 2     |
| 1:A:76:MET:N    | 1:A:77:PRO:HD3  | 0.46     | 2.26        | 5      | 12    |
| 1:C:52:SER:O    | 1:C:53:ALA:C    | 0.46     | 2.54        | 18     | 1     |
| 1:C:37:PRO:C    | 1:C:39:THR:N    | 0.46     | 2.68        | 10     | 11    |
| 1:A:118:THR:O   | 1:A:122:HIS:CD2 | 0.46     | 2.69        | 8      | 1     |
| 2:D:17:LYS:CD   | 2:D:17:LYS:H    | 0.46     | 2.24        | 8      | 2     |
| 2:D:119:GLY:O   | 2:D:122:PHE:N   | 0.46     | 2.47        | 19     | 2     |
| 2:B:114:LEU:H   | 2:B:114:LEU:CD1 | 0.46     | 2.24        | 9      | 1     |
| 2:B:139:ASN:OD1 | 2:D:146:HIS:C   | 0.46     | 2.53        | 6      | 1     |
| 1:C:27:GLU:OE2  | 1:C:112:HIS:CE1 | 0.46     | 2.69        | 17     | 1     |
| 1:A:48:LEU:H    | 1:A:48:LEU:HD23 | 0.46     | 1.70        | 1      | 1     |
| 1:A:106:LEU:O   | 1:A:110:ALA:HB2 | 0.46     | 2.10        | 12     | 1     |
| 2:B:58:PRO:O    | 2:B:60:VAL:N    | 0.46     | 2.48        | 11     | 1     |
| 1:A:115:ALA:C   | 1:A:117:PHE:H   | 0.46     | 2.14        | 15     | 2     |
| 1:C:7:LYS:O     | 1:C:11:LYS:HG2  | 0.46     | 2.11        | 1      | 2     |
| 1:C:46:PHE:CD1  | 1:C:46:PHE:C    | 0.46     | 2.85        | 9      | 2     |
| 1:A:5:ALA:O     | 1:A:9:ASN:ND2   | 0.46     | 2.49        | 14     | 3     |
| 2:B:97:HIS:HB3  | 1:C:38:THR:HG22 | 0.46     | 1.85        | 19     | 2     |
| 2:B:114:LEU:CD1 | 2:B:114:LEU:N   | 0.46     | 2.78        | 9      | 1     |
| 1:C:91:LEU:CD1  | 1:C:91:LEU:H    | 0.46     | 2.23        | 9      | 2     |
| 1:A:46:PHE:O    | 1:A:48:LEU:CG   | 0.46     | 2.64        | 18     | 5     |
| 2:D:91:LEU:O    | 2:D:95:LYS:CB   | 0.46     | 2.63        | 9      | 7     |
| 2:D:40:ARG:C    | 2:D:42:PHE:N    | 0.46     | 2.69        | 15     | 2     |
| 1:A:105:LEU:CD1 | 1:A:105:LEU:C   | 0.46     | 2.80        | 16     | 1     |
| 1:A:65:ALA:O    | 1:A:68:ASN:OD1  | 0.46     | 2.33        | 9      | 1     |
| 2:D:96:LEU:O    | 2:D:96:LEU:HD13 | 0.46     | 2.11        | 4      | 1     |
| 1:C:3:SER:H     | 1:C:6:ASP:CG    | 0.46     | 2.13        | 20     | 1     |
| 2:D:133:VAL:C   | 2:D:135:ALA:N   | 0.46     | 2.69        | 12     | 1     |
| 1:C:46:PHE:O    | 1:C:48:LEU:CG   | 0.46     | 2.64        | 18     | 5     |
| 3:B:147:HEC:CMC | 2:D:31:LEU:HD21 | 0.46     | 2.41        | 15     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:15:TRP:HE1   | 2:B:72:SER:HG    | 0.46     | 1.46        | 15     | 2     |
| 1:A:5:ALA:C      | 1:A:7:LYS:N      | 0.46     | 2.67        | 12     | 3     |
| 1:C:137:THR:CG2  | 1:C:137:THR:O    | 0.46     | 2.63        | 12     | 1     |
| 2:B:142:ALA:O    | 2:B:145:TYR:N    | 0.46     | 2.48        | 12     | 1     |
| 1:C:84:SER:O     | 1:C:88:ALA:CB    | 0.45     | 2.64        | 13     | 4     |
| 3:B:147:HEC:HMC3 | 2:D:31:LEU:CD2   | 0.45     | 2.41        | 15     | 1     |
| 2:D:17:LYS:CD    | 2:D:17:LYS:N     | 0.45     | 2.79        | 13     | 2     |
| 2:D:94:ASP:C     | 2:D:97:HIS:HE2   | 0.45     | 2.15        | 15     | 1     |
| 1:A:6:ASP:CG     | 1:A:127:LYS:HZ1  | 0.45     | 2.14        | 16     | 1     |
| 2:D:57:ASN:C     | 2:D:57:ASN:HD22  | 0.45     | 2.14        | 9      | 1     |
| 1:C:129:LEU:CD1  | 1:C:129:LEU:C    | 0.45     | 2.84        | 7      | 2     |
| 1:A:117:PHE:HA   | 2:B:30:ARG:HH22  | 0.45     | 1.71        | 17     | 1     |
| 1:C:48:LEU:CD2   | 1:C:48:LEU:H     | 0.45     | 2.24        | 1      | 1     |
| 2:B:110:LEU:C    | 2:B:110:LEU:HD23 | 0.45     | 2.32        | 12     | 1     |
| 1:C:86:LEU:CD1   | 1:C:90:LYS:NZ    | 0.45     | 2.78        | 13     | 1     |
| 1:A:94:ASP:CB    | 2:D:99:ASP:OD1   | 0.45     | 2.65        | 2      | 1     |
| 2:B:40:ARG:CZ    | 1:C:92:ARG:CD    | 0.45     | 2.94        | 18     | 1     |
| 2:D:80:ASN:O     | 2:D:82:LYS:N     | 0.45     | 2.49        | 10     | 1     |
| 2:D:6:GLU:CD     | 2:D:6:GLU:N      | 0.45     | 2.69        | 19     | 2     |
| 1:A:7:LYS:O      | 1:A:11:LYS:HG2   | 0.45     | 2.11        | 8      | 2     |
| 1:C:108:THR:HG23 | 1:C:109:LEU:N    | 0.45     | 2.27        | 16     | 1     |
| 2:D:111:VAL:HG12 | 2:D:130:TYR:CD1  | 0.45     | 2.47        | 14     | 1     |
| 1:C:65:ALA:O     | 1:C:68:ASN:OD1   | 0.45     | 2.33        | 9      | 1     |
| 2:B:96:LEU:HD13  | 2:B:96:LEU:O     | 0.45     | 2.11        | 4      | 1     |
| 1:C:58:HIS:CD2   | 1:C:58:HIS:C     | 0.45     | 2.88        | 3      | 1     |
| 1:C:86:LEU:HD21  | 3:C:142:HEC:HBD2 | 0.45     | 1.88        | 13     | 1     |
| 2:D:106:LEU:HD11 | 3:D:147:HEC:CAB  | 0.45     | 2.29        | 2      | 1     |
| 2:B:6:GLU:N      | 2:B:6:GLU:CD     | 0.45     | 2.69        | 19     | 2     |
| 1:A:92:ARG:HH21  | 2:D:40:ARG:CZ    | 0.45     | 2.12        | 15     | 1     |
| 2:B:40:ARG:C     | 2:B:42:PHE:N     | 0.45     | 2.69        | 15     | 1     |
| 1:A:38:THR:O     | 1:A:40:LYS:N     | 0.45     | 2.49        | 16     | 3     |
| 2:D:121:GLU:O    | 2:D:123:THR:N    | 0.45     | 2.48        | 9      | 1     |
| 1:A:88:ALA:O     | 1:A:89:HIS:CG    | 0.45     | 2.70        | 4      | 1     |
| 2:D:109:VAL:O    | 2:D:112:CYS:SG   | 0.45     | 2.71        | 20     | 1     |
| 2:B:135:ALA:HB3  | 2:D:146:HIS:HB3  | 0.45     | 1.88        | 3      | 1     |
| 1:C:78:ASN:ND2   | 1:C:79:ALA:N     | 0.45     | 2.64        | 17     | 1     |
| 1:C:2:LEU:N      | 1:C:2:LEU:CD1    | 0.45     | 2.79        | 1      | 2     |
| 1:A:2:LEU:N      | 1:A:2:LEU:CD1    | 0.45     | 2.79        | 1      | 1     |
| 2:D:42:PHE:CD1   | 3:D:147:HEC:C2B  | 0.45     | 2.98        | 12     | 1     |
| 2:B:146:HIS:N    | 2:B:146:HIS:HD1  | 0.45     | 2.09        | 11     | 1     |
| 2:D:20:VAL:HG12  | 2:D:20:VAL:O     | 0.45     | 2.10        | 11     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:D:32:LEU:CD2   | 2:D:38:THR:OG1   | 0.45     | 2.64        | 2      | 1     |
| 2:B:124:PRO:N    | 2:B:125:PRO:HD2  | 0.45     | 2.27        | 16     | 15    |
| 1:A:27:GLU:OE1   | 1:A:27:GLU:CA    | 0.45     | 2.63        | 15     | 1     |
| 1:A:49:SER:CB    | 1:A:52:SER:OG    | 0.45     | 2.65        | 14     | 1     |
| 2:D:77:HIS:C     | 2:D:79:ASP:N     | 0.45     | 2.70        | 14     | 1     |
| 1:C:122:HIS:CD2  | 2:D:34:VAL:HG13  | 0.45     | 2.47        | 19     | 1     |
| 2:D:96:LEU:C     | 2:D:97:HIS:CD2   | 0.45     | 2.90        | 19     | 1     |
| 1:C:86:LEU:CD1   | 1:C:86:LEU:C     | 0.45     | 2.82        | 19     | 1     |
| 1:C:2:LEU:CD2    | 1:C:128:PHE:CD2  | 0.45     | 3.00        | 9      | 1     |
| 1:C:1:VAL:O      | 1:C:2:LEU:O      | 0.45     | 2.35        | 2      | 4     |
| 2:B:40:ARG:C     | 1:C:92:ARG:NH1   | 0.45     | 2.69        | 17     | 1     |
| 1:A:91:LEU:O     | 1:A:92:ARG:C     | 0.45     | 2.53        | 12     | 2     |
| 1:C:18:GLY:O     | 1:C:19:ALA:CB    | 0.45     | 2.64        | 11     | 2     |
| 1:A:3:SER:N      | 1:A:4:PRO:HD2    | 0.45     | 2.26        | 9      | 6     |
| 2:B:105:LEU:O    | 2:B:108:ASN:N    | 0.45     | 2.50        | 10     | 1     |
| 2:B:80:ASN:O     | 2:B:82:LYS:N     | 0.45     | 2.49        | 10     | 1     |
| 2:D:144:LYS:C    | 2:D:146:HIS:H    | 0.45     | 2.15        | 19     | 5     |
| 3:B:147:HEC:C1C  | 2:D:106:LEU:CD1  | 0.45     | 2.77        | 15     | 1     |
| 1:A:84:SER:O     | 1:A:88:ALA:CB    | 0.45     | 2.65        | 15     | 2     |
| 2:B:143:HIS:CD2  | 2:B:143:HIS:O    | 0.45     | 2.70        | 16     | 2     |
| 1:A:93:VAL:O     | 2:D:40:ARG:NH1   | 0.45     | 2.49        | 14     | 1     |
| 1:C:48:LEU:HD22  | 1:C:49:SER:N     | 0.45     | 2.27        | 9      | 2     |
| 2:D:114:LEU:CD1  | 2:D:114:LEU:N    | 0.45     | 2.78        | 9      | 1     |
| 1:A:1:VAL:O      | 1:A:2:LEU:O      | 0.45     | 2.35        | 1      | 3     |
| 1:C:101:LEU:HD22 | 3:C:142:HEC:HAB  | 0.45     | 1.89        | 1      | 1     |
| 1:C:34:LEU:CD1   | 1:C:35:SER:N     | 0.45     | 2.79        | 1      | 1     |
| 1:C:117:PHE:CE2  | 2:D:116:HIS:NE2  | 0.45     | 2.58        | 13     | 1     |
| 1:A:18:GLY:O     | 1:A:19:ALA:CB    | 0.45     | 2.64        | 11     | 1     |
| 2:D:146:HIS:N    | 2:D:146:HIS:HD1  | 0.45     | 2.09        | 11     | 1     |
| 2:D:17:LYS:N     | 2:D:17:LYS:CD    | 0.45     | 2.79        | 14     | 5     |
| 2:D:31:LEU:HD23  | 3:D:147:HEC:HBC2 | 0.45     | 1.89        | 10     | 1     |
| 2:D:47:ASP:N     | 2:D:47:ASP:OD1   | 0.45     | 2.49        | 10     | 1     |
| 2:B:13:ALA:C     | 2:B:15:TRP:N     | 0.45     | 2.67        | 15     | 3     |
| 2:D:143:HIS:O    | 2:D:143:HIS:CD2  | 0.45     | 2.70        | 16     | 1     |
| 2:D:90:GLU:O     | 2:D:94:ASP:CB    | 0.45     | 2.65        | 16     | 1     |
| 2:B:111:VAL:HG12 | 2:B:130:TYR:CD1  | 0.45     | 2.47        | 14     | 1     |
| 1:A:122:HIS:CD2  | 2:B:34:VAL:HG13  | 0.45     | 2.47        | 19     | 1     |
| 1:C:94:ASP:OD2   | 1:C:96:VAL:CG2   | 0.45     | 2.64        | 9      | 1     |
| 2:B:139:ASN:N    | 2:B:139:ASN:HD22 | 0.45     | 2.10        | 6      | 1     |
| 1:A:113:LEU:CD1  | 1:A:113:LEU:O    | 0.45     | 2.64        | 20     | 1     |
| 1:C:32:MET:SD    | 1:C:32:MET:C     | 0.45     | 2.95        | 12     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:52:SER:O     | 1:A:53:ALA:C     | 0.45     | 2.54        | 18     | 1     |
| 2:B:8:LYS:O      | 2:B:10:ALA:N     | 0.45     | 2.50        | 19     | 6     |
| 2:B:44:SER:C     | 2:B:46:GLY:N     | 0.45     | 2.69        | 3      | 6     |
| 2:B:36:PRO:C     | 2:B:38:THR:N     | 0.45     | 2.70        | 15     | 3     |
| 2:B:40:ARG:CZ    | 1:C:93:VAL:O     | 0.45     | 2.65        | 14     | 1     |
| 2:B:77:HIS:C     | 2:B:79:ASP:N     | 0.45     | 2.70        | 14     | 1     |
| 1:A:127:LYS:CD   | 1:A:127:LYS:C    | 0.45     | 2.84        | 14     | 4     |
| 1:C:61:LYS:HG3   | 3:C:142:HEC:CAA  | 0.45     | 2.42        | 19     | 1     |
| 2:B:8:LYS:CG     | 2:B:9:SER:N      | 0.45     | 2.80        | 19     | 1     |
| 1:A:48:LEU:HD22  | 1:A:49:SER:N     | 0.45     | 2.27        | 9      | 2     |
| 1:A:2:LEU:CD2    | 1:A:128:PHE:CD2  | 0.45     | 3.00        | 9      | 1     |
| 1:C:50:HIS:C     | 1:C:50:HIS:ND1   | 0.45     | 2.70        | 9      | 1     |
| 2:D:93:CYS:SG    | 2:D:145:TYR:CE1  | 0.45     | 3.09        | 9      | 1     |
| 2:D:110:LEU:HD23 | 2:D:110:LEU:C    | 0.45     | 2.32        | 9      | 2     |
| 2:D:94:ASP:OD1   | 2:D:94:ASP:N     | 0.45     | 2.49        | 6      | 2     |
| 1:A:58:HIS:C     | 1:A:58:HIS:CD2   | 0.45     | 2.88        | 3      | 1     |
| 2:B:102:ASN:C    | 2:B:104:ARG:N    | 0.45     | 2.70        | 17     | 1     |
| 1:A:78:ASN:ND2   | 1:A:79:ALA:N     | 0.45     | 2.65        | 17     | 1     |
| 2:B:101:GLU:O    | 2:B:102:ASN:OD1  | 0.45     | 2.35        | 18     | 1     |
| 2:B:47:ASP:N     | 2:B:47:ASP:OD1   | 0.45     | 2.49        | 10     | 1     |
| 1:A:92:ARG:HH21  | 2:D:40:ARG:HE    | 0.45     | 0.56        | 15     | 1     |
| 2:D:127:GLN:O    | 2:D:131:GLN:OE1  | 0.45     | 2.35        | 16     | 1     |
| 1:A:109:LEU:C    | 1:A:109:LEU:CD1  | 0.45     | 2.81        | 16     | 1     |
| 1:C:49:SER:CB    | 1:C:52:SER:OG    | 0.45     | 2.65        | 14     | 1     |
| 2:B:96:LEU:C     | 2:B:97:HIS:CD2   | 0.45     | 2.90        | 19     | 1     |
| 1:A:94:ASP:OD2   | 1:A:96:VAL:CG2   | 0.45     | 2.64        | 9      | 1     |
| 2:B:111:VAL:CG1  | 2:B:130:TYR:CD1  | 0.45     | 3.00        | 5      | 1     |
| 1:A:100:LEU:O    | 1:A:102:SER:N    | 0.45     | 2.50        | 20     | 1     |
| 2:B:146:HIS:HD2  | 2:D:139:ASN:OD1  | 0.45     | 1.94        | 17     | 1     |
| 1:A:34:LEU:CD1   | 1:A:35:SER:N     | 0.45     | 2.80        | 1      | 1     |
| 2:D:123:THR:O    | 2:D:127:GLN:OE1  | 0.45     | 2.35        | 1      | 1     |
| 1:C:33:PHE:CE1   | 3:C:142:HEC:C1D  | 0.45     | 3.00        | 12     | 1     |
| 2:D:42:PHE:CD1   | 3:D:147:HEC:C1B  | 0.45     | 3.00        | 12     | 1     |
| 1:C:97:ASN:N     | 1:C:97:ASN:OD1   | 0.45     | 2.50        | 18     | 1     |
| 2:D:101:GLU:O    | 2:D:102:ASN:OD1  | 0.45     | 2.35        | 18     | 1     |
| 3:B:147:HEC:C2C  | 2:D:106:LEU:HD12 | 0.45     | 2.41        | 15     | 1     |
| 1:C:118:THR:O    | 1:C:122:HIS:CD2  | 0.45     | 2.69        | 8      | 1     |
| 1:A:98:PHE:CD1   | 1:A:98:PHE:C     | 0.45     | 2.87        | 8      | 1     |
| 2:B:127:GLN:O    | 2:B:131:GLN:OE1  | 0.45     | 2.35        | 16     | 1     |
| 1:A:33:PHE:O     | 1:A:36:PHE:O     | 0.45     | 2.35        | 14     | 1     |
