



# Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1KUL / pdb\_00001kul  
Title : GLUCOAMYLASE, GRANULAR STARCH-BINDING DOMAIN, NMR, 5 STRUCTURES  
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Deposited on : 1996-01-12

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| wwPDB-RCI                      | : | v_1n_11_5_13_A (Berjanski et al., 2005)                          |
| PANAV                          | : | Wang et al. (2010)                                               |
| wwPDB-ShiftChecker             | : | v1.2                                                             |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

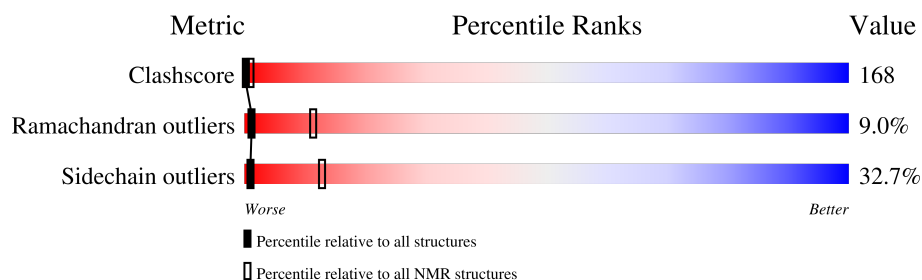
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*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            | 229148                      | 14424                     |
| Ramachandran outliers | 224038                      | 12848                     |
| Sidechain outliers    | 223484                      | 12823                     |

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     | 108    |                  |

## 2 Ensemble composition and analysis

This entry contains 5 models. Model 2 is the overall representative, medoid model (most similar to other models).

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:514-A:601, A:608-A:616<br>(97) | 0.61              | 2            |

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 1 clusters. No single-model clusters were found.

| Cluster number | Models        |
|----------------|---------------|
| 1              | 1, 2, 3, 4, 5 |

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

There is only 1 type of molecule in this entry. The entry contains 1613 atoms, of which 775 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called GLUCOAMYLASE.

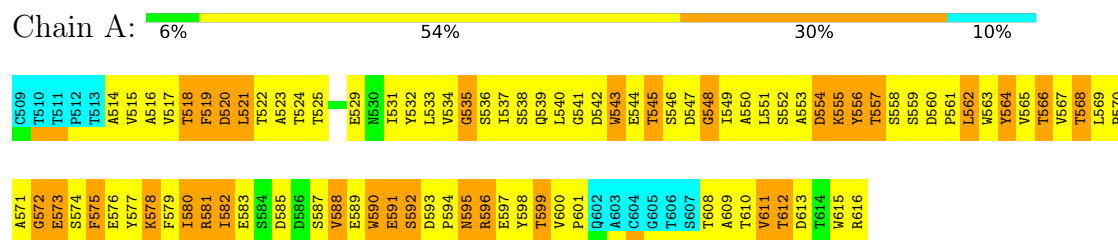
| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 108      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1613  | 527 | 775 | 127 | 182 | 2 |       |