| 2:B:110:LEU:HD23 | 2:B:110:LEU:C    | 0.45     | 2.32        | 9      | 2     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 2:B:96:LEU:HD12 | 2:B:98:VAL:CG2   | 0.45     | 2.42        | 6      | 1     |
| 1:C:94:ASP:OD1  | 1:C:94:ASP:N     | 0.45     | 2.48        | 7      | 3     |
| 2:B:83:GLY:O    | 2:B:86:ALA:N     | 0.45     | 2.43        | 4      | 1     |
| 1:C:117:PHE:HA  | 2:D:30:ARG:HH22  | 0.45     | 1.71        | 17     | 1     |
| 1:C:46:PHE:CD1  | 3:C:142:HEC:CMA  | 0.45     | 2.88        | 12     | 1     |
| 2:B:133:VAL:C   | 2:B:135:ALA:N    | 0.45     | 2.68        | 12     | 1     |
| 1:A:32:MET:SD   | 1:A:32:MET:C     | 0.45     | 2.95        | 12     | 1     |
| 2:B:37:TRP:CD1  | 2:B:38:THR:HG23  | 0.45     | 2.47        | 10     | 2     |
| 1:C:27:GLU:CA   | 1:C:27:GLU:OE1   | 0.45     | 2.62        | 15     | 1     |
| 1:A:137:THR:O   | 1:A:138:SER:O    | 0.45     | 2.36        | 3      | 3     |
| 1:A:101:LEU:CD1 | 3:A:142:HEC:C4B  | 0.45     | 2.91        | 19     | 1     |
| 2:B:56:GLY:O    | 2:B:57:ASN:HB2   | 0.45     | 2.12        | 19     | 1     |
| 2:D:67:VAL:CG2  | 3:D:147:HEC:NA   | 0.45     | 2.80        | 9      | 1     |
| 2:B:111:VAL:CG1 | 2:B:130:TYR:CE1  | 0.45     | 3.00        | 5      | 1     |
| 1:A:68:ASN:HD21 | 1:A:79:ALA:CB    | 0.45     | 2.25        | 5      | 1     |
| 1:C:100:LEU:O   | 1:C:102:SER:N    | 0.45     | 2.50        | 20     | 1     |
| 1:A:115:ALA:O   | 1:A:121:VAL:CG2  | 0.45     | 2.60        | 1      | 1     |
| 2:B:123:THR:O   | 2:B:127:GLN:OE1  | 0.45     | 2.35        | 1      | 1     |
| 2:B:67:VAL:HG13 | 3:B:147:HEC:C3B  | 0.44     | 2.34        | 18     | 1     |
| 2:B:114:LEU:O   | 2:B:116:HIS:N    | 0.44     | 2.50        | 20     | 2     |
| 1:A:137:THR:O   | 1:A:138:SER:CB   | 0.44     | 2.63        | 15     | 1     |
| 2:D:127:GLN:O   | 2:D:130:TYR:N    | 0.44     | 2.51        | 1      | 2     |
| 2:D:21:ASP:OD1  | 2:D:21:ASP:N     | 0.44     | 2.50        | 9      | 2     |
| 1:A:17:VAL:O    | 1:A:18:GLY:O     | 0.44     | 2.35        | 11     | 3     |
| 2:B:39:GLN:O    | 2:B:39:GLN:OE1   | 0.44     | 2.36        | 16     | 1     |
| 2:D:96:LEU:HD12 | 2:D:98:VAL:HG23  | 0.44     | 1.87        | 6      | 2     |
| 1:A:92:ARG:O    | 1:A:93:VAL:C     | 0.44     | 2.55        | 17     | 2     |
| 2:D:8:LYS:CG    | 2:D:9:SER:N      | 0.44     | 2.79        | 19     | 1     |
| 2:B:114:LEU:H   | 2:B:114:LEU:HD12 | 0.44     | 1.71        | 9      | 1     |
| 2:B:102:ASN:ND2 | 3:B:147:HEC:HMC2 | 0.44     | 2.27        | 7      | 1     |
| 2:D:142:ALA:C   | 2:D:144:LYS:N    | 0.44     | 2.69        | 20     | 1     |
| 2:B:102:ASN:O   | 2:B:104:ARG:N    | 0.44     | 2.50        | 17     | 1     |
| 1:C:48:LEU:CD1  | 3:C:142:HEC:HAA1 | 0.44     | 2.42        | 12     | 1     |
| 2:D:36:PRO:C    | 3:D:147:HEC:C2C  | 0.44     | 2.82        | 12     | 1     |
| 2:B:97:HIS:CE1  | 1:C:41:THR:HG22  | 0.44     | 2.48        | 11     | 1     |
| 1:A:127:LYS:C   | 1:A:129:LEU:N    | 0.44     | 2.70        | 2      | 7     |
| 2:B:21:ASP:C    | 2:B:65:LYS:HZ3   | 0.44     | 2.15        | 10     | 1     |
| 1:C:34:LEU:C    | 1:C:36:PHE:N     | 0.44     | 2.69        | 6      | 3     |
| 1:A:94:ASP:O    | 1:A:97:ASN:OD1   | 0.44     | 2.35        | 16     | 1     |
| 2:D:96:LEU:HD12 | 2:D:98:VAL:CG2   | 0.44     | 2.42        | 6      | 1     |
| 1:C:60:LYS:O    | 1:C:64:ASP:CG    | 0.44     | 2.56        | 6      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:62:VAL:HG12  | 1:A:63:ALA:N     | 0.44     | 2.28        | 1      | 3     |
| 3:A:142:HEC:HMB1 | 3:A:142:HEC:CBB  | 0.44     | 2.31        | 11     | 2     |
| 1:C:32:MET:CE    | 3:C:142:HEC:C3B  | 0.44     | 2.95        | 12     | 1     |
| 1:C:120:ALA:O    | 1:C:124:SER:OG   | 0.44     | 2.33        | 10     | 5     |
| 2:B:132:LYS:CB   | 2:B:132:LYS:NZ   | 0.44     | 2.80        | 18     | 1     |
| 2:D:40:ARG:O     | 2:D:42:PHE:N     | 0.44     | 2.50        | 15     | 2     |
| 2:B:42:PHE:CE1   | 2:B:45:PHE:CZ    | 0.44     | 3.06        | 16     | 1     |
| 1:C:94:ASP:C     | 1:C:96:VAL:N     | 0.44     | 2.71        | 4      | 6     |
| 2:B:95:LYS:O     | 2:B:97:HIS:CD2   | 0.44     | 2.70        | 19     | 1     |
| 1:A:60:LYS:O     | 1:A:64:ASP:CG    | 0.44     | 2.56        | 6      | 3     |
| 2:B:21:ASP:N     | 2:B:21:ASP:OD1   | 0.44     | 2.50        | 9      | 1     |
| 2:B:97:HIS:CG    | 1:C:38:THR:HG22  | 0.44     | 2.38        | 7      | 1     |
| 1:C:88:ALA:O     | 1:C:89:HIS:CG    | 0.44     | 2.70        | 4      | 1     |
| 2:B:146:HIS:CE1  | 2:D:135:ALA:HB3  | 0.44     | 2.47        | 17     | 1     |
| 2:D:102:ASN:O    | 2:D:104:ARG:N    | 0.44     | 2.50        | 17     | 1     |
| 2:B:97:HIS:CD2   | 2:B:97:HIS:O     | 0.44     | 2.70        | 2      | 1     |
| 1:C:113:LEU:O    | 1:C:113:LEU:CD1  | 0.44     | 2.66        | 18     | 1     |
| 2:D:132:LYS:CB   | 2:D:132:LYS:NZ   | 0.44     | 2.80        | 18     | 1     |
| 2:D:8:LYS:O      | 2:D:10:ALA:N     | 0.44     | 2.50        | 19     | 7     |
| 1:C:48:LEU:N     | 1:C:48:LEU:CD1   | 0.44     | 2.80        | 8      | 1     |
| 1:A:94:ASP:O     | 1:A:97:ASN:ND2   | 0.44     | 2.50        | 8      | 1     |
| 2:B:101:GLU:C    | 2:B:102:ASN:ND2  | 0.44     | 2.71        | 8      | 1     |
| 1:C:32:MET:C     | 1:C:34:LEU:N     | 0.44     | 2.69        | 16     | 1     |
| 2:B:119:GLY:C    | 2:B:121:GLU:H    | 0.44     | 2.16        | 16     | 2     |
| 1:C:33:PHE:O     | 1:C:36:PHE:O     | 0.44     | 2.35        | 14     | 1     |
| 2:B:67:VAL:CG1   | 3:B:147:HEC:C3B  | 0.44     | 2.96        | 19     | 1     |
| 1:C:2:LEU:HD12   | 1:C:6:ASP:OD2    | 0.44     | 2.12        | 19     | 1     |
| 2:B:106:LEU:HD13 | 3:B:147:HEC:HAB  | 0.44     | 1.85        | 3      | 2     |
| 2:B:146:HIS:C    | 2:B:146:HIS:ND1  | 0.44     | 2.71        | 7      | 1     |
| 2:B:82:LYS:HZ2   | 2:B:143:HIS:CD2  | 0.44     | 2.31        | 11     | 2     |
| 1:C:132:VAL:O    | 1:C:136:LEU:HD13 | 0.44     | 2.13        | 20     | 1     |
| 1:A:45:HIS:CD2   | 1:A:45:HIS:O     | 0.44     | 2.71        | 3      | 1     |
| 1:C:110:ALA:C    | 1:C:112:HIS:N    | 0.44     | 2.69        | 1      | 1     |
| 2:B:96:LEU:N     | 2:B:96:LEU:HD12  | 0.44     | 2.27        | 18     | 1     |
| 2:B:31:LEU:HD23  | 3:B:147:HEC:HBC2 | 0.44     | 1.89        | 10     | 1     |
| 1:C:137:THR:O    | 1:C:138:SER:O    | 0.44     | 2.36        | 3      | 3     |
| 2:D:2:HIS:CD2    | 2:D:2:HIS:C      | 0.44     | 2.90        | 14     | 1     |
| 2:D:56:GLY:O     | 2:D:57:ASN:ND2   | 0.44     | 2.51        | 19     | 1     |
| 2:B:67:VAL:CG2   | 3:B:147:HEC:NA   | 0.44     | 2.80        | 9      | 1     |
| 1:C:34:LEU:CD1   | 1:C:34:LEU:C     | 0.44     | 2.82        | 9      | 1     |
| 1:A:68:ASN:HD21  | 1:A:80:LEU:HD21  | 0.44     | 1.73        | 9      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 2:B:121:GLU:O   | 2:B:123:THR:N    | 0.44     | 2.48        | 9      | 1     |
| 1:A:118:THR:OG1 | 1:A:121:VAL:CB   | 0.44     | 2.66        | 20     | 2     |
| 2:B:58:PRO:C    | 2:B:60:VAL:N     | 0.44     | 2.71        | 11     | 1     |
| 1:C:74:ASP:O    | 1:C:75:ASP:CG    | 0.44     | 2.56        | 18     | 5     |
| 1:A:74:ASP:O    | 1:A:75:ASP:CG    | 0.44     | 2.56        | 18     | 5     |
| 1:C:127:LYS:C   | 1:C:129:LEU:N    | 0.44     | 2.70        | 2      | 7     |
| 2:D:44:SER:C    | 2:D:46:GLY:N     | 0.44     | 2.69        | 3      | 6     |
| 2:B:144:LYS:C   | 2:B:146:HIS:H    | 0.44     | 2.15        | 19     | 6     |
| 1:C:94:ASP:O    | 1:C:97:ASN:ND2   | 0.44     | 2.50        | 8      | 1     |
| 2:B:90:GLU:O    | 2:B:94:ASP:CB    | 0.44     | 2.65        | 16     | 1     |
| 1:C:29:LEU:HD13 | 1:C:58:HIS:CD2   | 0.44     | 2.48        | 14     | 1     |
| 2:D:95:LYS:O    | 2:D:97:HIS:CD2   | 0.44     | 2.70        | 19     | 1     |
| 2:B:67:VAL:HA   | 3:B:147:HEC:HBB  | 0.44     | 1.89        | 9      | 1     |
| 1:C:66:LEU:C    | 1:C:66:LEU:HD12  | 0.44     | 2.32        | 9      | 1     |
| 1:A:91:LEU:CD1  | 1:A:91:LEU:N     | 0.44     | 2.80        | 9      | 1     |
| 1:C:87:HIS:O    | 1:C:90:LYS:O     | 0.44     | 2.36        | 5      | 1     |
| 2:B:127:GLN:N   | 2:B:127:GLN:OE1  | 0.44     | 2.51        | 1      | 1     |
| 2:D:37:TRP:CD1  | 2:D:38:THR:HG23  | 0.44     | 2.47        | 10     | 2     |
| 1:A:84:SER:O    | 1:A:88:ALA:HB2   | 0.44     | 2.12        | 10     | 3     |
| 2:B:2:HIS:CE1   | 2:D:146:HIS:CD2  | 0.44     | 2.83        | 15     | 1     |
| 2:B:40:ARG:O    | 2:B:42:PHE:N     | 0.44     | 2.50        | 15     | 2     |
| 1:C:89:HIS:O    | 1:C:90:LYS:C     | 0.44     | 2.56        | 15     | 2     |
| 1:A:98:PHE:CZ   | 1:A:136:LEU:HD23 | 0.44     | 2.48        | 15     | 1     |
| 2:B:131:GLN:H   | 2:B:131:GLN:CD   | 0.44     | 2.16        | 16     | 2     |
| 1:C:101:LEU:O   | 1:C:101:LEU:HD23 | 0.44     | 2.13        | 19     | 1     |
| 1:C:115:ALA:HB1 | 1:C:121:VAL:HG13 | 0.44     | 1.89        | 1      | 3     |
| 1:A:33:PHE:CZ   | 1:A:46:PHE:CZ    | 0.44     | 3.06        | 9      | 1     |
| 2:B:130:TYR:O   | 2:B:133:VAL:HG12 | 0.44     | 2.13        | 9      | 1     |
| 1:C:68:ASN:HD21 | 1:C:80:LEU:HD21  | 0.44     | 1.73        | 9      | 1     |
| 1:C:91:LEU:N    | 1:C:91:LEU:CD1   | 0.44     | 2.80        | 9      | 1     |
| 1:A:50:HIS:ND1  | 1:A:50:HIS:C     | 0.44     | 2.70        | 9      | 1     |
| 1:C:78:ASN:O    | 1:C:81:SER:OG    | 0.44     | 2.36        | 9      | 1     |
| 2:B:99:ASP:O    | 2:B:102:ASN:OD1  | 0.44     | 2.36        | 6      | 2     |
| 1:A:106:LEU:CD1 | 1:A:122:HIS:CE1  | 0.44     | 2.99        | 4      | 1     |
| 1:C:68:ASN:HD21 | 1:C:79:ALA:CB    | 0.44     | 2.25        | 5      | 1     |
| 2:D:111:VAL:CG1 | 2:D:130:TYR:CD1  | 0.44     | 3.00        | 5      | 1     |
| 1:A:65:ALA:HB3  | 3:A:142:HEC:HMB3 | 0.44     | 1.90        | 20     | 1     |
| 1:A:110:ALA:C   | 1:A:112:HIS:H    | 0.44     | 2.15        | 1      | 1     |
| 1:C:62:VAL:HG12 | 1:C:63:ALA:N     | 0.44     | 2.28        | 1      | 2     |
| 1:C:113:LEU:CD1 | 1:C:113:LEU:C    | 0.44     | 2.86        | 12     | 1     |
| 1:C:127:LYS:CG  | 1:C:128:PHE:N    | 0.44     | 2.81        | 4      | 11    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:C:103:HIS:CB   | 2:D:108:ASN:ND2  | 0.44     | 2.80        | 10     | 1     |
| 2:D:145:TYR:O    | 2:D:146:HIS:O    | 0.44     | 2.36        | 10     | 2     |
| 2:B:145:TYR:O    | 2:B:146:HIS:O    | 0.44     | 2.36        | 10     | 2     |
| 2:D:114:LEU:O    | 2:D:116:HIS:N    | 0.44     | 2.50        | 20     | 2     |
| 1:C:106:LEU:N    | 1:C:106:LEU:CD1  | 0.44     | 2.80        | 8      | 2     |
| 2:D:101:GLU:C    | 2:D:102:ASN:ND2  | 0.44     | 2.71        | 8      | 1     |
| 2:D:131:GLN:CD   | 2:D:131:GLN:H    | 0.44     | 2.16        | 16     | 2     |
| 1:C:52:SER:C     | 1:C:54:GLN:H     | 0.44     | 2.15        | 1      | 5     |
| 1:A:52:SER:C     | 1:A:54:GLN:H     | 0.44     | 2.16        | 1      | 4     |
| 2:D:130:TYR:O    | 2:D:133:VAL:HG12 | 0.44     | 2.13        | 9      | 1     |
| 1:A:94:ASP:C     | 1:A:96:VAL:N     | 0.44     | 2.71        | 4      | 5     |
| 2:B:57:ASN:C     | 2:B:57:ASN:ND2   | 0.44     | 2.71        | 9      | 1     |
| 2:D:57:ASN:ND2   | 2:D:57:ASN:C     | 0.44     | 2.71        | 9      | 1     |
| 2:D:102:ASN:ND2  | 3:D:147:HEC:HMC2 | 0.44     | 2.27        | 7      | 1     |
| 1:A:132:VAL:O    | 1:A:136:LEU:HD13 | 0.44     | 2.13        | 20     | 1     |
| 1:A:101:LEU:HD22 | 3:A:142:HEC:HAB  | 0.44     | 1.89        | 1      | 1     |
| 1:A:121:VAL:CG1  | 1:A:122:HIS:CE1  | 0.44     | 3.01        | 12     | 1     |
| 2:B:108:ASN:O    | 2:B:112:CYS:SG   | 0.44     | 2.71        | 12     | 1     |
| 2:D:110:LEU:O    | 2:D:113:VAL:N    | 0.44     | 2.51        | 12     | 1     |
| 1:C:99:LYS:NZ    | 1:C:99:LYS:CB    | 0.44     | 2.81        | 2      | 1     |
| 3:A:142:HEC:CBB  | 3:A:142:HEC:HMB1 | 0.44     | 2.37        | 16     | 4     |
| 2:B:82:LYS:NZ    | 2:B:143:HIS:ND1  | 0.44     | 2.66        | 16     | 1     |
| 2:B:4:THR:O      | 2:B:7:GLU:N      | 0.44     | 2.46        | 16     | 3     |
| 2:B:2:HIS:CD2    | 2:B:2:HIS:C      | 0.44     | 2.90        | 14     | 1     |
| 2:B:67:VAL:HA    | 3:B:147:HEC:C4A  | 0.44     | 2.43        | 19     | 1     |
| 1:A:57:GLY:O     | 1:A:61:LYS:CE    | 0.44     | 2.66        | 9      | 1     |
| 1:C:68:ASN:ND2   | 1:C:80:LEU:HD21  | 0.44     | 2.28        | 9      | 1     |
| 2:D:139:ASN:HD22 | 2:D:139:ASN:N    | 0.44     | 2.10        | 6      | 1     |