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

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

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: GLUCOAMYLASE

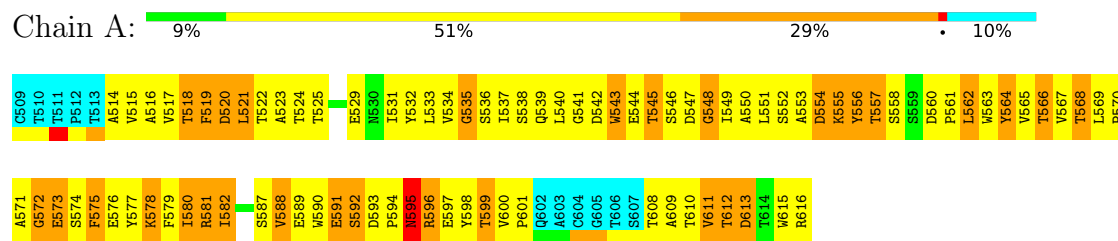


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

#### 4.2.1 Score per residue for model 1

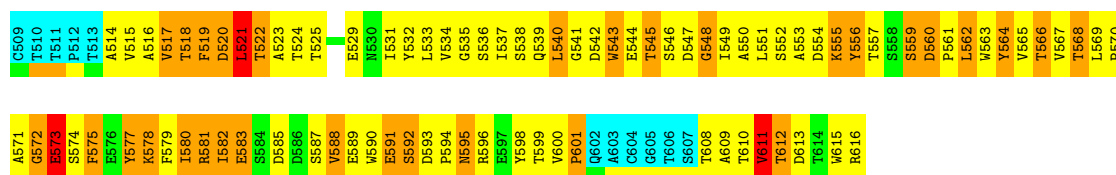
#### • Molecule 1: GLUCOAMYLASE



#### 4.2.2 Score per residue for model 2 (medoid)

#### • Molecule 1: GLUCOAMYLASE

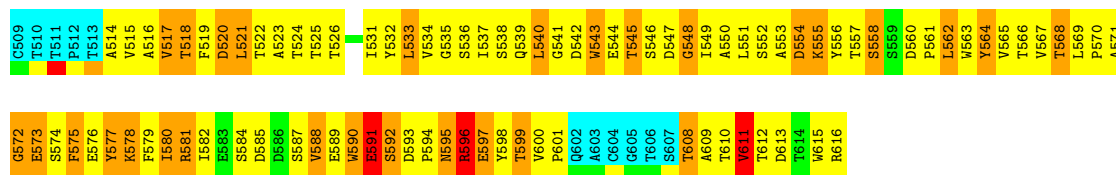




### 4.2.3 Score per residue for model 3

- Molecule 1: GLUCOAMYLASE

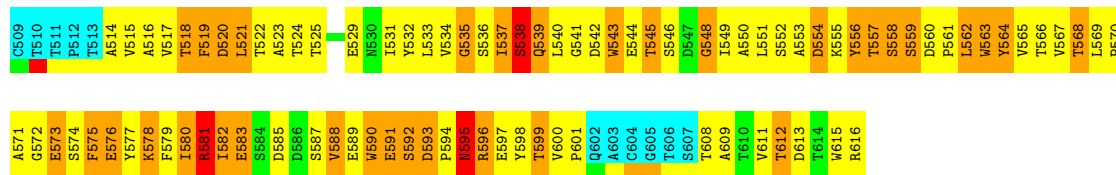
Chain A: 7% 53% 27% 10%



### 4.2.4 Score per residue for model 4

- Molecule 1: GLUCOAMYLASE

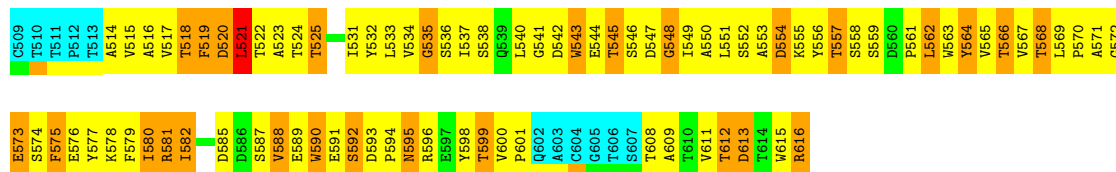
Chain A: 8% 47% 31% 10%



### 4.2.5 Score per residue for model 5

- Molecule 1: GLUCOAMYLASE

Chain A: 12% 52% 25% 10%



## 5 Refinement protocol and experimental data overview

Of the 100 calculated structures, 5 were deposited, based on the following criterion: ?.

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

| Software name | Classification | Version |
|---------------|----------------|---------|
| X-PLOR        | refinement     | 3.1     |

No chemical shift data was provided.

## 6 Model quality i

### 6.1 Standard geometry i

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

| Mol | Chain | Bond lengths |                      | Bond angles |                       |
|-----|-------|--------------|----------------------|-------------|-----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                  |
| 1   | A     | 1.44±0.01    | 1±1/787 ( 0.1± 0.1%) | 1.36±0.02   | 1±1/1081 ( 0.1± 0.1%) |
| All | All   | 1.44         | 5/3935 ( 0.1%)       | 1.36        | 7/5405 ( 0.1%)        |

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

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 3.0±0.0   |
| All | All   | 0         | 15        |

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 |
| 1   | A     | 535 | GLY  | N-CA  | 5.75 | 1.50        | 1.45     | 1      | 3     |
| 1   | A     | 521 | LEU  | N-CA  | 5.73 | 1.53        | 1.46     | 2      | 2     |

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 |
| 1   | A     | 519 | PHE  | CA-CB-CG | -6.38 | 107.42      | 113.80   | 5      | 4     |
| 1   | A     | 590 | TRP  | N-CA-C   | 5.29  | 115.12      | 108.45   | 5      | 2     |
| 1   | A     | 563 | TRP  | CB-CA-C  | -5.07 | 101.88      | 113.33   | 4      | 1     |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 581 | ARG  | Sidechain | 5              |
| 1   | A     | 596 | ARG  | Sidechain | 5              |
| 1   | A     | 616 | ARG  | Sidechain | 5              |

## 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     | 767   | 709      | 709      | 248±11  |
| All | All   | 3835  | 3545     | 3545     | 1239    |