| 2:D:33:VAL:CG1   | 2:D:34:VAL:H     | 0.44     | 2.23        | 3      | 1     |
| 2:B:33:VAL:CG1   | 2:B:34:VAL:H     | 0.44     | 2.23        | 3      | 1     |
| 2:B:97:HIS:ND1   | 1:C:37:PRO:O     | 0.44     | 2.51        | 3      | 1     |
| 2:D:102:ASN:C    | 2:D:104:ARG:N    | 0.44     | 2.70        | 17     | 1     |
| 1:A:27:GLU:CG    | 1:A:108:THR:OG1  | 0.44     | 2.66        | 1      | 1     |
| 2:D:42:PHE:CE2   | 3:D:147:HEC:CMB  | 0.44     | 2.91        | 12     | 1     |
| 2:D:145:TYR:CD2  | 2:D:145:TYR:O    | 0.44     | 2.71        | 12     | 1     |
| 1:A:69:ALA:CB    | 1:A:76:MET:SD    | 0.43     | 3.06        | 10     | 2     |
| 1:A:127:LYS:O    | 1:A:129:LEU:N    | 0.43     | 2.51        | 2      | 4     |
| 2:D:32:LEU:HB3   | 3:D:147:HEC:CMB  | 0.43     | 2.39        | 15     | 1     |
| 2:B:73:ASP:OD2   | 2:B:84:THR:OG1   | 0.43     | 2.37        | 15     | 1     |
| 1:C:108:THR:C    | 1:C:110:ALA:N    | 0.43     | 2.70        | 5      | 3     |
| 2:D:42:PHE:CE1   | 2:D:45:PHE:CZ    | 0.43     | 3.06        | 16     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:32:MET:C     | 1:A:34:LEU:N     | 0.43     | 2.69        | 16     | 1     |
| 2:D:19:ASN:C     | 2:D:21:ASP:H     | 0.43     | 2.16        | 11     | 4     |
| 2:B:19:ASN:C     | 2:B:21:ASP:H     | 0.43     | 2.16        | 11     | 3     |
| 2:B:90:GLU:O     | 2:B:94:ASP:N     | 0.43     | 2.45        | 16     | 1     |
| 2:D:67:VAL:CG1   | 3:D:147:HEC:C3B  | 0.43     | 2.96        | 19     | 1     |
| 1:A:101:LEU:O    | 1:A:101:LEU:HD23 | 0.43     | 2.12        | 19     | 1     |
| 1:A:115:ALA:HB1  | 1:A:121:VAL:HG13 | 0.43     | 1.90        | 19     | 3     |
| 1:C:127:LYS:HG3  | 1:C:128:PHE:N    | 0.43     | 2.28        | 19     | 3     |
| 1:A:127:LYS:HG3  | 1:A:128:PHE:N    | 0.43     | 2.28        | 3      | 3     |
| 2:D:99:ASP:O     | 2:D:102:ASN:OD1  | 0.43     | 2.36        | 13     | 2     |
| 1:A:91:LEU:H     | 1:A:91:LEU:CD1   | 0.43     | 2.25        | 11     | 1     |
| 2:D:41:PHE:C     | 2:D:42:PHE:CD1   | 0.43     | 2.91        | 6      | 2     |
| 1:C:76:MET:N     | 1:C:77:PRO:HD3   | 0.43     | 2.27        | 10     | 13    |
| 1:A:127:LYS:CG   | 1:A:128:PHE:N    | 0.43     | 2.81        | 4      | 9     |
| 2:D:82:LYS:CD    | 2:D:82:LYS:N     | 0.43     | 2.81        | 18     | 2     |
| 1:C:82:ALA:O     | 1:C:83:LEU:C     | 0.43     | 2.57        | 13     | 11    |
| 1:A:73:VAL:O     | 1:A:74:ASP:OD1   | 0.43     | 2.37        | 16     | 4     |
| 1:A:92:ARG:NH2   | 2:D:40:ARG:CG    | 0.43     | 2.81        | 15     | 1     |
| 2:D:73:ASP:OD2   | 2:D:84:THR:OG1   | 0.43     | 2.36        | 15     | 1     |
| 1:A:108:THR:C    | 1:A:110:ALA:N    | 0.43     | 2.70        | 5      | 2     |
| 1:C:17:VAL:O     | 1:C:18:GLY:O     | 0.43     | 2.36        | 16     | 3     |
| 2:B:75:LEU:HD12  | 2:B:75:LEU:H     | 0.43     | 1.73        | 16     | 1     |
| 2:D:56:GLY:O     | 2:D:57:ASN:HB2   | 0.43     | 2.12        | 19     | 1     |
| 1:C:56:LYS:CG    | 1:C:57:GLY:N     | 0.43     | 2.81        | 19     | 1     |
| 2:B:67:VAL:HG13  | 3:B:147:HEC:HMB3 | 0.43     | 1.90        | 9      | 1     |
| 1:C:33:PHE:CZ    | 1:C:46:PHE:CZ    | 0.43     | 3.06        | 9      | 1     |
| 1:C:2:LEU:CD2    | 1:C:6:ASP:OD1    | 0.43     | 2.67        | 9      | 1     |
| 1:A:23:GLU:O     | 1:A:27:GLU:OE1   | 0.43     | 2.36        | 9      | 1     |
| 2:D:102:ASN:C    | 2:D:102:ASN:HD22 | 0.43     | 2.16        | 7      | 1     |
| 2:D:111:VAL:CG1  | 2:D:130:TYR:CE1  | 0.43     | 3.00        | 5      | 1     |
| 1:A:88:ALA:C     | 1:A:90:LYS:H     | 0.43     | 2.16        | 17     | 1     |
| 1:A:115:ALA:CB   | 1:A:122:HIS:NE2  | 0.43     | 2.81        | 12     | 1     |
| 1:A:118:THR:O    | 1:A:121:VAL:HG12 | 0.43     | 2.13        | 12     | 2     |
| 1:A:38:THR:O     | 1:A:41:THR:CG2   | 0.43     | 2.67        | 15     | 2     |
| 1:C:127:LYS:O    | 1:C:129:LEU:N    | 0.43     | 2.51        | 2      | 3     |
| 1:A:46:PHE:CD1   | 1:A:46:PHE:C     | 0.43     | 2.92        | 8      | 1     |
| 1:A:108:THR:HG23 | 1:A:109:LEU:N    | 0.43     | 2.27        | 16     | 1     |
| 1:C:94:ASP:O     | 1:C:97:ASN:OD1   | 0.43     | 2.36        | 16     | 1     |
| 2:B:56:GLY:O     | 2:B:57:ASN:ND2   | 0.43     | 2.51        | 19     | 1     |
| 1:A:68:ASN:ND2   | 1:A:80:LEU:HD21  | 0.43     | 2.28        | 9      | 1     |
| 2:B:43:GLU:CD    | 2:B:44:SER:H     | 0.43     | 2.17        | 9      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 2:B:77:HIS:O    | 2:B:78:LEU:C     | 0.43     | 2.54        | 6      | 1     |
| 1:C:115:ALA:O   | 1:C:121:VAL:HG11 | 0.43     | 2.13        | 20     | 1     |
| 1:A:115:ALA:O   | 1:A:121:VAL:HG11 | 0.43     | 2.13        | 20     | 1     |
| 2:D:79:ASP:OD1  | 2:D:80:ASN:N     | 0.43     | 2.51        | 17     | 1     |
| 1:C:110:ALA:C   | 1:C:112:HIS:H    | 0.43     | 2.15        | 1      | 1     |
| 1:C:121:VAL:CG1 | 1:C:122:HIS:CE1  | 0.43     | 3.01        | 12     | 1     |
| 2:B:41:PHE:O    | 2:B:42:PHE:CG    | 0.43     | 2.72        | 11     | 1     |
| 2:B:123:THR:C   | 2:B:127:GLN:HE22 | 0.43     | 2.17        | 11     | 1     |
| 1:A:84:SER:OG   | 1:A:135:VAL:O    | 0.43     | 2.37        | 18     | 1     |
| 2:D:90:GLU:O    | 2:D:94:ASP:OD2   | 0.43     | 2.36        | 18     | 1     |
| 1:C:84:SER:O    | 1:C:88:ALA:HB2   | 0.43     | 2.12        | 10     | 3     |
| 1:C:38:THR:O    | 1:C:41:THR:CG2   | 0.43     | 2.67        | 15     | 2     |
| 2:D:36:PRO:C    | 2:D:38:THR:N     | 0.43     | 2.70        | 15     | 2     |
| 1:A:85:ASP:O    | 1:A:89:HIS:CB    | 0.43     | 2.67        | 16     | 1     |
| 1:A:29:LEU:HD13 | 1:A:58:HIS:CD2   | 0.43     | 2.48        | 14     | 1     |
| 2:D:26:GLU:O    | 2:D:28:LEU:N     | 0.43     | 2.52        | 14     | 1     |
| 1:C:92:ARG:O    | 1:C:93:VAL:C     | 0.43     | 2.55        | 17     | 2     |
| 1:A:2:LEU:HD12  | 1:A:6:ASP:OD2    | 0.43     | 2.12        | 19     | 1     |
| 2:D:143:HIS:CD2 | 2:D:143:HIS:O    | 0.43     | 2.72        | 9      | 1     |
| 1:C:118:THR:OG1 | 1:C:121:VAL:CB   | 0.43     | 2.66        | 20     | 2     |
| 1:C:134:THR:O   | 1:C:137:THR:OG1  | 0.43     | 2.36        | 7      | 1     |
| 1:A:113:LEU:CD1 | 1:A:113:LEU:C    | 0.43     | 2.86        | 12     | 2     |
| 1:C:32:MET:SD   | 3:C:142:HEC:CHC  | 0.43     | 3.06        | 12     | 1     |
| 2:D:42:PHE:HB3  | 3:D:147:HEC:HMA2 | 0.43     | 1.66        | 12     | 1     |
| 1:C:31:ARG:HH11 | 1:C:31:ARG:CG    | 0.43     | 2.26        | 12     | 1     |
| 2:D:31:LEU:O    | 2:D:35:TYR:O     | 0.43     | 2.37        | 12     | 1     |
| 1:C:52:SER:OG   | 1:C:55:VAL:HG23  | 0.43     | 2.14        | 11     | 1     |
| 2:B:40:ARG:HD2  | 1:C:92:ARG:NE    | 0.43     | 2.22        | 18     | 1     |
| 2:B:110:LEU:O   | 2:B:110:LEU:HD23 | 0.43     | 2.13        | 3      | 2     |
| 1:A:82:ALA:O    | 1:A:83:LEU:C     | 0.43     | 2.57        | 13     | 13    |
| 2:B:21:ASP:OD1  | 2:B:21:ASP:N     | 0.43     | 2.51        | 8      | 1     |
| 1:A:130:ALA:O   | 1:A:134:THR:OG1  | 0.43     | 2.34        | 8      | 1     |
| 2:D:82:LYS:NZ   | 2:D:143:HIS:ND1  | 0.43     | 2.66        | 16     | 1     |
| 2:D:75:LEU:H    | 2:D:75:LEU:HD12  | 0.43     | 1.73        | 16     | 1     |
| 2:D:134:VAL:O   | 2:D:136:GLY:N    | 0.43     | 2.51        | 19     | 3     |
| 2:D:4:THR:OG1   | 2:D:7:GLU:OE2    | 0.43     | 2.35        | 19     | 1     |
| 1:C:23:GLU:O    | 1:C:27:GLU:OE1   | 0.43     | 2.36        | 9      | 1     |
| 1:A:98:PHE:N    | 1:A:98:PHE:CD1   | 0.43     | 2.85        | 17     | 1     |
| 2:B:79:ASP:OD1  | 2:B:80:ASN:N     | 0.43     | 2.51        | 17     | 1     |
| 1:C:27:GLU:CG   | 1:C:108:THR:OG1  | 0.43     | 2.66        | 1      | 1     |
| 1:C:115:ALA:CB  | 1:C:122:HIS:NE2  | 0.43     | 2.81        | 12     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:110:LEU:O    | 2:B:113:VAL:N    | 0.43     | 2.49        | 13     | 2     |
| 1:A:31:ARG:NH1   | 1:A:31:ARG:CG    | 0.43     | 2.80        | 12     | 1     |
| 2:B:14:LEU:O     | 2:B:17:LYS:N     | 0.43     | 2.52        | 12     | 1     |
| 1:A:80:LEU:N     | 1:A:80:LEU:CD1   | 0.43     | 2.81        | 18     | 1     |
| 1:A:58:HIS:HD1   | 1:A:58:HIS:C     | 0.43     | 2.17        | 18     | 1     |
| 1:C:6:ASP:OD2    | 1:C:127:LYS:CE   | 0.43     | 2.67        | 10     | 1     |
| 1:A:6:ASP:OD2    | 1:A:127:LYS:CE   | 0.43     | 2.67        | 10     | 1     |
| 3:B:147:HEC:HBC2 | 2:D:31:LEU:HD23  | 0.43     | 1.91        | 15     | 1     |
| 1:C:11:LYS:H     | 1:C:11:LYS:CD    | 0.43     | 2.27        | 15     | 2     |
| 1:A:49:SER:O     | 1:A:52:SER:OG    | 0.43     | 2.36        | 14     | 1     |
| 2:B:56:GLY:O     | 2:B:57:ASN:CG    | 0.43     | 2.57        | 19     | 1     |
| 2:B:134:VAL:O    | 2:B:136:GLY:N    | 0.43     | 2.51        | 19     | 2     |
| 2:B:76:ALA:O     | 2:B:77:HIS:ND1   | 0.43     | 2.51        | 19     | 2     |
| 2:D:36:PRO:O     | 2:D:39:GLN:N     | 0.43     | 2.44        | 19     | 1     |
| 2:B:57:ASN:ND2   | 2:B:60:VAL:H     | 0.43     | 2.12        | 9      | 1     |
| 2:D:57:ASN:ND2   | 2:D:60:VAL:H     | 0.43     | 2.12        | 9      | 1     |
| 2:D:102:ASN:O    | 2:D:105:LEU:N    | 0.43     | 2.51        | 7      | 1     |
| 2:D:23:VAL:O     | 2:D:27:ALA:CB    | 0.43     | 2.67        | 5      | 1     |
| 1:C:71:ALA:C     | 1:C:72:HIS:CG    | 0.43     | 2.92        | 17     | 1     |
| 1:A:14:TRP:NE1   | 1:A:67:THR:OG1   | 0.43     | 2.49        | 17     | 1     |
| 2:B:127:GLN:O    | 2:B:130:TYR:N    | 0.43     | 2.51        | 1      | 1     |
| 2:D:36:PRO:O     | 3:D:147:HEC:C1C  | 0.43     | 2.67        | 12     | 1     |
| 2:B:145:TYR:O    | 2:B:145:TYR:CD2  | 0.43     | 2.71        | 12     | 1     |
| 2:D:142:ALA:O    | 2:D:145:TYR:N    | 0.43     | 2.48        | 12     | 1     |
| 2:D:19:ASN:N     | 2:D:19:ASN:HD22  | 0.43     | 2.12        | 11     | 1     |
| 1:C:2:LEU:C      | 1:C:3:SER:OG     | 0.43     | 2.57        | 18     | 1     |
| 2:B:82:LYS:CD    | 2:B:82:LYS:N     | 0.43     | 2.81        | 18     | 1     |
| 1:C:84:SER:OG    | 1:C:135:VAL:O    | 0.43     | 2.37        | 18     | 1     |
| 2:D:99:ASP:N     | 2:D:99:ASP:OD1   | 0.43     | 2.51        | 10     | 1     |
| 2:B:17:LYS:N     | 2:B:17:LYS:HD2   | 0.43     | 2.29        | 15     | 1     |
| 2:B:85:PHE:CZ    | 2:B:137:VAL:HG13 | 0.43     | 2.49        | 16     | 1     |
| 2:B:104:ARG:O    | 2:B:108:ASN:OD1  | 0.43     | 2.37        | 3      | 3     |
| 2:D:67:VAL:HA    | 3:D:147:HEC:HHB  | 0.43     | 1.89        | 9      | 1     |
| 2:B:131:GLN:O    | 2:B:135:ALA:N    | 0.43     | 2.49        | 9      | 1     |
| 1:A:96:VAL:CG1   | 2:D:99:ASP:OD1   | 0.43     | 2.66        | 6      | 1     |
| 1:C:1:VAL:HG12   | 1:C:1:VAL:O      | 0.43     | 2.13        | 6      | 1     |
| 2:B:102:ASN:O    | 2:B:105:LEU:N    | 0.43     | 2.51        | 7      | 1     |
| 2:B:127:GLN:HE22 | 2:B:131:GLN:CG   | 0.43     | 2.27        | 4      | 1     |
| 2:B:119:GLY:O    | 2:B:121:GLU:N    | 0.43     | 2.52        | 5      | 1     |
| 1:A:100:LEU:C    | 1:A:102:SER:N    | 0.43     | 2.72        | 20     | 1     |
| 2:D:110:LEU:HD23 | 2:D:110:LEU:O    | 0.43     | 2.13        | 3      | 2     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 2:B:104:ARG:NH2 | 2:D:146:HIS:C    | 0.43     | 2.72        | 17     | 1     |
| 1:C:75:ASP:O    | 1:C:78:ASN:OD1   | 0.43     | 2.37        | 17     | 1     |
| 2:D:41:PHE:O    | 2:D:42:PHE:CG    | 0.43     | 2.72        | 11     | 1     |
| 1:A:52:SER:OG   | 1:A:55:VAL:HG23  | 0.43     | 2.14        | 11     | 1     |
| 2:B:41:PHE:C    | 2:B:42:PHE:CD1   | 0.43     | 2.91        | 6      | 2     |
| 2:B:90:GLU:O    | 2:B:94:ASP:OD2   | 0.43     | 2.36        | 18     | 1     |
| 1:C:6:ASP:OD1   | 1:C:6:ASP:N      | 0.43     | 2.50        | 10     | 1     |
| 1:C:98:PHE:CZ   | 1:C:136:LEU:HD23 | 0.43     | 2.48        | 15     | 1     |
| 1:A:89:HIS:O    | 1:A:90:LYS:C     | 0.43     | 2.56        | 15     | 2     |
| 1:A:118:THR:OG1 | 1:A:121:VAL:HG23 | 0.43     | 2.14        | 15     | 1     |
| 2:D:67:VAL:HA   | 3:D:147:HEC:C4A  | 0.43     | 2.43        | 19     | 1     |
| 2:D:50:THR:O    | 2:D:52:ASP:N     | 0.43     | 2.52        | 9      | 1     |
| 1:A:78:ASN:O    | 1:A:81:SER:OG    | 0.43     | 2.36        | 9      | 1     |
| 1:C:14:TRP:NE1  | 1:C:67:THR:OG1   | 0.43     | 2.49        | 17     | 2     |
| 2:B:102:ASN:C   | 2:B:102:ASN:HD22 | 0.43     | 2.16        | 7      | 1     |
| 2:B:45:PHE:O    | 2:B:46:GLY:O     | 0.43     | 2.37        | 4      | 1     |
| 1:A:1:VAL:CG2   | 1:A:131:SER:OG   | 0.43     | 2.67        | 4      | 1     |
| 2:B:119:GLY:C   | 2:B:121:GLU:N    | 0.43     | 2.72        | 5      | 1     |
| 2:D:119:GLY:O   | 2:D:121:GLU:N    | 0.43     | 2.52        | 5      | 1     |
| 1:C:45:HIS:CD2  | 1:C:45:HIS:O     | 0.43     | 2.71        | 3      | 1     |
| 1:C:11:LYS:NZ   | 1:C:70:VAL:HG13  | 0.43     | 2.29        | 1      | 1     |
| 2:D:14:LEU:O    | 2:D:17:LYS:N     | 0.43     | 2.52        | 12     | 1     |
| 2:D:26:GLU:O    | 2:D:30:ARG:NH1   | 0.43     | 2.52        | 11     | 1     |
| 1:A:118:THR:OG1 | 1:A:118:THR:O    | 0.43     | 2.36        | 18     | 2     |
| 1:C:73:VAL:O    | 1:C:74:ASP:OD1   | 0.43     | 2.37        | 16     | 3     |
| 1:C:85:ASP:O    | 1:C:89:HIS:CB    | 0.43     | 2.67        | 16     | 1     |
| 2:D:85:PHE:CZ   | 2:D:137:VAL:HG13 | 0.43     | 2.49        | 16     | 1     |
| 2:D:82:LYS:NZ   | 2:D:143:HIS:CG   | 0.43     | 2.87        | 16     | 1     |
| 2:B:37:TRP:O    | 2:B:39:GLN:N     | 0.43     | 2.51        | 14     | 1     |
| 1:C:57:GLY:O    | 1:C:61:LYS:CE    | 0.43     | 2.66        | 9      | 1     |
| 1:C:127:LYS:HD2 | 1:C:128:PHE:N    | 0.43     | 2.29        | 7      | 2     |
| 1:C:1:VAL:CG2   | 1:C:131:SER:OG   | 0.43     | 2.67        | 4      | 1     |
| 1:C:64:ASP:O    | 1:C:68:ASN:N     | 0.43     | 2.41        | 4      | 1     |
| 1:A:96:VAL:HG21 | 2:D:99:ASP:CG    | 0.43     | 2.34        | 5      | 1     |
| 1:C:103:HIS:CD2 | 2:D:108:ASN:ND2  | 0.43     | 2.86        | 5      | 1     |
| 2:B:23:VAL:O    | 2:B:27:ALA:CB    | 0.43     | 2.67        | 5      | 1     |
| 1:A:103:HIS:CD2 | 2:B:108:ASN:ND2  | 0.43     | 2.86        | 5      | 1     |
| 1:C:130:ALA:O   | 1:C:134:THR:CB   | 0.43     | 2.67        | 20     | 1     |
| 2:D:106:LEU:O   | 2:D:106:LEU:HD23 | 0.43     | 2.13        | 3      | 1     |
| 1:C:118:THR:O   | 1:C:121:VAL:HG12 | 0.43     | 2.13        | 12     | 2     |
| 2:D:105:LEU:O   | 2:D:108:ASN:N    | 0.43     | 2.50        | 10     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:D:100:PRO:C    | 2:D:102:ASN:HD22 | 0.43     | 2.17        | 15     | 1     |
| 2:D:114:LEU:C    | 2:D:116:HIS:N    | 0.43     | 2.71        | 20     | 2     |
| 1:C:118:THR:OG1  | 1:C:121:VAL:HG23 | 0.43     | 2.14        | 15     | 1     |
| 2:D:17:LYS:HD2   | 2:D:17:LYS:H     | 0.43     | 1.74        | 8      | 1     |
| 2:D:119:GLY:C    | 2:D:121:GLU:H    | 0.43     | 2.16        | 16     | 2     |
| 2:B:6:GLU:N      | 2:B:6:GLU:OE1    | 0.43     | 2.52        | 19     | 1     |
| 1:A:2:LEU:CD2    | 1:A:6:ASP:OD1    | 0.43     | 2.67        | 9      | 1     |
| 1:A:91:LEU:H     | 1:A:91:LEU:HD12  | 0.43     | 1.71        | 9      | 1     |
| 1:A:27:GLU:N     | 1:A:27:GLU:CD    | 0.43     | 2.72        | 9      | 1     |
| 2:D:5:PRO:O      | 2:D:9:SER:OG     | 0.43     | 2.34        | 6      | 2     |
| 2:D:127:GLN:HE22 | 2:D:131:GLN:CG   | 0.43     | 2.27        | 4      | 1     |
| 2:D:42:PHE:CG    | 2:D:43:GLU:N     | 0.43     | 2.87        | 5      | 3     |
| 1:A:130:ALA:O    | 1:A:134:THR:CB   | 0.43     | 2.67        | 20     | 1     |
| 2:B:106:LEU:CD2  | 2:B:106:LEU:C    | 0.43     | 2.86        | 3      | 1     |
| 1:A:71:ALA:C     | 1:A:72:HIS:CG    | 0.43     | 2.92        | 17     | 1     |
| 1:A:75:ASP:O     | 1:A:78:ASN:OD1   | 0.43     | 2.37        | 17     | 1     |
| 2:B:68:LEU:C     | 2:B:68:LEU:HD23  | 0.43     | 2.33        | 17     | 1     |
| 1:A:17:VAL:HG11  | 1:A:21:ALA:HB2   | 0.43     | 1.91        | 1      | 1     |
| 1:A:118:THR:O    | 1:A:118:THR:OG1  | 0.43     | 2.37        | 13     | 2     |
| 1:A:46:PHE:O     | 1:A:47:ASP:OD1   | 0.43     | 2.37        | 2      | 1     |
| 1:A:47:ASP:OD1   | 1:A:47:ASP:O     | 0.43     | 2.37        | 2      | 1     |
| 2:D:104:ARG:O    | 2:D:108:ASN:ND2  | 0.43     | 2.52        | 2      | 1     |
| 2:B:96:LEU:O     | 2:B:97:HIS:C     | 0.42     | 2.57        | 20     | 5     |
| 2:D:96:LEU:O     | 2:D:97:HIS:C     | 0.42     | 2.57        | 20     | 6     |
| 2:D:117:HIS:O    | 2:D:117:HIS:ND1  | 0.42     | 2.49        | 10     | 1     |
| 2:B:48:LEU:O     | 2:B:49:SER:C     | 0.42     | 2.58        | 10     | 2     |
| 2:B:82:LYS:HZ1   | 2:D:82:LYS:HZ1   | 0.42     | 0.50        | 15     | 1     |
| 2:B:82:LYS:NZ    | 2:B:143:HIS:CG   | 0.42     | 2.87        | 16     | 1     |
| 2:B:80:ASN:ND2   | 2:B:80:ASN:O     | 0.42     | 2.52        | 14     | 1     |
| 2:D:80:ASN:ND2   | 2:D:80:ASN:O     | 0.42     | 2.52        | 14     | 1     |
| 1:A:61:LYS:HB3   | 3:A:142:HEC:CMA  | 0.42     | 2.44        | 17     | 2     |
| 1:A:56:LYS:CG    | 1:A:57:GLY:N     | 0.42     | 2.81        | 19     | 1     |
| 1:C:63:ALA:O     | 1:C:67:THR:OG1   | 0.42     | 2.30        | 9      | 2     |
| 3:C:142:HEC:HBB3 | 3:C:142:HEC:CMB  | 0.42     | 2.39        | 6      | 1     |
| 1:A:117:PHE:CE1  | 2:B:116:HIS:CE1  | 0.42     | 3.07        | 4      | 1     |
| 1:C:32:MET:HE3   | 3:C:142:HEC:CBC  | 0.42     | 2.44        | 5      | 2     |
| 2:B:42:PHE:CG    | 2:B:43:GLU:N     | 0.42     | 2.87        | 5      | 2     |
| 2:B:146:HIS:ND1  | 2:D:135:ALA:HB1  | 0.42     | 2.28        | 3      | 1     |
| 1:A:98:PHE:CD1   | 1:A:99:LYS:N     | 0.42     | 2.87        | 3      | 1     |
| 1:C:31:ARG:CG    | 1:C:31:ARG:NH1   | 0.42     | 2.80        | 12     | 1     |
| 2:D:146:HIS:OXT  | 2:D:146:HIS:ND1  | 0.42     | 2.52        | 11     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:C:69:ALA:CB    | 1:C:76:MET:SD    | 0.42     | 3.07        | 10     | 2     |
| 2:B:77:HIS:C     | 2:B:79:ASP:H     | 0.42     | 2.17        | 14     | 2     |
| 2:B:40:ARG:C     | 2:B:42:PHE:H     | 0.42     | 2.17        | 15     | 1     |
| 2:B:20:VAL:C     | 2:B:22:GLU:H     | 0.42     | 2.18        | 15     | 1     |
| 1:C:9:ASN:C      | 1:C:124:SER:OG   | 0.42     | 2.57        | 8      | 1     |
| 2:D:42:PHE:CZ    | 2:D:45:PHE:CD2   | 0.42     | 3.07        | 8      | 1     |
| 2:B:80:ASN:O     | 2:B:80:ASN:OD1   | 0.42     | 2.38        | 8      | 1     |
| 2:B:17:LYS:N     | 2:B:17:LYS:CD    | 0.42     | 2.79        | 14     | 2     |
| 2:D:37:TRP:C     | 2:D:39:GLN:H     | 0.42     | 2.17        | 14     | 1     |
| 2:B:26:GLU:O     | 2:B:28:LEU:N     | 0.42     | 2.52        | 14     | 1     |
| 2:B:67:VAL:CG1   | 3:B:147:HEC:NB   | 0.42     | 2.76        | 19     | 1     |
| 1:C:53:ALA:O     | 1:C:54:GLN:C     | 0.42     | 2.58        | 19     | 2     |
| 2:D:76:ALA:O     | 2:D:77:HIS:ND1   | 0.42     | 2.51        | 19     | 2     |
| 3:C:142:HEC:HMB1 | 3:C:142:HEC:CBB  | 0.42     | 2.34        | 1      | 2     |
| 2:B:3:LEU:H      | 2:B:3:LEU:CD1    | 0.42     | 2.03        | 6      | 1     |
| 1:A:31:ARG:O     | 1:A:35:SER:OG    | 0.42     | 2.37        | 4      | 1     |
| 1:A:87:HIS:O     | 1:A:90:LYS:O     | 0.42     | 2.36        | 5      | 1     |
| 1:C:107:VAL:HG11 | 2:D:127:GLN:NE2  | 0.42     | 2.29        | 17     | 1     |
| 1:C:98:PHE:CD1   | 1:C:98:PHE:N     | 0.42     | 2.85        | 17     | 1     |
| 2:B:104:ARG:O    | 2:B:108:ASN:ND2  | 0.42     | 2.52        | 2      | 1     |
| 1:A:113:LEU:HD12 | 1:A:113:LEU:C    | 0.42     | 2.35        | 18     | 1     |
| 2:D:88:LEU:HD12  | 2:D:88:LEU:N     | 0.42     | 2.29        | 18     | 2     |
| 2:D:110:LEU:O    | 2:D:110:LEU:HD23 | 0.42     | 2.15        | 18     | 1     |
| 1:A:7:LYS:O      | 1:A:8:THR:C      | 0.42     | 2.58        | 1      | 3     |
| 2:B:100:PRO:C    | 2:B:102:ASN:HD22 | 0.42     | 2.18        | 15     | 1     |
| 1:C:84:SER:CB    | 1:C:138:SER:HG   | 0.42     | 2.26        | 16     | 1     |
| 2:B:114:LEU:CD1  | 2:B:130:TYR:OH   | 0.42     | 2.67        | 14     | 1     |
| 2:D:56:GLY:O     | 2:D:57:ASN:CG    | 0.42     | 2.56        | 19     | 1     |
| 2:D:58:PRO:C     | 2:D:60:VAL:N     | 0.42     | 2.71        | 11     | 2     |
| 2:B:4:THR:OG1    | 2:B:7:GLU:OE2    | 0.42     | 2.35        | 19     | 1     |
| 2:B:36:PRO:O     | 2:B:39:GLN:N     | 0.42     | 2.44        | 19     | 1     |
| 2:B:112:CYS:O    | 2:B:116:HIS:CE1  | 0.42     | 2.72        | 9      | 1     |
| 2:D:75:LEU:HD12  | 2:D:75:LEU:H     | 0.42     | 1.74        | 9      | 1     |
| 2:D:26:GLU:N     | 2:D:26:GLU:OE2   | 0.42     | 2.53        | 20     | 1     |
| 1:A:61:LYS:CG    | 3:A:142:HEC:HAA2 | 0.42     | 2.44        | 17     | 1     |
| 1:A:41:THR:CB    | 2:D:94:ASP:O     | 0.42     | 2.67        | 1      | 1     |
| 2:B:19:ASN:N     | 2:B:19:ASN:HD22  | 0.42     | 2.12        | 11     | 1     |
| 1:C:46:PHE:O     | 1:C:47:ASP:OD1   | 0.42     | 2.37        | 2      | 1     |
| 2:B:96:LEU:N     | 2:B:96:LEU:CD1   | 0.42     | 2.82        | 18     | 1     |
| 2:B:80:ASN:C     | 2:B:82:LYS:N     | 0.42     | 2.72        | 10     | 1     |
| 2:D:17:LYS:HD2   | 2:D:17:LYS:N     | 0.42     | 2.29        | 15     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:9:ASN:C      | 1:A:124:SER:OG   | 0.42     | 2.58        | 8      | 1     |
| 1:A:34:LEU:C     | 1:A:34:LEU:CD1   | 0.42     | 2.82        | 9      | 1     |
| 1:A:1:VAL:HG12   | 1:A:1:VAL:O      | 0.42     | 2.13        | 6      | 1     |
| 2:B:97:HIS:ND1   | 1:C:38:THR:HA    | 0.42     | 2.29        | 7      | 1     |
| 2:D:26:GLU:O     | 2:D:30:ARG:CG    | 0.42     | 2.67        | 7      | 1     |
| 2:B:42:PHE:CD2   | 2:B:45:PHE:CD1   | 0.42     | 3.07        | 4      | 1     |
| 2:B:109:VAL:O    | 2:B:112:CYS:SG   | 0.42     | 2.71        | 20     | 1     |
| 2:D:105:LEU:O    | 2:D:105:LEU:HD23 | 0.42     | 2.15        | 20     | 1     |
| 1:A:47:ASP:CG    | 1:A:54:GLN:HE22  | 0.42     | 2.18        | 17     | 1     |
| 1:C:47:ASP:CG    | 1:C:54:GLN:HE22  | 0.42     | 2.18        | 17     | 1     |
| 1:C:17:VAL:HG11  | 1:C:21:ALA:HB2   | 0.42     | 1.91        | 1      | 1     |
| 2:B:144:LYS:C    | 2:B:146:HIS:HD1  | 0.42     | 2.17        | 11     | 1     |
| 2:B:26:GLU:O     | 2:B:30:ARG:NH1   | 0.42     | 2.52        | 11     | 1     |
| 1:C:93:VAL:CG1   | 1:C:94:ASP:H     | 0.42     | 2.21        | 18     | 1     |
| 1:C:118:THR:OG1  | 1:C:118:THR:O    | 0.42     | 2.36        | 18     | 1     |
| 1:C:113:LEU:C    | 1:C:113:LEU:HD12 | 0.42     | 2.35        | 18     | 1     |
| 1:C:80:LEU:CD1   | 1:C:80:LEU:N     | 0.42     | 2.81        | 18     | 1     |
| 1:A:103:HIS:CB   | 2:B:108:ASN:ND2  | 0.42     | 2.81        | 10     | 1     |
| 2:B:19:ASN:O     | 2:B:20:VAL:C     | 0.42     | 2.58        | 10     | 4     |
| 2:B:145:TYR:O    | 2:B:146:HIS:C    | 0.42     | 2.58        | 5      | 4     |
| 2:D:84:THR:C     | 2:D:86:ALA:H     | 0.42     | 2.18        | 15     | 3     |
| 1:A:36:PHE:CD2   | 1:A:100:LEU:HD21 | 0.42     | 2.50        | 15     | 1     |
| 1:A:115:ALA:HB1  | 1:A:121:VAL:CG1  | 0.42     | 2.44        | 5      | 4     |
| 1:C:115:ALA:HB1  | 1:C:121:VAL:CG1  | 0.42     | 2.44        | 5      | 4     |
| 2:D:104:ARG:O    | 2:D:108:ASN:OD1  | 0.42     | 2.37        | 3      | 3     |
| 1:C:103:HIS:O    | 1:C:103:HIS:CD2  | 0.42     | 2.73        | 19     | 1     |
| 2:D:112:CYS:O    | 2:D:116:HIS:CE1  | 0.42     | 2.72        | 9      | 1     |
| 2:D:114:LEU:HD12 | 2:D:114:LEU:H    | 0.42     | 1.71        | 9      | 1     |
| 2:B:50:THR:O     | 2:B:52:ASP:N     | 0.42     | 2.52        | 9      | 2     |
| 1:A:50:HIS:ND1   | 1:A:50:HIS:O     | 0.42     | 2.53        | 6      | 1     |
| 2:D:119:GLY:C    | 2:D:121:GLU:N    | 0.42     | 2.72        | 5      | 1     |
| 1:C:61:LYS:CG    | 3:C:142:HEC:HAA2 | 0.42     | 2.44        | 17     | 1     |
| 1:A:47:ASP:OD2   | 1:A:54:GLN:OE1   | 0.42     | 2.37        | 17     | 1     |
| 1:C:88:ALA:C     | 1:C:90:LYS:H     | 0.42     | 2.16        | 17     | 1     |
| 1:C:97:ASN:C     | 1:C:99:LYS:N     | 0.42     | 2.73        | 13     | 1     |
| 1:C:91:LEU:H     | 1:C:91:LEU:HD12  | 0.42     | 1.74        | 11     | 1     |
| 2:D:46:GLY:O     | 2:D:47:ASP:O     | 0.42     | 2.37        | 11     | 1     |
| 1:C:36:PHE:CD2   | 1:C:100:LEU:HD21 | 0.42     | 2.50        | 15     | 1     |
| 2:D:80:ASN:O     | 2:D:80:ASN:OD1   | 0.42     | 2.38        | 8      | 1     |
| 2:D:39:GLN:OE1   | 2:D:39:GLN:O     | 0.42     | 2.36        | 16     | 1     |
| 2:D:114:LEU:CD1  | 2:D:130:TYR:OH   | 0.42     | 2.68        | 14     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:D:43:GLU:CD    | 2:D:44:SER:H     | 0.42     | 2.17        | 9      | 1     |