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 168.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:534:VAL:HG11 | 1:A:590:TRP:CH2  | 1.06     | 1.86        | 5      | 5     |
| 1:A:532:TYR:CE2  | 1:A:550:ALA:HB2  | 1.02     | 1.89        | 4      | 5     |
| 1:A:580:ILE:HG22 | 1:A:590:TRP:CD1  | 0.99     | 1.92        | 3      | 5     |
| 1:A:540:LEU:CD1  | 1:A:567:VAL:HG11 | 0.98     | 1.88        | 2      | 3     |
| 1:A:515:VAL:HG21 | 1:A:600:VAL:HG13 | 0.97     | 1.30        | 5      | 1     |
| 1:A:598:TYR:CZ   | 1:A:609:ALA:HB1  | 0.96     | 1.96        | 1      | 5     |
| 1:A:517:VAL:HG22 | 1:A:609:ALA:CB   | 0.96     | 1.91        | 1      | 5     |
| 1:A:537:ILE:HD11 | 1:A:569:LEU:CD2  | 0.96     | 1.91        | 2      | 4     |
| 1:A:521:LEU:HD12 | 1:A:613:ASP:O    | 0.96     | 1.60        | 1      | 5     |
| 1:A:562:LEU:HD22 | 1:A:562:LEU:O    | 0.95     | 1.61        | 4      | 3     |
| 1:A:515:VAL:CG2  | 1:A:600:VAL:HG13 | 0.94     | 1.91        | 5      | 5     |
| 1:A:537:ILE:HD11 | 1:A:569:LEU:HD22 | 0.93     | 1.37        | 5      | 4     |
| 1:A:519:PHE:CD2  | 1:A:533:LEU:HD23 | 0.93     | 1.98        | 3      | 1     |
| 1:A:515:VAL:HG21 | 1:A:601:PRO:HD2  | 0.92     | 1.41        | 1      | 2     |
| 1:A:577:TYR:OH   | 1:A:611:VAL:HG21 | 0.92     | 1.62        | 3      | 2     |
| 1:A:598:TYR:CE2  | 1:A:609:ALA:HB1  | 0.91     | 2.00        | 4      | 4     |
| 1:A:521:LEU:HD21 | 1:A:531:ILE:HG21 | 0.89     | 1.44        | 4      | 4     |
| 1:A:533:LEU:HD12 | 1:A:578:LYS:O    | 0.88     | 1.68        | 4      | 2     |
| 1:A:532:TYR:CZ   | 1:A:550:ALA:HB2  | 0.87     | 2.04        | 1      | 4     |
| 1:A:521:LEU:CD2  | 1:A:531:ILE:HG21 | 0.86     | 1.98        | 4      | 3     |
| 1:A:569:LEU:O    | 1:A:600:VAL:HG21 | 0.86     | 1.70        | 2      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:582:ILE:N    | 1:A:582:ILE:HD12 | 0.86     | 1.86        | 5      | 5     |
| 1:A:564:TYR:O    | 1:A:565:VAL:HG23 | 0.85     | 1.71        | 2      | 4     |
| 1:A:540:LEU:HD12 | 1:A:577:TYR:CE2  | 0.85     | 2.07        | 4      | 1     |
| 1:A:517:VAL:HG22 | 1:A:609:ALA:HB3  | 0.85     | 1.49        | 1      | 4     |
| 1:A:537:ILE:HD13 | 1:A:575:PHE:CD1  | 0.85     | 2.06        | 3      | 4     |
| 1:A:533:LEU:HD12 | 1:A:534:VAL:N    | 0.85     | 1.87        | 3      | 1     |
| 1:A:523:ALA:HB2  | 1:A:615:TRP:HB3  | 0.84     | 1.49        | 4      | 5     |
| 1:A:553:ALA:HB1  | 1:A:556:TYR:HB3  | 0.84     | 1.47        | 5      | 3     |
| 1:A:562:LEU:HD13 | 1:A:562:LEU:N    | 0.84     | 1.87        | 1      | 3     |
| 1:A:545:THR:CB   | 1:A:580:ILE:HG21 | 0.84     | 2.03        | 3      | 1     |
| 1:A:580:ILE:HB   | 1:A:582:ILE:HD11 | 0.83     | 1.51        | 5      | 5     |
| 1:A:540:LEU:HD11 | 1:A:567:VAL:HG11 | 0.83     | 1.48        | 2      | 3     |
| 1:A:610:THR:O    | 1:A:611:VAL:HG23 | 0.83     | 1.74        | 2      | 3     |
| 1:A:540:LEU:HD12 | 1:A:577:TYR:CD2  | 0.83     | 2.09        | 4      | 1     |
| 1:A:519:PHE:O    | 1:A:564:TYR:HA   | 0.82     | 1.75        | 3      | 4     |
| 1:A:533:LEU:HD12 | 1:A:533:LEU:C    | 0.81     | 2.01        | 3      | 1     |
| 1:A:566:THR:O    | 1:A:566:THR:HG23 | 0.80     | 1.75        | 3      | 5     |
| 1:A:540:LEU:HD13 | 1:A:577:TYR:CZ   | 0.80     | 2.12        | 1      | 1     |