| 2:B:75:LEU:H     | 2:B:75:LEU:HD12  | 0.42     | 1.74        | 9      | 1     |
| 2:D:42:PHE:CD2   | 2:D:45:PHE:CD1   | 0.42     | 3.07        | 4      | 1     |
| 2:D:116:HIS:HD1  | 2:D:116:HIS:C    | 0.42     | 2.18        | 11     | 2     |
| 2:B:114:LEU:C    | 2:B:116:HIS:N    | 0.42     | 2.71        | 20     | 1     |
| 2:B:105:LEU:O    | 2:B:105:LEU:HD23 | 0.42     | 2.15        | 20     | 1     |
| 2:D:106:LEU:CD2  | 2:D:106:LEU:C    | 0.42     | 2.86        | 3      | 1     |
| 1:C:118:THR:O    | 1:C:118:THR:OG1  | 0.42     | 2.38        | 17     | 2     |
| 1:C:36:PHE:C     | 3:C:142:HEC:HMC1 | 0.42     | 2.34        | 12     | 1     |
| 1:A:31:ARG:CG    | 1:A:31:ARG:HH11  | 0.42     | 2.27        | 12     | 1     |
| 2:B:63:HIS:NE2   | 3:B:147:HEC:HHA  | 0.42     | 2.24        | 2      | 1     |
| 2:D:105:LEU:N    | 2:D:105:LEU:CD2  | 0.42     | 2.83        | 2      | 1     |
| 2:B:3:LEU:HD13   | 2:B:8:LYS:HG3    | 0.42     | 1.91        | 10     | 1     |
| 2:D:3:LEU:HD13   | 2:D:8:LYS:HG3    | 0.42     | 1.91        | 10     | 1     |
| 1:A:48:LEU:C     | 1:A:50:HIS:H     | 0.42     | 2.18        | 15     | 1     |
| 2:B:42:PHE:CZ    | 2:B:45:PHE:CD2   | 0.42     | 3.07        | 8      | 1     |
| 2:B:17:LYS:H     | 2:B:17:LYS:HE2   | 0.42     | 1.74        | 8      | 1     |
| 2:D:100:PRO:O    | 2:D:102:ASN:OD1  | 0.42     | 2.37        | 19     | 1     |
| 1:A:103:HIS:O    | 1:A:103:HIS:CD2  | 0.42     | 2.73        | 19     | 1     |
| 1:C:2:LEU:HD11   | 1:C:127:LYS:HE3  | 0.42     | 1.91        | 9      | 1     |
| 2:D:30:ARG:O     | 2:D:31:LEU:C     | 0.42     | 2.58        | 9      | 1     |
| 1:A:127:LYS:HD2  | 1:A:128:PHE:N    | 0.42     | 2.29        | 7      | 1     |
| 1:C:113:LEU:C    | 1:C:113:LEU:CD1  | 0.42     | 2.87        | 7      | 1     |
| 2:B:26:GLU:O     | 2:B:30:ARG:CG    | 0.42     | 2.67        | 7      | 1     |
| 2:D:45:PHE:O     | 2:D:46:GLY:O     | 0.42     | 2.37        | 4      | 1     |
| 1:C:98:PHE:CD1   | 1:C:99:LYS:N     | 0.42     | 2.87        | 3      | 1     |
| 1:C:47:ASP:OD2   | 1:C:54:GLN:OE1   | 0.42     | 2.37        | 17     | 1     |
| 1:A:97:ASN:C     | 1:A:99:LYS:N     | 0.42     | 2.73        | 13     | 1     |
| 2:D:77:HIS:C     | 2:D:79:ASP:H     | 0.42     | 2.18        | 18     | 3     |
| 1:A:11:LYS:CD    | 1:A:11:LYS:H     | 0.42     | 2.27        | 15     | 1     |
| 2:D:143:HIS:CG   | 2:D:143:HIS:O    | 0.42     | 2.73        | 16     | 1     |
| 2:B:143:HIS:CG   | 2:B:143:HIS:O    | 0.42     | 2.73        | 16     | 1     |
| 2:D:26:GLU:C     | 2:D:28:LEU:N     | 0.42     | 2.73        | 14     | 1     |
| 2:B:52:ASP:C     | 2:B:54:VAL:N     | 0.42     | 2.73        | 4      | 3     |
| 2:D:55:MET:O     | 2:D:57:ASN:OD1   | 0.42     | 2.37        | 19     | 1     |
| 2:B:106:LEU:HD12 | 3:B:147:HEC:C1C  | 0.42     | 2.41        | 9      | 1     |
| 1:C:27:GLU:CD    | 1:C:27:GLU:N     | 0.42     | 2.72        | 9      | 1     |
| 1:C:108:THR:O    | 1:C:109:LEU:C    | 0.42     | 2.58        | 7      | 1     |
| 2:B:130:TYR:O    | 2:B:132:LYS:N    | 0.42     | 2.53        | 7      | 1     |
| 2:B:71:PHE:O     | 2:B:75:LEU:CD2   | 0.42     | 2.68        | 4      | 1     |
| 2:B:106:LEU:HD23 | 2:B:106:LEU:O    | 0.42     | 2.13        | 3      | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:C:119:PRO:HA  | 2:D:33:VAL:HG21  | 0.42     | 1.92        | 3      | 1     |
| 2:D:65:LYS:O    | 2:D:69:GLY:N     | 0.42     | 2.53        | 3      | 1     |
| 2:B:104:ARG:NH2 | 2:D:146:HIS:O    | 0.42     | 2.53        | 17     | 1     |
| 1:C:115:ALA:HB2 | 1:C:122:HIS:CE1  | 0.42     | 2.50        | 17     | 1     |
| 1:A:81:SER:O    | 1:A:85:ASP:OD1   | 0.42     | 2.37        | 17     | 1     |
| 2:B:145:TYR:O   | 2:B:145:TYR:CG   | 0.42     | 2.72        | 18     | 1     |
| 1:C:7:LYS:CG    | 1:C:8:THR:N      | 0.42     | 2.83        | 9      | 2     |
| 1:A:86:LEU:HD11 | 3:A:142:HEC:HBD1 | 0.42     | 1.92        | 15     | 1     |
| 1:C:86:LEU:HD11 | 3:C:142:HEC:HBD1 | 0.42     | 1.92        | 15     | 1     |
| 1:C:48:LEU:C    | 1:C:50:HIS:H     | 0.42     | 2.17        | 15     | 1     |
| 1:C:34:LEU:C    | 1:C:36:PHE:H     | 0.42     | 2.16        | 12     | 2     |
| 1:A:34:LEU:C    | 1:A:36:PHE:H     | 0.42     | 2.17        | 12     | 2     |
| 2:D:17:LYS:H    | 2:D:17:LYS:HE2   | 0.42     | 1.74        | 8      | 1     |
| 1:C:49:SER:O    | 1:C:50:HIS:CB    | 0.42     | 2.68        | 19     | 1     |
| 1:A:53:ALA:O    | 1:A:54:GLN:C     | 0.42     | 2.58        | 19     | 1     |
| 2:B:100:PRO:O   | 2:B:102:ASN:OD1  | 0.42     | 2.37        | 19     | 2     |
| 2:D:6:GLU:OE1   | 2:D:6:GLU:N      | 0.42     | 2.52        | 19     | 1     |
| 2:B:30:ARG:O    | 2:B:31:LEU:C     | 0.42     | 2.58        | 9      | 1     |
| 1:A:12:ALA:O    | 1:A:15:GLY:N     | 0.42     | 2.51        | 9      | 2     |
| 1:C:50:HIS:ND1  | 1:C:50:HIS:O     | 0.42     | 2.53        | 6      | 1     |
| 1:C:94:ASP:C    | 1:C:96:VAL:H     | 0.42     | 2.18        | 4      | 2     |
| 2:B:139:ASN:O   | 2:B:142:ALA:N    | 0.42     | 2.49        | 5      | 1     |
| 2:D:14:LEU:CD1  | 2:D:14:LEU:N     | 0.42     | 2.82        | 20     | 1     |
| 1:A:94:ASP:OD2  | 2:D:40:ARG:CZ    | 0.42     | 2.68        | 3      | 1     |
| 1:C:81:SER:O    | 1:C:85:ASP:OD1   | 0.42     | 2.37        | 17     | 2     |
| 1:A:63:ALA:O    | 1:A:67:THR:OG1   | 0.42     | 2.34        | 17     | 1     |
| 1:A:11:LYS:NZ   | 1:A:70:VAL:HG13  | 0.42     | 2.29        | 1      | 1     |
| 2:B:31:LEU:O    | 2:B:35:TYR:O     | 0.42     | 2.37        | 12     | 1     |
| 2:D:123:THR:C   | 2:D:127:GLN:HE22 | 0.42     | 2.17        | 11     | 1     |
| 2:B:105:LEU:N   | 2:B:105:LEU:CD2  | 0.42     | 2.83        | 2      | 1     |
| 1:A:92:ARG:NE   | 2:D:40:ARG:HD2   | 0.42     | 2.20        | 18     | 1     |
| 1:C:129:LEU:O   | 1:C:133:SER:CB   | 0.42     | 2.67        | 18     | 1     |
| 1:A:129:LEU:O   | 1:A:133:SER:CB   | 0.42     | 2.67        | 18     | 1     |
| 1:A:2:LEU:C     | 1:A:3:SER:OG     | 0.42     | 2.57        | 18     | 1     |
| 2:D:80:ASN:C    | 2:D:82:LYS:N     | 0.42     | 2.72        | 10     | 1     |
| 2:D:145:TYR:O   | 2:D:146:HIS:C    | 0.42     | 2.57        | 16     | 4     |
| 1:C:117:PHE:O   | 1:C:117:PHE:CG   | 0.42     | 2.73        | 10     | 1     |
| 2:B:42:PHE:O    | 2:B:45:PHE:N     | 0.42     | 2.48        | 10     | 1     |
| 2:D:90:GLU:O    | 2:D:94:ASP:N     | 0.42     | 2.45        | 16     | 2     |
| 1:C:3:SER:OG    | 1:C:6:ASP:OD1    | 0.42     | 2.37        | 16     | 1     |
| 2:D:52:ASP:C    | 2:D:54:VAL:N     | 0.42     | 2.73        | 4      | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:95:PRO:O     | 1:A:96:VAL:C     | 0.42     | 2.58        | 5      | 4     |
| 2:D:81:LEU:O     | 2:D:84:THR:OG1   | 0.42     | 2.37        | 6      | 1     |
| 2:D:146:HIS:C    | 2:D:146:HIS:ND1  | 0.42     | 2.71        | 7      | 1     |
| 1:A:115:ALA:HB2  | 1:A:122:HIS:CE1  | 0.42     | 2.50        | 17     | 1     |
| 2:D:18:VAL:O     | 2:D:20:VAL:N     | 0.42     | 2.53        | 12     | 1     |
| 1:C:109:LEU:O    | 1:C:113:LEU:N    | 0.41     | 2.53        | 14     | 6     |
| 1:A:7:LYS:CG     | 1:A:8:THR:N      | 0.41     | 2.83        | 18     | 2     |
| 2:D:40:ARG:C     | 2:D:42:PHE:H     | 0.41     | 2.17        | 15     | 1     |
| 1:C:97:ASN:N     | 1:C:97:ASN:ND2   | 0.41     | 2.68        | 15     | 1     |
| 2:B:37:TRP:CG    | 2:B:38:THR:N     | 0.41     | 2.88        | 16     | 1     |
| 1:C:101:LEU:HD23 | 3:C:142:HEC:HBB3 | 0.41     | 1.91        | 14     | 1     |
| 2:B:81:LEU:O     | 2:B:84:THR:OG1   | 0.41     | 2.37        | 6      | 1     |
| 2:D:87:THR:OG1   | 2:D:88:LEU:N     | 0.41     | 2.53        | 6      | 1     |
| 1:C:31:ARG:O     | 1:C:35:SER:OG    | 0.41     | 2.37        | 4      | 1     |
| 2:B:26:GLU:OE2   | 2:B:26:GLU:N     | 0.41     | 2.52        | 20     | 1     |
| 2:D:71:PHE:CE2   | 2:D:134:VAL:HG11 | 0.41     | 2.50        | 3      | 1     |
| 1:A:63:ALA:O     | 1:A:67:THR:CB    | 0.41     | 2.68        | 17     | 1     |
| 1:C:110:ALA:O    | 1:C:112:HIS:N    | 0.41     | 2.53        | 1      | 1     |
| 1:C:32:MET:O     | 1:C:33:PHE:C     | 0.41     | 2.59        | 18     | 2     |
| 1:A:3:SER:H      | 1:A:4:PRO:CD     | 0.41     | 2.28        | 10     | 1     |
| 1:C:21:ALA:C     | 1:C:23:GLU:H     | 0.41     | 2.19        | 10     | 5     |
| 1:C:7:LYS:O      | 1:C:8:THR:C      | 0.41     | 2.58        | 15     | 5     |
| 2:D:30:ARG:O     | 2:D:34:VAL:HG22  | 0.41     | 2.15        | 8      | 1     |
| 2:B:30:ARG:O     | 2:B:34:VAL:HG22  | 0.41     | 2.15        | 8      | 1     |
| 2:B:102:ASN:ND2  | 3:B:147:HEC:CMC  | 0.41     | 2.83        | 14     | 1     |
| 1:C:86:LEU:HD21  | 3:C:142:HEC:CGD  | 0.41     | 2.45        | 7      | 1     |
| 1:C:50:HIS:C     | 1:C:52:SER:N     | 0.41     | 2.73        | 17     | 1     |
| 1:A:47:ASP:O     | 1:A:52:SER:CB    | 0.41     | 2.69        | 13     | 1     |
| 2:D:52:ASP:OD1   | 2:D:53:ALA:N     | 0.41     | 2.53        | 13     | 1     |
| 1:C:50:HIS:CG    | 1:C:51:GLY:H     | 0.41     | 2.33        | 11     | 1     |
| 2:D:146:HIS:N    | 2:D:146:HIS:ND1  | 0.41     | 2.68        | 11     | 1     |
| 1:A:103:HIS:HB3  | 2:B:108:ASN:ND2  | 0.41     | 2.30        | 10     | 1     |
| 2:D:20:VAL:C     | 2:D:22:GLU:H     | 0.41     | 2.18        | 15     | 2     |
| 1:A:11:LYS:HD2   | 1:A:11:LYS:N     | 0.41     | 2.31        | 8      | 1     |
| 1:C:61:LYS:HB3   | 3:C:142:HEC:CMA  | 0.41     | 2.44        | 17     | 2     |
| 2:B:55:MET:O     | 2:B:57:ASN:OD1   | 0.41     | 2.37        | 19     | 1     |
| 2:D:93:CYS:O     | 2:D:97:HIS:CG    | 0.41     | 2.74        | 7      | 1     |
| 2:D:130:TYR:O    | 2:D:132:LYS:N    | 0.41     | 2.53        | 7      | 1     |
| 2:D:71:PHE:O     | 2:D:75:LEU:CD2   | 0.41     | 2.68        | 4      | 1     |
| 2:D:22:GLU:O     | 2:D:23:VAL:C     | 0.41     | 2.59        | 20     | 1     |
| 2:B:103:PHE:C    | 2:B:105:LEU:N    | 0.41     | 2.74        | 1      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 3:A:142:HEC:CMB  | 3:A:142:HEC:HBB3 | 0.41     | 2.40        | 12     | 1     |
| 1:C:47:ASP:O     | 1:C:52:SER:CB    | 0.41     | 2.69        | 13     | 1     |
| 1:A:91:LEU:HD12  | 1:A:91:LEU:H     | 0.41     | 1.74        | 11     | 1     |
| 1:A:109:LEU:O    | 1:A:113:LEU:N    | 0.41     | 2.53        | 17     | 6     |
| 2:D:19:ASN:O     | 2:D:20:VAL:C     | 0.41     | 2.59        | 9      | 5     |
| 1:A:134:THR:O    | 1:A:138:SER:CB   | 0.41     | 2.69        | 10     | 1     |
| 2:B:139:ASN:ND2  | 2:B:139:ASN:O    | 0.41     | 2.52        | 15     | 1     |
| 1:C:84:SER:OG    | 1:C:136:LEU:O    | 0.41     | 2.36        | 20     | 2     |
| 1:A:84:SER:OG    | 1:A:136:LEU:O    | 0.41     | 2.37        | 16     | 1     |
| 2:B:7:GLU:CD     | 2:B:7:GLU:N      | 0.41     | 2.74        | 19     | 1     |
| 2:D:7:GLU:CD     | 2:D:7:GLU:N      | 0.41     | 2.74        | 19     | 1     |
| 2:D:131:GLN:O    | 2:D:135:ALA:N    | 0.41     | 2.49        | 9      | 1     |
| 2:D:92:HIS:O     | 2:D:145:TYR:OH   | 0.41     | 2.35        | 6      | 1     |
| 2:B:30:ARG:HH21  | 2:B:33:VAL:HG11  | 0.41     | 1.75        | 7      | 1     |
| 1:A:64:ASP:O     | 1:A:68:ASN:N     | 0.41     | 2.41        | 4      | 1     |
| 2:B:14:LEU:N     | 2:B:14:LEU:CD1   | 0.41     | 2.82        | 20     | 1     |
| 2:B:146:HIS:HB3  | 2:D:135:ALA:HB3  | 0.41     | 1.91        | 3      | 1     |
| 2:B:14:LEU:HD23  | 2:B:17:LYS:HD3   | 0.41     | 1.92        | 3      | 1     |
| 1:A:29:LEU:O     | 1:A:30:GLU:C     | 0.41     | 2.58        | 3      | 1     |
| 1:A:88:ALA:C     | 1:A:90:LYS:N     | 0.41     | 2.73        | 17     | 1     |
| 2:D:71:PHE:O     | 2:D:74:GLY:N     | 0.41     | 2.50        | 12     | 1     |
| 1:A:32:MET:O     | 1:A:35:SER:N     | 0.41     | 2.53        | 18     | 1     |
| 1:A:62:VAL:HG22  | 3:A:142:HEC:C2B  | 0.41     | 2.45        | 8      | 1     |
| 2:B:17:LYS:HD2   | 2:B:17:LYS:H     | 0.41     | 1.74        | 8      | 1     |
| 2:B:97:HIS:O     | 2:B:98:VAL:C     | 0.41     | 2.59        | 16     | 1     |
| 2:D:37:TRP:CG    | 2:D:38:THR:N     | 0.41     | 2.89        | 16     | 1     |
| 2:B:47:ASP:OD1   | 2:B:47:ASP:N     | 0.41     | 2.47        | 16     | 1     |
| 1:A:101:LEU:HD23 | 3:A:142:HEC:HBB3 | 0.41     | 1.91        | 14     | 2     |
| 1:C:101:LEU:CD1  | 3:C:142:HEC:HMC3 | 0.41     | 2.34        | 7      | 1     |
| 1:C:95:PRO:O     | 1:C:96:VAL:C     | 0.41     | 2.58        | 5      | 2     |
| 2:B:131:GLN:CD   | 2:B:131:GLN:N    | 0.41     | 2.74        | 5      | 1     |
| 1:A:113:LEU:HD13 | 1:A:113:LEU:C    | 0.41     | 2.36        | 5      | 1     |
| 2:D:84:THR:C     | 2:D:86:ALA:N     | 0.41     | 2.73        | 20     | 1     |
| 1:C:100:LEU:C    | 1:C:102:SER:N    | 0.41     | 2.72        | 20     | 1     |
| 2:B:135:ALA:HB1  | 2:D:146:HIS:ND1  | 0.41     | 2.30        | 3      | 1     |
| 1:C:63:ALA:O     | 1:C:67:THR:CB    | 0.41     | 2.68        | 17     | 1     |
| 2:D:103:PHE:C    | 2:D:105:LEU:N    | 0.41     | 2.74        | 1      | 1     |
| 2:D:104:ARG:NH1  | 2:D:104:ARG:CB   | 0.41     | 2.84        | 12     | 1     |
| 1:C:126:ASP:CG   | 2:D:35:TYR:CD2   | 0.41     | 2.93        | 13     | 1     |
| 2:D:96:LEU:O     | 2:D:98:VAL:N     | 0.41     | 2.54        | 13     | 1     |
| 1:A:21:ALA:C     | 1:A:23:GLU:H     | 0.41     | 2.19        | 10     | 4     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 3:B:147:HEC:CMC | 2:D:31:LEU:CD2   | 0.41     | 2.99        | 15     | 1     |
| 2:B:84:THR:C    | 2:B:86:ALA:H     | 0.41     | 2.18        | 15     | 2     |
| 1:A:17:VAL:HG13 | 1:A:24:TYR:CD2   | 0.41     | 2.50        | 16     | 1     |
| 1:C:18:GLY:C    | 1:C:20:HIS:N     | 0.41     | 2.74        | 16     | 1     |
| 2:D:38:THR:O    | 2:D:41:PHE:N     | 0.41     | 2.46        | 19     | 1     |
| 2:D:37:TRP:CE2  | 2:D:38:THR:HG23  | 0.41     | 2.51        | 6      | 2     |
| 1:A:2:LEU:HD11  | 1:A:127:LYS:HE3  | 0.41     | 1.92        | 9      | 1     |
| 2:D:41:PHE:CD1  | 2:D:41:PHE:N     | 0.41     | 2.89        | 6      | 1     |
| 2:B:45:PHE:C    | 2:B:47:ASP:H     | 0.41     | 2.18        | 5      | 1     |
| 1:A:97:ASN:CB   | 3:A:142:HEC:CMC  | 0.41     | 2.97        | 17     | 1     |
| 1:A:19:ALA:O    | 1:A:20:HIS:CG    | 0.41     | 2.73        | 17     | 1     |
| 1:A:75:ASP:OD2  | 1:A:78:ASN:OD1   | 0.41     | 2.38        | 17     | 1     |
| 1:C:97:ASN:O    | 1:C:99:LYS:N     | 0.41     | 2.54        | 13     | 1     |
| 2:B:52:ASP:OD1  | 2:B:53:ALA:N     | 0.41     | 2.53        | 13     | 1     |
| 2:D:144:LYS:C   | 2:D:146:HIS:HD1  | 0.41     | 2.17        | 11     | 1     |
| 2:B:46:GLY:O    | 2:B:47:ASP:O     | 0.41     | 2.37        | 11     | 1     |
| 2:B:121:GLU:C   | 2:B:123:THR:H    | 0.41     | 2.18        | 15     | 1     |
| 2:B:131:GLN:N   | 2:B:131:GLN:CD   | 0.41     | 2.74        | 16     | 1     |
| 2:D:77:HIS:O    | 2:D:79:ASP:N     | 0.41     | 2.54        | 14     | 1     |
| 1:A:2:LEU:HD21  | 1:A:6:ASP:OD1    | 0.41     | 2.16        | 9      | 1     |
| 1:A:86:LEU:HD21 | 3:A:142:HEC:CGD  | 0.41     | 2.45        | 7      | 1     |
| 2:D:42:PHE:C    | 2:D:44:SER:H     | 0.41     | 2.19        | 7      | 1     |
| 1:C:106:LEU:CD1 | 1:C:122:HIS:CE1  | 0.41     | 2.99        | 4      | 1     |
| 2:D:8:LYS:O     | 2:D:9:SER:C      | 0.41     | 2.59        | 4      | 1     |
| 1:C:65:ALA:HB3  | 3:C:142:HEC:HMB3 | 0.41     | 1.90        | 20     | 1     |
| 2:B:82:LYS:N    | 2:B:82:LYS:CD    | 0.41     | 2.83        | 3      | 1     |
| 2:D:133:VAL:O   | 2:D:134:VAL:C    | 0.41     | 2.59        | 12     | 1     |
| 1:A:17:VAL:HG13 | 1:A:24:TYR:CE2   | 0.41     | 2.51        | 12     | 1     |
| 3:C:142:HEC:CMB | 3:C:142:HEC:HBB3 | 0.41     | 2.36        | 11     | 1     |
| 1:A:92:ARG:HB3  | 2:D:40:ARG:HE    | 0.41     | 1.73        | 18     | 1     |
| 1:C:134:THR:O   | 1:C:138:SER:CB   | 0.41     | 2.69        | 10     | 1     |
| 1:C:62:VAL:HG22 | 3:C:142:HEC:C2B  | 0.41     | 2.45        | 8      | 1     |
| 1:A:32:MET:O    | 1:A:33:PHE:C     | 0.41     | 2.59        | 16     | 1     |
| 2:B:37:TRP:C    | 2:B:39:GLN:H     | 0.41     | 2.17        | 14     | 1     |
| 2:B:8:LYS:C     | 2:B:10:ALA:N     | 0.41     | 2.74        | 19     | 1     |
| 2:D:67:VAL:HG13 | 3:D:147:HEC:HMB3 | 0.41     | 1.91        | 9      | 1     |
| 1:A:83:LEU:N    | 1:A:83:LEU:HD23  | 0.41     | 2.31        | 11     | 2     |
| 1:C:117:PHE:CE1 | 2:D:116:HIS:CE1  | 0.41     | 3.07        | 4      | 1     |
| 1:C:46:PHE:CE2  | 1:C:55:VAL:HG22  | 0.41     | 2.51        | 5      | 1     |
| 2:D:45:PHE:C    | 2:D:47:ASP:H     | 0.41     | 2.18        | 5      | 1     |
| 1:C:3:SER:OG    | 1:C:4:PRO:CD     | 0.41     | 2.69        | 20     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 2:B:22:GLU:O    | 2:B:23:VAL:C     | 0.41     | 2.59        | 20     | 1     |
| 2:B:26:GLU:CD   | 2:B:26:GLU:N     | 0.41     | 2.74        | 20     | 1     |
| 2:D:20:VAL:O    | 2:D:20:VAL:HG12  | 0.41     | 2.16        | 20     | 1     |
| 2:B:73:ASP:O    | 2:B:77:HIS:N     | 0.41     | 2.53        | 17     | 1     |
| 1:A:110:ALA:O   | 1:A:112:HIS:N    | 0.41     | 2.53        | 1      | 1     |
| 2:B:66:LYS:O    | 3:B:147:HEC:HMA3 | 0.41     | 2.15        | 12     | 1     |
| 1:C:47:ASP:O    | 1:C:47:ASP:OD1   | 0.41     | 2.37        | 2      | 1     |
| 1:A:92:ARG:HD2  | 2:D:40:ARG:NH1   | 0.41     | 2.31        | 18     | 1     |
| 2:B:106:LEU:O   | 2:B:106:LEU:HD13 | 0.41     | 2.15        | 18     | 1     |
| 1:C:32:MET:O    | 1:C:35:SER:N     | 0.41     | 2.53        | 18     | 1     |
| 1:C:103:HIS:HB3 | 2:D:108:ASN:ND2  | 0.41     | 2.30        | 10     | 1     |
| 2:B:97:HIS:CE1  | 1:C:94:ASP:OD2   | 0.41     | 2.74        | 10     | 1     |
| 1:A:37:PRO:O    | 1:A:38:THR:C     | 0.41     | 2.59        | 10     | 1     |
| 1:A:27:GLU:OE2  | 1:A:112:HIS:CD2  | 0.41     | 2.74        | 10     | 1     |
| 2:D:21:ASP:C    | 2:D:65:LYS:NZ    | 0.41     | 2.74        | 10     | 1     |
| 3:B:147:HEC:CHB | 2:D:67:VAL:HA    | 0.41     | 2.46        | 15     | 1     |
| 1:A:75:ASP:C    | 1:A:77:PRO:HD2   | 0.41     | 2.37        | 15     | 1     |
| 1:A:31:ARG:NH2  | 1:A:34:LEU:CD1   | 0.41     | 2.84        | 16     | 1     |
| 2:D:102:ASN:ND2 | 3:D:147:HEC:CMC  | 0.41     | 2.83        | 14     | 1     |
| 1:C:86:LEU:HD11 | 3:C:142:HEC:O1D  | 0.41     | 2.16        | 14     | 1     |
| 2:B:13:ALA:O    | 2:B:16:GLY:N     | 0.41     | 2.52        | 14     | 1     |
| 2:D:37:TRP:O    | 2:D:39:GLN:N     | 0.41     | 2.51        | 14     | 1     |
| 2:B:37:TRP:CE2  | 2:B:38:THR:HG23  | 0.41     | 2.51        | 6      | 2     |
| 2:B:134:VAL:C   | 2:B:136:GLY:N    | 0.41     | 2.73        | 19     | 1     |
| 1:C:48:LEU:CD2  | 1:C:48:LEU:C     | 0.41     | 2.90        | 9      | 1     |
| 1:C:120:ALA:O   | 1:C:121:VAL:C    | 0.41     | 2.59        | 9      | 1     |
| 2:D:44:SER:C    | 2:D:46:GLY:H     | 0.41     | 2.19        | 6      | 1     |
| 2:B:93:CYS:O    | 2:B:97:HIS:CG    | 0.41     | 2.74        | 7      | 1     |
| 1:C:24:TYR:CD1  | 1:C:112:HIS:CE1  | 0.41     | 3.09        | 7      | 1     |
| 1:A:94:ASP:C    | 1:A:96:VAL:H     | 0.41     | 2.18        | 4      | 2     |
| 1:A:98:PHE:CE1  | 1:A:133:SER:CB   | 0.41     | 3.04        | 7      | 1     |
| 1:A:46:PHE:CE2  | 1:A:55:VAL:HG22  | 0.41     | 2.51        | 5      | 2     |
| 1:A:3:SER:OG    | 1:A:4:PRO:CD     | 0.41     | 2.69        | 20     | 1     |
| 2:D:14:LEU:CD1  | 2:D:14:LEU:H     | 0.41     | 2.29        | 20     | 1     |
| 2:B:71:PHE:CE2  | 2:B:134:VAL:HG11 | 0.41     | 2.50        | 3      | 1     |
| 1:A:117:PHE:O   | 1:A:117:PHE:CD2  | 0.41     | 2.74        | 17     | 1     |
| 1:C:117:PHE:CD2 | 1:C:117:PHE:O    | 0.41     | 2.74        | 17     | 1     |
| 1:C:75:ASP:OD2  | 1:C:78:ASN:OD1   | 0.41     | 2.38        | 17     | 1     |
| 1:A:4:PRO:O     | 1:A:5:ALA:C      | 0.41     | 2.60        | 17     | 1     |
| 2:B:97:HIS:NE2  | 1:C:41:THR:CB    | 0.41     | 2.84        | 12     | 1     |
| 2:B:133:VAL:O   | 2:B:134:VAL:C    | 0.41     | 2.59        | 12     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:99:ASP:CB    | 1:C:96:VAL:HG11  | 0.41     | 2.41        | 11     | 1     |
| 1:C:3:SER:H      | 1:C:4:PRO:CD     | 0.41     | 2.29        | 2      | 1     |
| 1:A:78:ASN:C     | 1:A:78:ASN:HD22  | 0.41     | 2.18        | 2      | 1     |
| 2:B:97:HIS:C     | 2:B:97:HIS:ND1   | 0.41     | 2.74        | 18     | 1     |
| 2:B:88:LEU:O     | 2:B:92:HIS:CG    | 0.41     | 2.74        | 18     | 1     |
| 1:A:115:ALA:O    | 1:A:117:PHE:N    | 0.41     | 2.53        | 15     | 1     |
| 2:D:131:GLN:N    | 2:D:131:GLN:CD   | 0.41     | 2.74        | 16     | 1     |
| 1:A:38:THR:O     | 1:A:39:THR:C     | 0.41     | 2.59        | 16     | 1     |
| 1:C:38:THR:O     | 1:C:39:THR:C     | 0.41     | 2.59        | 16     | 1     |
| 2:D:71:PHE:O     | 2:D:71:PHE:CD1   | 0.41     | 2.74        | 16     | 1     |
| 1:A:86:LEU:HD11  | 3:A:142:HEC:O1D  | 0.41     | 2.16        | 14     | 1     |
| 2:B:52:ASP:O     | 2:B:54:VAL:N     | 0.41     | 2.54        | 14     | 3     |
| 1:A:125:LEU:O    | 1:A:129:LEU:HB3  | 0.41     | 2.16        | 7      | 1     |
| 2:D:30:ARG:HH21  | 2:D:33:VAL:HG11  | 0.41     | 1.76        | 7      | 1     |
| 2:D:131:GLN:CD   | 2:D:131:GLN:N    | 0.41     | 2.74        | 5      | 1     |
| 1:A:1:VAL:C      | 1:A:2:LEU:HD12   | 0.41     | 2.37        | 5      | 1     |
| 2:B:41:PHE:C     | 2:B:43:GLU:H     | 0.41     | 2.19        | 3      | 1     |
| 1:C:23:GLU:O     | 1:C:26:ALA:HB3   | 0.41     | 2.16        | 17     | 1     |
| 1:C:19:ALA:O     | 1:C:20:HIS:CG    | 0.41     | 2.73        | 17     | 1     |
| 1:C:88:ALA:C     | 1:C:90:LYS:N     | 0.41     | 2.73        | 17     | 1     |
| 1:C:4:PRO:O      | 1:C:5:ALA:C      | 0.41     | 2.60        | 17     | 1     |
| 1:A:90:LYS:O     | 1:A:91:LEU:CB    | 0.41     | 2.67        | 1      | 1     |
| 1:A:48:LEU:H     | 1:A:48:LEU:CD2   | 0.41     | 2.24        | 1      | 1     |
| 1:C:13:ALA:O     | 1:C:17:VAL:CG2   | 0.41     | 2.68        | 13     | 1     |
| 2:B:96:LEU:O     | 2:B:98:VAL:N     | 0.41     | 2.54        | 13     | 1     |
| 1:A:83:LEU:HD23  | 1:A:83:LEU:N     | 0.41     | 2.31        | 13     | 1     |
| 1:C:83:LEU:HD23  | 1:C:83:LEU:N     | 0.41     | 2.31        | 11     | 1     |
| 1:C:17:VAL:HG13  | 1:C:24:TYR:CD2   | 0.40     | 2.50        | 16     | 1     |
| 1:C:116:GLU:O    | 1:C:117:PHE:C    | 0.40     | 2.60        | 14     | 1     |
| 2:B:106:LEU:HD22 | 3:B:147:HEC:HBB3 | 0.40     | 0.43        | 19     | 1     |
| 1:A:2:LEU:CD2    | 1:A:131:SER:OG   | 0.40     | 2.68        | 19     | 1     |
| 2:B:41:PHE:CD1   | 2:B:41:PHE:N     | 0.40     | 2.90        | 7      | 2     |
| 2:B:87:THR:OG1   | 2:B:88:LEU:N     | 0.40     | 2.53        | 6      | 1     |
| 1:A:4:PRO:C      | 1:A:6:ASP:H      | 0.40     | 2.20        | 7      | 1     |
| 2:B:42:PHE:C     | 2:B:44:SER:H     | 0.40     | 2.20        | 7      | 1     |
| 2:D:83:GLY:O     | 2:D:86:ALA:N     | 0.40     | 2.43        | 4      | 1     |
| 2:D:89:SER:OG    | 2:D:140:ALA:O    | 0.40     | 2.37        | 5      | 1     |
| 2:B:105:LEU:C    | 2:B:107:GLY:N    | 0.40     | 2.75        | 1      | 1     |
| 1:A:109:LEU:HD23 | 1:A:109:LEU:H    | 0.40     | 1.75        | 12     | 1     |
| 1:C:10:VAL:HG21  | 1:C:128:PHE:CD1  | 0.40     | 2.51        | 13     | 1     |
| 2:D:106:LEU:HD13 | 2:D:106:LEU:O    | 0.40     | 2.15        | 18     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:8:LYS:O      | 2:B:9:SER:C      | 0.40     | 2.59        | 18     | 1     |
| 2:B:21:ASP:C     | 2:B:65:LYS:NZ    | 0.40     | 2.74        | 10     | 1     |
| 1:C:115:ALA:O    | 1:C:117:PHE:N    | 0.40     | 2.53        | 15     | 1     |
| 2:D:139:ASN:ND2  | 2:D:139:ASN:O    | 0.40     | 2.52        | 15     | 1     |
| 1:C:80:LEU:C     | 1:C:82:ALA:N     | 0.40     | 2.75        | 8      | 1     |
| 1:C:31:ARG:NH2   | 1:C:34:LEU:CD1   | 0.40     | 2.84        | 16     | 1     |
| 1:A:18:GLY:C     | 1:A:20:HIS:N     | 0.40     | 2.74        | 16     | 1     |
| 2:B:26:GLU:C     | 2:B:28:LEU:N     | 0.40     | 2.73        | 14     | 1     |
| 1:A:7:LYS:NZ     | 1:A:7:LYS:CB     | 0.40     | 2.84        | 14     | 1     |
| 2:B:38:THR:O     | 2:B:41:PHE:N     | 0.40     | 2.46        | 19     | 1     |
| 2:D:134:VAL:C    | 2:D:136:GLY:N    | 0.40     | 2.73        | 19     | 1     |
| 2:B:59:LYS:CG    | 2:B:60:VAL:N     | 0.40     | 2.85        | 6      | 1     |
| 2:B:47:ASP:CG    | 2:B:48:LEU:H     | 0.40     | 2.19        | 20     | 1     |
| 2:B:2:HIS:ND1    | 2:B:2:HIS:C      | 0.40     | 2.74        | 3      | 1     |
| 1:C:126:ASP:OD2  | 2:D:35:TYR:CZ    | 0.40     | 2.75        | 17     | 1     |
| 1:C:17:VAL:HG13  | 1:C:24:TYR:CE2   | 0.40     | 2.51        | 12     | 1     |
| 1:A:30:GLU:O     | 1:A:30:GLU:OE2   | 0.40     | 2.40        | 12     | 1     |