| 1:A:549:ILE:HD12 | 1:A:567:VAL:HG22 | 0.79     | 1.54        | 2      | 2     |
| 1:A:515:VAL:CG1  | 1:A:609:ALA:HB2  | 0.78     | 2.09        | 1      | 4     |
| 1:A:562:LEU:HD13 | 1:A:562:LEU:H    | 0.78     | 1.36        | 2      | 3     |
| 1:A:517:VAL:HG21 | 1:A:569:LEU:HD12 | 0.78     | 1.55        | 5      | 3     |
| 1:A:515:VAL:HG13 | 1:A:608:THR:O    | 0.78     | 1.78        | 1      | 1     |
| 1:A:520:ASP:OD1  | 1:A:612:THR:HG23 | 0.78     | 1.79        | 1      | 1     |
| 1:A:545:THR:OG1  | 1:A:580:ILE:HG21 | 0.77     | 1.80        | 3      | 1     |
| 1:A:580:ILE:HG22 | 1:A:590:TRP:CG   | 0.76     | 2.15        | 3      | 5     |
| 1:A:578:LYS:NZ   | 1:A:580:ILE:HG23 | 0.76     | 1.96        | 4      | 1     |
| 1:A:516:ALA:HB1  | 1:A:566:THR:OG1  | 0.76     | 1.81        | 4      | 2     |
| 1:A:531:ILE:O    | 1:A:551:LEU:HD13 | 0.75     | 1.80        | 5      | 5     |
| 1:A:551:LEU:HA   | 1:A:565:VAL:CG2  | 0.75     | 2.12        | 3      | 5     |
| 1:A:521:LEU:O    | 1:A:562:LEU:HA   | 0.74     | 1.83        | 1      | 5     |
| 1:A:521:LEU:HB2  | 1:A:563:TRP:HB2  | 0.74     | 1.59        | 2      | 5     |
| 1:A:521:LEU:HA   | 1:A:613:ASP:O    | 0.74     | 1.83        | 1      | 5     |
| 1:A:531:ILE:HD13 | 1:A:563:TRP:CE2  | 0.74     | 2.17        | 1      | 4     |
| 1:A:517:VAL:CG2  | 1:A:569:LEU:HD12 | 0.72     | 2.13        | 5      | 2     |
| 1:A:517:VAL:HA   | 1:A:609:ALA:HB3  | 0.72     | 1.59        | 2      | 5     |
| 1:A:551:LEU:HA   | 1:A:565:VAL:HG21 | 0.72     | 1.62        | 5      | 5     |
| 1:A:519:PHE:CD2  | 1:A:533:LEU:HD22 | 0.72     | 2.19        | 4      | 1     |
| 1:A:519:PHE:CD2  | 1:A:533:LEU:CD2  | 0.71     | 2.73        | 3      | 4     |
| 1:A:569:LEU:HD11 | 1:A:577:TYR:CE2  | 0.71     | 2.21        | 1      | 2     |
| 1:A:545:THR:HB   | 1:A:580:ILE:HG21 | 0.70     | 1.63        | 3      | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:582:ILE:N    | 1:A:582:ILE:CD1  | 0.69     | 2.55        | 5      | 5     |
| 1:A:535:GLY:N    | 1:A:540:LEU:CB   | 0.69     | 2.55        | 5      | 5     |
| 1:A:552:SER:O    | 1:A:563:TRP:CE3  | 0.69     | 2.46        | 5      | 5     |
| 1:A:531:ILE:CG1  | 1:A:615:TRP:CE3  | 0.69     | 2.76        | 1      | 5     |
| 1:A:556:TYR:CD1  | 1:A:556:TYR:C    | 0.68     | 2.71        | 4      | 5     |
| 1:A:534:VAL:HG13 | 1:A:578:LYS:HE2  | 0.68     | 1.65        | 1      | 1     |
| 1:A:519:PHE:CG   | 1:A:533:LEU:HD23 | 0.68     | 2.23        | 3      | 1     |
| 1:A:521:LEU:HG   | 1:A:615:TRP:CB   | 0.68     | 2.18        | 3      | 5     |
| 1:A:537:ILE:HD13 | 1:A:575:PHE:CE1  | 0.68     | 2.24        | 1      | 2     |
| 1:A:519:PHE:CD2  | 1:A:565:VAL:O    | 0.68     | 2.46        | 1      | 4     |
| 1:A:518:THR:HG23 | 1:A:566:THR:HB   | 0.67     | 1.66        | 4      | 2     |
| 1:A:590:TRP:CD1  | 1:A:590:TRP:N    | 0.67     | 2.62        | 3      | 1     |
| 1:A:525:THR:N    | 1:A:556:TYR:OH   | 0.67     | 2.27        | 5      | 5     |
| 1:A:573:GLU:CB   | 1:A:575:PHE:CZ   | 0.67     | 2.77        | 4      | 4     |
| 1:A:532:TYR:CE2  | 1:A:550:ALA:CB   | 0.66     | 2.75        | 3      | 4     |
| 1:A:581:ARG:C    | 1:A:582:ILE:HD12 | 0.66     | 2.16        | 4      | 4     |
| 1:A:540:LEU:HD13 | 1:A:567:VAL:HG11 | 0.66     | 1.64        | 2      | 1     |
| 1:A:517:VAL:CG2  | 1:A:609:ALA:HB3  | 0.66     | 2.19        | 1      | 3     |
| 1:A:569:LEU:HD13 | 1:A:577:TYR:CZ   | 0.66     | 2.24        | 5      | 1     |
| 1:A:533:LEU:CB   | 1:A:551:LEU:HD11 | 0.66     | 2.21        | 4      | 4     |
| 1:A:521:LEU:HD12 | 1:A:613:ASP:C    | 0.66     | 2.16        | 3      | 5     |
| 1:A:580:ILE:CB   | 1:A:582:ILE:HD11 | 0.65     | 2.20        | 5      | 5     |
| 1:A:515:VAL:HG23 | 1:A:600:VAL:HG13 | 0.65     | 1.67        | 2      | 2     |
| 1:A:521:LEU:HG   | 1:A:615:TRP:HB2  | 0.65     | 1.68        | 4      | 3     |
| 1:A:562:LEU:N    | 1:A:562:LEU:CD1  | 0.65     | 2.60        | 4      | 3     |
| 1:A:532:TYR:CG   | 1:A:550:ALA:HA   | 0.65     | 2.27        | 2      | 5     |
| 1:A:515:VAL:HG12 | 1:A:609:ALA:HB2  | 0.65     | 1.69        | 2      | 5     |
| 1:A:598:TYR:CZ   | 1:A:609:ALA:CB   | 0.64     | 2.77        | 1      | 5     |
| 1:A:517:VAL:CA   | 1:A:609:ALA:HB3  | 0.64     | 2.22        | 2      | 5     |
| 1:A:580:ILE:CG2  | 1:A:590:TRP:CE2  | 0.64     | 2.80        | 5      | 4     |
| 1:A:537:ILE:CD1  | 1:A:569:LEU:HD22 | 0.64     | 2.23        | 2      | 3     |
| 1:A:570:PRO:O    | 1:A:571:ALA:HB3  | 0.64     | 1.93        | 3      | 4     |
| 1:A:515:VAL:CB   | 1:A:600:VAL:HG13 | 0.64     | 2.23        | 2      | 4     |
| 1:A:521:LEU:HD21 | 1:A:531:ILE:HG12 | 0.64     | 1.70        | 1      | 3     |
| 1:A:573:GLU:CB   | 1:A:575:PHE:CE2  | 0.64     | 2.80        | 4      | 4     |
| 1:A:569:LEU:HD13 | 1:A:577:TYR:CE2  | 0.63     | 2.27        | 5      | 1     |
| 1:A:569:LEU:CD2  | 1:A:577:TYR:OH   | 0.63     | 2.46        | 4      | 2     |
| 1:A:535:GLY:C    | 1:A:543:TRP:CZ2  | 0.63     | 2.77        | 4      | 5     |
| 1:A:598:TYR:CE2  | 1:A:609:ALA:CB   | 0.63     | 2.81        | 4      | 3     |
| 1:A:554:ASP:CG   | 1:A:564:TYR:HH   | 0.62     | 2.02        | 3      | 1     |
| 1:A:535:GLY:N    | 1:A:540:LEU:HB3  | 0.62     | 2.10        | 5      | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:536:SER:HA   | 1:A:543:TRP:CE2  | 0.62     | 2.29        | 1      | 5     |
| 1:A:531:ILE:HG12 | 1:A:615:TRP:CE3  | 0.62     | 2.29        | 2      | 5     |
| 1:A:523:ALA:O    | 1:A:556:TYR:CZ   | 0.62     | 2.52        | 5      | 5     |
| 1:A:531:ILE:HG13 | 1:A:615:TRP:CE3  | 0.62     | 2.30        | 1      | 5     |
| 1:A:577:TYR:N    | 1:A:577:TYR:CD1  | 0.62     | 2.66        | 5      | 3     |
| 1:A:542:ASP:O    | 1:A:543:TRP:CG   | 0.61     | 2.53        | 4      | 5     |
| 1:A:534:VAL:HG21 | 1:A:544:GLU:N    | 0.61     | 2.11        | 3      | 5     |
| 1:A:535:GLY:O    | 1:A:543:TRP:CD2  | 0.61     | 2.53        | 1      | 5     |
| 1:A:566:THR:O    | 1:A:566:THR:CG2  | 0.61     | 2.47        | 5      | 4     |
| 1:A:581:ARG:O    | 1:A:588:VAL:HA   | 0.61     | 1.95        | 2      | 5     |
| 1:A:582:ILE:HG13 | 1:A:588:VAL:HG11 | 0.61     | 1.71        | 2      | 5     |
| 1:A:578:LYS:HZ1  | 1:A:580:ILE:HG23 | 0.61     | 1.55        | 4      | 1     |
| 1:A:580:ILE:CG2  | 1:A:590:TRP:CD1  | 0.61     | 2.80        | 4      | 4     |
| 1:A:571:ALA:O    | 1:A:572:GLY:C    | 0.61     | 2.44        | 1      | 3     |
| 1:A:521:LEU:HD13 | 1:A:613:ASP:OD2  | 0.61     | 1.96        | 1      | 1     |
| 1:A:532:TYR:CD2  | 1:A:550:ALA:CA   | 0.61     | 2.83        | 3      | 5     |
| 1:A:535:GLY:O    | 1:A:543:TRP:CE2  | 0.61     | 2.54        | 2      | 5     |