| 1:A:77:PRO:O     | 1:A:81:SER:OG    | 0.40     | 2.35        | 13     | 1     |
| 1:C:76:MET:SD    | 1:C:132:VAL:HG22 | 0.40     | 2.56        | 13     | 1     |
| 2:B:95:LYS:O     | 2:B:96:LEU:HD12  | 0.40     | 2.17        | 13     | 1     |
| 1:A:96:VAL:HG21  | 2:D:99:ASP:OD1   | 0.40     | 2.15        | 13     | 1     |
| 1:A:38:THR:C     | 1:A:40:LYS:N     | 0.40     | 2.75        | 11     | 1     |
| 2:D:48:LEU:O     | 2:D:49:SER:C     | 0.40     | 2.58        | 10     | 2     |
| 1:A:121:VAL:HG12 | 1:A:122:HIS:N    | 0.40     | 2.31        | 15     | 1     |
| 1:C:47:ASP:O     | 1:C:48:LEU:C     | 0.40     | 2.59        | 19     | 1     |
| 2:D:8:LYS:C      | 2:D:10:ALA:N     | 0.40     | 2.74        | 19     | 1     |
| 2:B:44:SER:C     | 2:B:46:GLY:H     | 0.40     | 2.19        | 6      | 1     |
| 2:B:59:LYS:O     | 2:B:60:VAL:C     | 0.40     | 2.59        | 7      | 1     |
| 1:C:98:PHE:CE1   | 1:C:133:SER:CB   | 0.40     | 3.04        | 7      | 1     |
| 1:A:65:ALA:CB    | 3:A:142:HEC:CMB  | 0.40     | 2.99        | 20     | 1     |
| 2:B:110:LEU:HD23 | 2:B:110:LEU:O    | 0.40     | 2.17        | 1      | 1     |
| 2:B:97:HIS:CE1   | 1:C:41:THR:OG1   | 0.40     | 2.74        | 12     | 1     |
| 2:B:104:ARG:CB   | 2:B:104:ARG:NH1  | 0.40     | 2.84        | 12     | 1     |
| 1:A:126:ASP:CG   | 2:B:35:TYR:CD2   | 0.40     | 2.93        | 13     | 1     |
| 2:D:95:LYS:O     | 2:D:96:LEU:HD12  | 0.40     | 2.17        | 13     | 1     |
| 2:D:90:GLU:HA    | 2:D:144:LYS:HZ2  | 0.40     | 1.77        | 2      | 1     |
| 2:B:105:LEU:N    | 2:B:105:LEU:HD22 | 0.40     | 2.32        | 2      | 1     |
| 1:A:29:LEU:CD1   | 1:A:58:HIS:CG    | 0.40     | 3.05        | 18     | 1     |
| 1:A:99:LYS:O     | 1:A:103:HIS:CE1  | 0.40     | 2.75        | 10     | 1     |
| 1:A:117:PHE:CG   | 1:A:117:PHE:O    | 0.40     | 2.73        | 10     | 1     |
| 1:A:80:LEU:C     | 1:A:82:ALA:N     | 0.40     | 2.75        | 8      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:D:122:PHE:O    | 2:D:123:THR:C    | 0.40     | 2.60        | 16     | 1     |
| 1:A:93:VAL:HG13  | 1:A:93:VAL:O     | 0.40     | 2.17        | 19     | 1     |
| 1:C:131:SER:O    | 1:C:135:VAL:CG2  | 0.40     | 2.70        | 19     | 1     |
| 1:C:2:LEU:CD2    | 1:C:131:SER:OG   | 0.40     | 2.68        | 19     | 1     |
| 2:D:126:VAL:HG12 | 2:D:126:VAL:O    | 0.40     | 2.16        | 19     | 1     |
| 1:C:2:LEU:HD21   | 1:C:6:ASP:OD1    | 0.40     | 2.16        | 9      | 1     |
| 1:A:104:CYS:O    | 1:A:107:VAL:N    | 0.40     | 2.54        | 5      | 1     |
| 1:C:1:VAL:C      | 1:C:2:LEU:HD12   | 0.40     | 2.37        | 5      | 1     |
| 1:C:33:PHE:O     | 1:C:34:LEU:C     | 0.40     | 2.59        | 3      | 1     |
| 1:A:50:HIS:C     | 1:A:52:SER:N     | 0.40     | 2.73        | 17     | 1     |
| 1:A:119:PRO:CA   | 2:B:33:VAL:HG13  | 0.40     | 2.46        | 17     | 1     |
| 1:A:107:VAL:HG11 | 2:B:127:GLN:NE2  | 0.40     | 2.29        | 17     | 1     |
| 2:D:73:ASP:O     | 2:D:77:HIS:N     | 0.40     | 2.53        | 17     | 1     |
| 1:C:109:LEU:H    | 1:C:109:LEU:HD23 | 0.40     | 1.75        | 12     | 1     |
| 2:D:88:LEU:O     | 2:D:92:HIS:CG    | 0.40     | 2.74        | 18     | 1     |
| 1:C:99:LYS:O     | 1:C:103:HIS:CE1  | 0.40     | 2.75        | 10     | 1     |
| 2:D:97:HIS:O     | 2:D:98:VAL:C     | 0.40     | 2.59        | 16     | 1     |
| 2:B:122:PHE:O    | 2:B:123:THR:C    | 0.40     | 2.60        | 16     | 1     |
| 2:B:77:HIS:O     | 2:B:79:ASP:N     | 0.40     | 2.54        | 14     | 1     |
| 1:A:24:TYR:CD1   | 1:A:112:HIS:CE1  | 0.40     | 3.09        | 7      | 1     |
| 2:B:97:HIS:ND1   | 1:C:41:THR:HB    | 0.40     | 2.32        | 4      | 1     |
| 2:B:84:THR:C     | 2:B:86:ALA:N     | 0.40     | 2.73        | 20     | 1     |
| 2:D:26:GLU:N     | 2:D:26:GLU:CD    | 0.40     | 2.74        | 20     | 1     |
| 1:A:119:PRO:HA   | 2:B:33:VAL:HG21  | 0.40     | 1.92        | 3      | 1     |
| 2:B:146:HIS:C    | 2:D:104:ARG:NH2  | 0.40     | 2.74        | 17     | 1     |
| 1:C:119:PRO:CA   | 2:D:33:VAL:HG13  | 0.40     | 2.46        | 17     | 1     |
| 1:A:11:LYS:H     | 1:A:11:LYS:CD    | 0.40     | 2.26        | 1      | 1     |
| 2:B:18:VAL:O     | 2:B:20:VAL:N     | 0.40     | 2.53        | 12     | 1     |
| 2:B:79:ASP:O     | 2:B:80:ASN:CG    | 0.40     | 2.60        | 13     | 1     |
| 1:A:48:LEU:C     | 1:A:48:LEU:CD2   | 0.40     | 2.90        | 11     | 1     |
| 1:A:50:HIS:CG    | 1:A:51:GLY:H     | 0.40     | 2.33        | 11     | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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     | 134/141 (95%)     | 100±3 (74±2%) | 22±3 (16±2%) | 13±2 (9±2%) | 2           | 11 |
| 1   | C     | 134/141 (95%)     | 100±3 (74±2%) | 22±3 (16±2%) | 13±2 (9±2%) | 2           | 11 |
| 2   | B     | 144/146 (99%)     | 111±4 (77±3%) | 29±4 (20±3%) | 4±2 (3±1%)  | 9           | 42 |
| 2   | D     | 144/146 (99%)     | 111±4 (77±3%) | 29±4 (20±3%) | 4±2 (3±1%)  | 9           | 42 |
| All | All   | 11120/11480 (97%) | 8418 (76%)    | 2024 (18%)   | 678 (6%)    | 4           | 21 |

All 118 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | C     | 73  | VAL  | 20             |
| 1   | A     | 73  | VAL  | 20             |
| 1   | C     | 75  | ASP  | 19             |
| 1   | A     | 119 | PRO  | 19             |
| 1   | C     | 119 | PRO  | 19             |
| 1   | A     | 75  | ASP  | 19             |
| 1   | A     | 19  | ALA  | 17             |
| 1   | C     | 19  | ALA  | 17             |
| 1   | A     | 47  | ASP  | 16             |
| 1   | C     | 47  | ASP  | 16             |
| 1   | C     | 114 | PRO  | 16             |
| 1   | A     | 114 | PRO  | 16             |
| 1   | A     | 4   | PRO  | 15             |
| 1   | C     | 4   | PRO  | 15             |
| 2   | B     | 20  | VAL  | 12             |
| 2   | D     | 77  | HIS  | 12             |
| 2   | D     | 20  | VAL  | 12             |
| 2   | B     | 77  | HIS  | 12             |
| 1   | A     | 116 | GLU  | 11             |
| 1   | A     | 3   | SER  | 11             |
| 1   | C     | 116 | GLU  | 11             |
| 1   | C     | 3   | SER  | 11             |
| 1   | C     | 90  | LYS  | 10             |
| 1   | A     | 90  | LYS  | 10             |
| 1   | A     | 45  | HIS  | 8              |
| 1   | C     | 95  | PRO  | 8              |
| 1   | C     | 45  | HIS  | 8              |
| 1   | A     | 95  | PRO  | 8              |
| 2   | D     | 2   | HIS  | 7              |
| 1   | A     | 138 | SER  | 7              |
| 1   | A     | 53  | ALA  | 7              |
| 1   | C     | 53  | ALA  | 7              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2   | B     | 102 | ASN  | 7              |
| 1   | C     | 138 | SER  | 7              |
| 1   | C     | 96  | VAL  | 7              |
| 1   | A     | 96  | VAL  | 7              |
| 2   | D     | 102 | ASN  | 7              |
| 2   | B     | 2   | HIS  | 7              |
| 2   | D     | 100 | PRO  | 6              |
| 2   | B     | 100 | PRO  | 6              |
| 1   | C     | 93  | VAL  | 6              |
| 1   | A     | 50  | HIS  | 6              |
| 1   | A     | 93  | VAL  | 6              |
| 2   | B     | 47  | ASP  | 6              |
| 1   | C     | 50  | HIS  | 6              |
| 2   | D     | 47  | ASP  | 6              |
| 1   | C     | 5   | ALA  | 5              |
| 1   | A     | 2   | LEU  | 5              |
| 1   | A     | 5   | ALA  | 5              |
| 1   | C     | 52  | SER  | 5              |
| 1   | C     | 2   | LEU  | 5              |
| 2   | B     | 58  | PRO  | 5              |
| 1   | A     | 52  | SER  | 5              |
| 2   | D     | 58  | PRO  | 5              |
| 2   | D     | 38  | THR  | 4              |
| 1   | A     | 6   | ASP  | 4              |
| 2   | D     | 46  | GLY  | 4              |
| 2   | B     | 38  | THR  | 4              |
| 2   | B     | 46  | GLY  | 4              |
| 1   | C     | 54  | GLN  | 4              |
| 1   | A     | 92  | ARG  | 4              |
| 1   | A     | 54  | GLN  | 4              |
| 1   | C     | 92  | ARG  | 4              |
| 1   | A     | 88  | ALA  | 4              |
| 1   | C     | 6   | ASP  | 4              |
| 1   | C     | 88  | ALA  | 4              |
| 2   | B     | 80  | ASN  | 3              |
| 1   | C     | 91  | LEU  | 3              |
| 1   | A     | 48  | LEU  | 3              |
| 1   | C     | 48  | LEU  | 3              |
| 1   | A     | 91  | LEU  | 3              |
| 1   | A     | 18  | GLY  | 3              |
| 1   | C     | 18  | GLY  | 3              |
| 2   | D     | 80  | ASN  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 37  | PRO  | 2              |
| 1   | C     | 37  | PRO  | 2              |
| 2   | D     | 14  | LEU  | 2              |
| 1   | A     | 41  | THR  | 2              |
| 2   | B     | 14  | LEU  | 2              |
| 2   | B     | 43  | GLU  | 2              |
| 2   | D     | 145 | TYR  | 2              |
| 2   | D     | 15  | TRP  | 2              |
| 2   | D     | 39  | GLN  | 2              |
| 2   | B     | 39  | GLN  | 2              |
| 1   | C     | 38  | THR  | 2              |
| 1   | C     | 41  | THR  | 2              |
| 2   | B     | 145 | TYR  | 2              |
| 2   | B     | 15  | TRP  | 2              |
| 1   | A     | 38  | THR  | 2              |
| 2   | D     | 43  | GLU  | 2              |
| 1   | C     | 120 | ALA  | 1              |
| 2   | D     | 37  | TRP  | 1              |
| 2   | D     | 97  | HIS  | 1              |
| 2   | B     | 101 | GLU  | 1              |
| 2   | D     | 134 | VAL  | 1              |
| 2   | B     | 37  | TRP  | 1              |
| 2   | B     | 108 | ASN  | 1              |
| 1   | C     | 33  | PHE  | 1              |
| 2   | D     | 5   | PRO  | 1              |
| 1   | A     | 33  | PHE  | 1              |
| 1   | A     | 94  | ASP  | 1              |
| 1   | A     | 35  | SER  | 1              |
| 2   | B     | 57  | ASN  | 1              |
| 2   | D     | 57  | ASN  | 1              |
| 2   | B     | 5   | PRO  | 1              |
| 1   | C     | 35  | SER  | 1              |
| 2   | D     | 42  | PHE  | 1              |
| 2   | B     | 40  | ARG  | 1              |
| 2   | B     | 97  | HIS  | 1              |
| 2   | D     | 101 | GLU  | 1              |
| 1   | C     | 94  | ASP  | 1              |
| 2   | D     | 108 | ASN  | 1              |
| 2   | D     | 122 | PHE  | 1              |
| 2   | B     | 134 | VAL  | 1              |
| 1   | A     | 120 | ALA  | 1              |
| 2   | B     | 42  | PHE  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2   | D     | 40  | ARG  | 1              |
| 2   | B     | 122 | PHE  | 1              |

### 6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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     | 107/113 (95%)   | 94±3 (88±2%)  | 13±3 (12±2%) | 11          | 53 |
| 1   | C     | 107/113 (95%)   | 94±3 (88±2%)  | 13±3 (12±2%) | 11          | 53 |
| 2   | B     | 117/118 (99%)   | 104±2 (89±2%) | 13±2 (11±2%) | 12          | 55 |
| 2   | D     | 117/118 (99%)   | 104±2 (89±2%) | 13±2 (11±2%) | 12          | 55 |
| All | All   | 8960/9240 (97%) | 7927 (88%)    | 1033 (12%)   | 11          | 54 |

All 224 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | C     | 127 | LYS  | 20             |
| 1   | A     | 127 | LYS  | 20             |
| 1   | A     | 3   | SER  | 20             |
| 1   | C     | 3   | SER  | 20             |
| 1   | A     | 14  | TRP  | 19             |
| 1   | C     | 14  | TRP  | 19             |
| 2   | B     | 122 | PHE  | 18             |
| 2   | D     | 3   | LEU  | 18             |
| 2   | D     | 122 | PHE  | 18             |
| 2   | B     | 3   | LEU  | 18             |
| 1   | C     | 61  | LYS  | 15             |
| 1   | C     | 113 | LEU  | 15             |
| 1   | A     | 61  | LYS  | 15             |
| 1   | A     | 113 | LEU  | 15             |
| 2   | D     | 17  | LYS  | 14             |
| 2   | B     | 17  | LYS  | 14             |
| 2   | B     | 14  | LEU  | 13             |
| 2   | D     | 14  | LEU  | 13             |
| 1   | A     | 46  | PHE  | 12             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2   | B     | 95  | LYS  | 12             |
| 1   | C     | 136 | LEU  | 12             |
| 1   | A     | 136 | LEU  | 12             |
| 2   | B     | 116 | HIS  | 12             |
| 1   | C     | 46  | PHE  | 12             |
| 2   | D     | 116 | HIS  | 12             |