| 1:A:598:TYR:CD1  | 1:A:610:THR:O    | 0.61     | 2.54        | 2      | 3     |
| 1:A:589:GLU:O    | 1:A:590:TRP:CD1  | 0.60     | 2.54        | 5      | 4     |
| 1:A:560:ASP:CG   | 1:A:562:LEU:HD12 | 0.60     | 2.20        | 4      | 1     |
| 1:A:588:VAL:HG23 | 1:A:590:TRP:CD1  | 0.60     | 2.31        | 3      | 5     |
| 1:A:520:ASP:OD2  | 1:A:612:THR:HG23 | 0.60     | 1.97        | 2      | 3     |
| 1:A:554:ASP:OD2  | 1:A:564:TYR:CD2  | 0.60     | 2.54        | 1      | 3     |
| 1:A:514:ALA:HB2  | 1:A:570:PRO:HB3  | 0.60     | 1.74        | 3      | 1     |
| 1:A:549:ILE:HG21 | 1:A:565:VAL:HG11 | 0.60     | 1.74        | 3      | 1     |
| 1:A:532:TYR:CD2  | 1:A:550:ALA:HA   | 0.60     | 2.32        | 3      | 2     |
| 1:A:531:ILE:O    | 1:A:551:LEU:CD1  | 0.60     | 2.50        | 2      | 5     |
| 1:A:521:LEU:HB2  | 1:A:563:TRP:CB   | 0.60     | 2.27        | 5      | 3     |
| 1:A:573:GLU:HB2  | 1:A:575:PHE:CZ   | 0.60     | 2.31        | 4      | 4     |
| 1:A:531:ILE:HD13 | 1:A:563:TRP:NE1  | 0.59     | 2.11        | 1      | 2     |
| 1:A:519:PHE:O    | 1:A:564:TYR:CA   | 0.59     | 2.49        | 4      | 1     |
| 1:A:564:TYR:O    | 1:A:565:VAL:CG2  | 0.59     | 2.49        | 2      | 4     |
| 1:A:524:THR:HA   | 1:A:556:TYR:CE1  | 0.59     | 2.31        | 4      | 5     |
| 1:A:593:ASP:N    | 1:A:594:PRO:CD   | 0.59     | 2.65        | 3      | 3     |
| 1:A:581:ARG:O    | 1:A:588:VAL:HB   | 0.59     | 1.98        | 4      | 5     |
| 1:A:514:ALA:HB1  | 1:A:569:LEU:O    | 0.59     | 1.98        | 4      | 1     |
| 1:A:518:THR:HA   | 1:A:565:VAL:O    | 0.59     | 1.97        | 1      | 5     |
| 1:A:535:GLY:C    | 1:A:543:TRP:CH2  | 0.59     | 2.81        | 4      | 5     |
| 1:A:519:PHE:O    | 1:A:564:TYR:CB   | 0.59     | 2.51        | 4      | 1     |
| 1:A:531:ILE:HG13 | 1:A:615:TRP:CZ3  | 0.59     | 2.33        | 1      | 5     |
| 1:A:549:ILE:HD12 | 1:A:567:VAL:CG2  | 0.59     | 2.25        | 2      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:579:PHE:C    | 1:A:579:PHE:CD1  | 0.59     | 2.80        | 1      | 2     |
| 1:A:533:LEU:HB2  | 1:A:551:LEU:HD11 | 0.59     | 1.74        | 4      | 1     |
| 1:A:543:TRP:CE3  | 1:A:543:TRP:HA   | 0.59     | 2.32        | 1      | 5     |
| 1:A:549:ILE:CG2  | 1:A:565:VAL:HG11 | 0.58     | 2.28        | 3      | 1     |
| 1:A:556:TYR:CD1  | 1:A:561:PRO:HA   | 0.58     | 2.33        | 3      | 5     |
| 1:A:573:GLU:HB3  | 1:A:575:PHE:CE2  | 0.58     | 2.34        | 2      | 4     |
| 1:A:579:PHE:CE1  | 1:A:615:TRP:CE3  | 0.58     | 2.92        | 3      | 2     |
| 1:A:535:GLY:HA3  | 1:A:577:TYR:CE2  | 0.58     | 2.33        | 4      | 1     |
| 1:A:570:PRO:HD2  | 1:A:575:PHE:CE1  | 0.58     | 2.34        | 4      | 1     |
| 1:A:580:ILE:CG2  | 1:A:590:TRP:CG   | 0.57     | 2.86        | 3      | 5     |
| 1:A:588:VAL:CG2  | 1:A:590:TRP:CD1  | 0.57     | 2.87        | 2      | 5     |
| 1:A:575:PHE:CB   | 1:A:577:TYR:OH   | 0.57     | 2.52        | 5      | 1     |
| 1:A:554:ASP:OD1  | 1:A:564:TYR:CZ   | 0.57     | 2.57        | 3      | 1     |
| 1:A:554:ASP:OD2  | 1:A:564:TYR:CE1  | 0.57     | 2.57        | 4      | 1     |
| 1:A:578:LYS:NZ   | 1:A:590:TRP:CE3  | 0.57     | 2.73        | 4      | 1     |
| 1:A:520:ASP:HA   | 1:A:563:TRP:O    | 0.57     | 1.99        | 4      | 4     |
| 1:A:541:GLY:O    | 1:A:542:ASP:CB   | 0.57     | 2.53        | 4      | 4     |
| 1:A:568:THR:O    | 1:A:569:LEU:HD23 | 0.57     | 1.99        | 5      | 4     |
| 1:A:563:TRP:O    | 1:A:564:TYR:CB   | 0.57     | 2.53        | 4      | 2     |
| 1:A:569:LEU:HD21 | 1:A:577:TYR:CZ   | 0.56     | 2.35        | 4      | 1     |
| 1:A:563:TRP:O    | 1:A:564:TYR:HB3  | 0.56     | 1.99        | 3      | 2     |
| 1:A:615:TRP:CD1  | 1:A:615:TRP:C    | 0.56     | 2.84        | 5      | 5     |
| 1:A:575:PHE:HB2  | 1:A:577:TYR:CE1  | 0.56     | 2.35        | 5      | 1     |
| 1:A:534:VAL:CG1  | 1:A:590:TRP:CH2  | 0.56     | 2.79        | 2      | 4     |
| 1:A:525:THR:HG22 | 1:A:526:THR:N    | 0.56     | 2.15        | 3      | 1     |
| 1:A:535:GLY:O    | 1:A:542:ASP:O    | 0.56     | 2.23        | 1      | 5     |
| 1:A:593:ASP:CB   | 1:A:594:PRO:CD   | 0.56     | 2.83        | 1      | 2     |
| 1:A:533:LEU:HD13 | 1:A:578:LYS:O    | 0.56     | 2.00        | 3      | 1     |
| 1:A:557:THR:O    | 1:A:558:SER:CB   | 0.56     | 2.54        | 3      | 1     |
| 1:A:515:VAL:HG21 | 1:A:600:VAL:CG1  | 0.56     | 2.19        | 5      | 1     |
| 1:A:564:TYR:C    | 1:A:565:VAL:HG23 | 0.56     | 2.26        | 4      | 2     |
| 1:A:524:THR:C    | 1:A:556:TYR:OH   | 0.56     | 2.49        | 4      | 5     |
| 1:A:582:ILE:HG13 | 1:A:588:VAL:CG1  | 0.56     | 2.31        | 1      | 5     |
| 1:A:571:ALA:O    | 1:A:572:GLY:O    | 0.56     | 2.24        | 2      | 3     |
| 1:A:598:TYR:OH   | 1:A:609:ALA:CB   | 0.56     | 2.53        | 5      | 4     |
| 1:A:580:ILE:CG2  | 1:A:590:TRP:NE1  | 0.56     | 2.69        | 5      | 4     |
| 1:A:531:ILE:CD1  | 1:A:563:TRP:CE2  | 0.55     | 2.90        | 1      | 2     |
| 1:A:519:PHE:CE2  | 1:A:533:LEU:CD2  | 0.55     | 2.90        | 4      | 1     |
| 1:A:578:LYS:CG   | 1:A:591:GLU:HB3  | 0.55     | 2.32        | 5      | 2     |
| 1:A:587:SER:C    | 1:A:588:VAL:CG1  | 0.55     | 2.80        | 4      | 5     |
| 1:A:534:VAL:C    | 1:A:540:LEU:HD13 | 0.55     | 2.26        | 4      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:543:TRP:CZ3  | 1:A:578:LYS:HD2  | 0.55     | 2.36        | 4      | 1     |
| 1:A:615:TRP:CD1  | 1:A:615:TRP:O    | 0.55     | 2.60        | 5      | 2     |
| 1:A:523:ALA:CB   | 1:A:615:TRP:HB3  | 0.55     | 2.32        | 5      | 4     |
| 1:A:548:GLY:O    | 1:A:549:ILE:CG1  | 0.55     | 2.55        | 5      | 3     |
| 1:A:534:VAL:HG11 | 1:A:590:TRP:CZ3  | 0.55     | 2.35        | 2      | 2     |
| 1:A:585:ASP:CG   | 1:A:587:SER:HG   | 0.55     | 2.10        | 5      | 1     |
| 1:A:593:ASP:HB2  | 1:A:594:PRO:HD3  | 0.55     | 1.79        | 4      | 2     |
| 1:A:521:LEU:O    | 1:A:562:LEU:CA   | 0.54     | 2.55        | 1      | 1     |
| 1:A:521:LEU:CD2  | 1:A:531:ILE:CG2  | 0.54     | 2.82        | 4      | 2     |
| 1:A:580:ILE:HG22 | 1:A:589:GLU:O    | 0.54     | 2.01        | 2      | 4     |
| 1:A:521:LEU:HB2  | 1:A:563:TRP:CD1  | 0.54     | 2.36        | 5      | 1     |
| 1:A:517:VAL:HG13 | 1:A:610:THR:N    | 0.54     | 2.18        | 1      | 2     |
| 1:A:545:THR:HB   | 1:A:590:TRP:CZ2  | 0.54     | 2.38        | 4      | 4     |
| 1:A:560:ASP:O    | 1:A:562:LEU:CD1  | 0.54     | 2.56        | 4      | 3     |
| 1:A:593:ASP:N    | 1:A:594:PRO:HD2  | 0.54     | 2.17        | 3      | 3     |
| 1:A:521:LEU:O    | 1:A:562:LEU:CB   | 0.54     | 2.56        | 1      | 1     |
| 1:A:532:TYR:C    | 1:A:551:LEU:CD1  | 0.54     | 2.81        | 4      | 4     |
| 1:A:531:ILE:HD12 | 1:A:531:ILE:N    | 0.54     | 2.17        | 5      | 5     |
| 1:A:581:ARG:HA   | 1:A:615:TRP:CH2  | 0.54     | 2.37        | 1      | 4     |
| 1:A:533:LEU:C    | 1:A:533:LEU:CD1  | 0.54     | 2.74        | 3      | 1     |
| 1:A:514:ALA:CA   | 1:A:569:LEU:O    | 0.54     | 2.56        | 4      | 1     |
| 1:A:554:ASP:OD2  | 1:A:564:TYR:CZ   | 0.54     | 2.61        | 4      | 1     |
| 1:A:573:GLU:HB3  | 1:A:575:PHE:CE1  | 0.54     | 2.37        | 5      | 1     |
| 1:A:515:VAL:HG21 | 1:A:601:PRO:CD   | 0.54     | 2.31        | 3      | 1     |
| 1:A:569:LEU:CD1  | 1:A:577:TYR:CE2  | 0.54     | 2.91        | 5      | 1     |
| 1:A:521:LEU:HG   | 1:A:615:TRP:HB3  | 0.54     | 1.80        | 5      | 4     |
| 1:A:540:LEU:N    | 1:A:540:LEU:HD12 | 0.54     | 2.18        | 1      | 1     |
| 1:A:580:ILE:O    | 1:A:582:ILE:CD1  | 0.54     | 2.56        | 4      | 4     |
| 1:A:515:VAL:HG11 | 1:A:601:PRO:HD2  | 0.54     | 1.79        | 2      | 1     |
| 1:A:534:VAL:HG22 | 1:A:543:TRP:CE3  | 0.53     | 2.38        | 4      | 3     |
| 1:A:535:GLY:CA   | 1:A:577:TYR:CD1  | 0.53     | 2.92        | 1      | 1     |
| 1:A:593:ASP:CB   | 1:A:594:PRO:HD3  | 0.53     | 2.33        | 1      | 2     |
| 1:A:515:VAL:HG23 | 1:A:600:VAL:CG1  | 0.53     | 2.33        | 2      | 2     |
| 1:A:573:GLU:HB3  | 1:A:575:PHE:CZ   | 0.53     | 2.38        | 4      | 3     |
| 1:A:581:ARG:HG2  | 1:A:615:TRP:CH2  | 0.53     | 2.38        | 1      | 2     |
| 1:A:535:GLY:CA   | 1:A:577:TYR:HB3  | 0.53     | 2.33        | 3      | 2     |
| 1:A:535:GLY:HA3  | 1:A:577:TYR:CE1  | 0.53     | 2.38        | 1      | 1     |
| 1:A:536:SER:N    | 1:A:543:TRP:CZ2  | 0.53     | 2.77        | 4      | 5     |
| 1:A:515:VAL:CG1  | 1:A:608:THR:O    | 0.53     | 2.57        | 2      | 3     |
| 1:A:540:LEU:CD1  | 1:A:577:TYR:CE2  | 0.53     | 2.89        | 4      | 2     |
| 1:A:521:LEU:CD2  | 1:A:531:ILE:HG12 | 0.53     | 2.33        | 2      | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:554:ASP:OD1  | 1:A:564:TYR:CB   | 0.53     | 2.57        | 2      | 1     |
| 1:A:545:THR:OG1  | 1:A:580:ILE:CG2  | 0.53     | 2.57        | 3      | 1     |
| 1:A:532:TYR:H    | 1:A:582:ILE:HD13 | 0.53     | 1.63        | 4      | 5     |
| 1:A:541:GLY:O    | 1:A:542:ASP:HB2  | 0.53     | 2.02        | 1      | 5     |
| 1:A:579:PHE:CD1  | 1:A:580:ILE:N    | 0.53     | 2.76        | 2      | 2     |
| 1:A:514:ALA:CB   | 1:A:569:LEU:O    | 0.53     | 2.57        | 4      | 1     |
| 1:A:535:GLY:N    | 1:A:540:LEU:HB2  | 0.53     | 2.19        | 4      | 4     |
| 1:A:556:TYR:CD1  | 1:A:561:PRO:CB   | 0.53     | 2.92        | 2      | 3     |
| 1:A:588:VAL:O    | 1:A:589:GLU:CG   | 0.53     | 2.57        | 3      | 1     |
| 1:A:525:THR:CG2  | 1:A:526:THR:N    | 0.53     | 2.71        | 3      | 1     |
| 1:A:578:LYS:NZ   | 1:A:579:PHE:O    | 0.52     | 2.43        | 1      | 1     |
| 1:A:598:TYR:CE1  | 1:A:609:ALA:HB1  | 0.52     | 2.39        | 1      | 1     |
| 1:A:544:GLU:O    | 1:A:548:GLY:N    | 0.52     | 2.41        | 3      | 2     |
| 1:A:581:ARG:CD   | 1:A:589:GLU:O    | 0.52     | 2.57        | 3      | 1     |
| 1:A:537:ILE:CD1  | 1:A:577:TYR:OH   | 0.52     | 2.58        | 4      | 1     |
| 1:A:611:VAL:HG12 | 1:A:611:VAL:O    | 0.52