| 2   | D     | 95  | LYS  | 12             |
| 1   | A     | 118 | THR  | 11             |
| 1   | C     | 118 | THR  | 11             |
| 2   | D     | 8   | LYS  | 11             |
| 2   | B     | 8   | LYS  | 11             |
| 2   | D     | 15  | TRP  | 10             |
| 1   | A     | 48  | LEU  | 10             |
| 1   | C     | 48  | LEU  | 10             |
| 2   | B     | 15  | TRP  | 10             |
| 1   | A     | 45  | HIS  | 9              |
| 1   | C     | 31  | ARG  | 9              |
| 1   | C     | 45  | HIS  | 9              |
| 1   | A     | 31  | ARG  | 9              |
| 2   | B     | 34  | VAL  | 8              |
| 2   | D     | 99  | ASP  | 8              |
| 2   | B     | 99  | ASP  | 8              |
| 2   | D     | 34  | VAL  | 8              |
| 1   | C     | 11  | LYS  | 7              |
| 2   | D     | 145 | TYR  | 7              |
| 2   | D     | 96  | LEU  | 7              |
| 2   | B     | 59  | LYS  | 7              |
| 2   | B     | 96  | LEU  | 7              |
| 2   | B     | 145 | TYR  | 7              |
| 2   | D     | 59  | LYS  | 7              |
| 1   | A     | 11  | LYS  | 7              |
| 2   | B     | 4   | THR  | 6              |
| 1   | A     | 122 | HIS  | 6              |
| 2   | D     | 144 | LYS  | 6              |
| 1   | A     | 94  | ASP  | 6              |
| 1   | A     | 105 | LEU  | 6              |
| 2   | D     | 4   | THR  | 6              |
| 2   | D     | 146 | HIS  | 6              |
| 1   | C     | 105 | LEU  | 6              |
| 1   | C     | 94  | ASP  | 6              |
| 1   | C     | 122 | HIS  | 6              |
| 2   | B     | 146 | HIS  | 6              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2   | B     | 144 | LYS  | 6              |
| 2   | D     | 37  | TRP  | 5              |
| 2   | B     | 84  | THR  | 5              |
| 1   | A     | 41  | THR  | 5              |
| 2   | D     | 97  | HIS  | 5              |
| 2   | B     | 37  | TRP  | 5              |
| 1   | C     | 98  | PHE  | 5              |
| 1   | C     | 41  | THR  | 5              |
| 2   | B     | 97  | HIS  | 5              |
| 1   | A     | 98  | PHE  | 5              |
| 2   | D     | 84  | THR  | 5              |
| 1   | C     | 33  | PHE  | 4              |
| 2   | B     | 11  | VAL  | 4              |
| 2   | D     | 2   | HIS  | 4              |
| 2   | B     | 130 | TYR  | 4              |
| 2   | B     | 127 | GLN  | 4              |
| 1   | A     | 78  | ASN  | 4              |
| 2   | B     | 102 | ASN  | 4              |
| 1   | A     | 33  | PHE  | 4              |
| 2   | D     | 127 | GLN  | 4              |
| 1   | A     | 7   | LYS  | 4              |
| 2   | D     | 11  | VAL  | 4              |
| 2   | D     | 55  | MET  | 4              |
| 2   | B     | 55  | MET  | 4              |
| 2   | D     | 130 | TYR  | 4              |
| 2   | D     | 102 | ASN  | 4              |
| 1   | C     | 78  | ASN  | 4              |
| 1   | C     | 7   | LYS  | 4              |
| 2   | B     | 2   | HIS  | 4              |
| 2   | B     | 80  | ASN  | 3              |
| 1   | C     | 97  | ASN  | 3              |
| 1   | A     | 56  | LYS  | 3              |
| 1   | C     | 75  | ASP  | 3              |
| 2   | B     | 65  | LYS  | 3              |
| 2   | D     | 123 | THR  | 3              |
| 1   | C     | 56  | LYS  | 3              |
| 1   | A     | 58  | HIS  | 3              |
| 1   | A     | 76  | MET  | 3              |
| 2   | D     | 35  | TYR  | 3              |
| 2   | B     | 117 | HIS  | 3              |
| 1   | C     | 66  | LEU  | 3              |
| 2   | B     | 123 | THR  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | C     | 58  | HIS  | 3              |
| 1   | A     | 50  | HIS  | 3              |
| 2   | B     | 35  | TYR  | 3              |
| 1   | A     | 75  | ASP  | 3              |
| 2   | D     | 80  | ASN  | 3              |
| 1   | C     | 50  | HIS  | 3              |
| 2   | D     | 117 | HIS  | 3              |
| 2   | B     | 30  | ARG  | 3              |
| 2   | D     | 65  | LYS  | 3              |
| 2   | D     | 30  | ARG  | 3              |
| 1   | C     | 76  | MET  | 3              |
| 1   | A     | 97  | ASN  | 3              |
| 1   | C     | 81  | SER  | 2              |
| 1   | C     | 90  | LYS  | 2              |
| 1   | A     | 90  | LYS  | 2              |
| 2   | D     | 57  | ASN  | 2              |
| 2   | D     | 50  | THR  | 2              |
| 1   | C     | 36  | PHE  | 2              |
| 2   | B     | 63  | HIS  | 2              |
| 2   | B     | 61  | LYS  | 2              |
| 2   | D     | 108 | ASN  | 2              |
| 1   | C     | 99  | LYS  | 2              |
| 1   | A     | 129 | LEU  | 2              |
| 2   | B     | 108 | ASN  | 2              |
| 2   | D     | 82  | LYS  | 2              |
| 2   | D     | 63  | HIS  | 2              |
| 2   | B     | 7   | GLU  | 2              |
| 2   | B     | 103 | PHE  | 2              |
| 1   | C     | 131 | SER  | 2              |
| 1   | A     | 32  | MET  | 2              |
| 2   | D     | 48  | LEU  | 2              |
| 1   | A     | 36  | PHE  | 2              |
| 1   | A     | 131 | SER  | 2              |
| 2   | B     | 57  | ASN  | 2              |
| 1   | C     | 109 | LEU  | 2              |
| 2   | D     | 139 | ASN  | 2              |
| 2   | B     | 82  | LYS  | 2              |
| 2   | B     | 133 | VAL  | 2              |
| 2   | D     | 21  | ASP  | 2              |
| 2   | B     | 52  | ASP  | 2              |
| 1   | A     | 66  | LEU  | 2              |
| 2   | B     | 94  | ASP  | 2              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 99  | LYS  | 2              |
| 2   | B     | 50  | THR  | 2              |
| 2   | D     | 61  | LYS  | 2              |
| 2   | D     | 133 | VAL  | 2              |
| 1   | C     | 89  | HIS  | 2              |
| 2   | D     | 94  | ASP  | 2              |
| 1   | A     | 89  | HIS  | 2              |
| 1   | C     | 129 | LEU  | 2              |
| 2   | B     | 21  | ASP  | 2              |
| 2   | D     | 103 | PHE  | 2              |
| 2   | D     | 52  | ASP  | 2              |
| 1   | C     | 32  | MET  | 2              |
| 2   | B     | 139 | ASN  | 2              |
| 1   | A     | 109 | LEU  | 2              |
| 2   | B     | 48  | LEU  | 2              |
| 2   | D     | 7   | GLU  | 2              |
| 1   | A     | 81  | SER  | 2              |
| 1   | A     | 47  | ASP  | 1              |
| 2   | D     | 28  | LEU  | 1              |
| 2   | B     | 9   | SER  | 1              |
| 1   | A     | 30  | GLU  | 1              |
| 1   | C     | 91  | LEU  | 1              |
| 1   | C     | 27  | GLU  | 1              |
| 1   | C     | 49  | SER  | 1              |
| 1   | C     | 47  | ASP  | 1              |
| 1   | C     | 116 | GLU  | 1              |
| 2   | B     | 71  | PHE  | 1              |
| 1   | A     | 138 | SER  | 1              |
| 1   | C     | 124 | SER  | 1              |
| 2   | D     | 114 | LEU  | 1              |
| 2   | D     | 43  | GLU  | 1              |
| 1   | A     | 124 | SER  | 1              |
| 2   | B     | 92  | HIS  | 1              |
| 2   | D     | 72  | SER  | 1              |
| 2   | D     | 66  | LYS  | 1              |
| 1   | A     | 1   | VAL  | 1              |
| 1   | A     | 112 | HIS  | 1              |
| 2   | B     | 72  | SER  | 1              |
| 1   | C     | 1   | VAL  | 1              |
| 2   | D     | 39  | GLN  | 1              |
| 1   | A     | 135 | VAL  | 1              |
| 1   | C     | 135 | VAL  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 84  | SER  | 1              |
| 1   | C     | 54  | GLN  | 1              |
| 1   | C     | 40  | LYS  | 1              |
| 2   | B     | 114 | LEU  | 1              |
| 1   | A     | 116 | GLU  | 1              |
| 1   | C     | 112 | HIS  | 1              |
| 1   | A     | 91  | LEU  | 1              |
| 1   | A     | 27  | GLU  | 1              |
| 1   | A     | 103 | HIS  | 1              |
| 2   | D     | 42  | PHE  | 1              |
| 1   | A     | 85  | ASP  | 1              |
| 2   | B     | 28  | LEU  | 1              |
| 1   | C     | 138 | SER  | 1              |
| 1   | C     | 83  | LEU  | 1              |
| 2   | D     | 71  | PHE  | 1              |
| 1   | A     | 108 | THR  | 1              |
| 1   | A     | 93  | VAL  | 1              |
| 1   | A     | 54  | GLN  | 1              |
| 1   | C     | 85  | ASP  | 1              |
| 2   | B     | 19  | ASN  | 1              |
| 2   | D     | 19  | ASN  | 1              |
| 2   | B     | 47  | ASP  | 1              |
| 1   | C     | 108 | THR  | 1              |
| 2   | B     | 39  | GLN  | 1              |
| 1   | A     | 40  | LYS  | 1              |
| 1   | C     | 103 | HIS  | 1              |
| 1   | C     | 93  | VAL  | 1              |
| 1   | C     | 30  | GLU  | 1              |
| 1   | C     | 84  | SER  | 1              |
| 2   | D     | 92  | HIS  | 1              |
| 1   | A     | 49  | SER  | 1              |
| 2   | B     | 42  | PHE  | 1              |
| 2   | D     | 9   | SER  | 1              |
| 2   | B     | 66  | LYS  | 1              |
| 2   | D     | 47  | ASP  | 1              |
| 1   | A     | 83  | LEU  | 1              |
| 2   | B     | 43  | GLU  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths |           |            |
|-----|------|-------|-----|------|--------------|-----------|------------|
|     |      |       |     |      | Counts       | RMSZ      | #Z>2       |
| 3   | HEC  | A     | 142 | -    | 24,50,50     | 1.74±0.03 | 1±1 (3±2%) |
| 3   | HEC  | B     | 147 | -    | 24,50,50     | 1.72±0.02 | 1±1 (3±2%) |
| 3   | HEC  | C     | 142 | -    | 24,50,50     | 1.74±0.03 | 1±1 (3±3%) |
| 3   | HEC  | D     | 147 | -    | 24,50,50     | 1.72±0.02 | 1±1 (3±3%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles |           |             |
|-----|------|-------|-----|------|-------------|-----------|-------------|
|     |      |       |     |      | Counts      | RMSZ      | #Z>2        |
| 3   | HEC  | A     | 142 | -    | 19,82,82    | 2.24±0.02 | 2±0 (10±0%) |
| 3   | HEC  | B     | 147 | -    | 19,82,82    | 2.27±0.02 | 2±0 (10±0%) |
| 3   | HEC  | C     | 142 | -    | 19,82,82    | 2.24±0.02 | 2±0 (10±0%) |
| 3   | HEC  | D     | 147 | -    | 19,82,82    | 2.27±0.02 | 2±0 (10±0%) |

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   | HEC  | A     | 142 | -    | -       | 0±0,6,54,54 | 0±0,0,8,8 |
| 3   | HEC  | B     | 147 | -    | -       | 0±0,6,54,54 | 0±0,0,8,8 |
| 3   | HEC  | C     | 142 | -    | -       | 0±0,6,54,54 | 0±0,0,8,8 |
| 3   | HEC  | D     | 147 | -    | -       | 0±0,6,54,54 | 0±0,0,8,8 |

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
|     |       |     |      |         |      |             |          | Worst  | Total |
| 3   | A     | 142 | HEC  | C3B-C2B | 5.28 | 1.35        | 1.40     | 5      | 13    |
| 3   | C     | 142 | HEC  | C3B-C2B | 5.25 | 1.35        | 1.40     | 18     | 13    |
| 3   | B     | 147 | HEC  | C3B-C2B | 5.20 | 1.35        | 1.40     | 18     | 10    |
| 3   | D     | 147 | HEC  | C3C-C2C | 5.19 | 1.35        | 1.40     | 14     | 9     |
| 3   | D     | 147 | HEC  | C3B-C2B | 5.17 | 1.35        | 1.40     | 18     | 8     |
| 3   | A     | 142 | HEC  | C3C-C2C | 5.09 | 1.35        | 1.40     | 20     | 3     |
| 3   | B     | 147 | HEC  | C3C-C2C | 5.08 | 1.35        | 1.40     | 1      | 5     |
| 3   | C     | 142 | HEC  | C3C-C2C | 5.08 | 1.35        | 1.40     | 19     | 6     |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
|     |       |     |      |             |      |             |          | Worst  | Total |
| 3   | D     | 147 | HEC  | CBB-CAB-C3B | 6.63 | 112.84      | 127.34   | 12     | 20    |
| 3   | B     | 147 | HEC  | CBB-CAB-C3B | 6.61 | 112.89      | 127.34   | 18     | 20    |
| 3   | A     | 142 | HEC  | CBB-CAB-C3B | 6.60 | 112.91      | 127.34   | 15     | 20    |
| 3   | C     | 142 | HEC  | CBB-CAB-C3B | 6.60 | 112.91      | 127.34   | 15     | 20    |
| 3   | B     | 147 | HEC  | CBC-CAC-C3C | 6.60 | 112.92      | 127.34   | 3      | 20    |
| 3   | C     | 142 | HEC  | CBC-CAC-C3C | 6.60 | 112.92      | 127.34   | 4      | 20    |
| 3   | A     | 142 | HEC  | CBC-CAC-C3C | 6.60 | 112.92      | 127.34   | 7      | 20    |
| 3   | D     | 147 | HEC  | CBC-CAC-C3C | 6.59 | 112.92      | 127.34   | 17     | 20    |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided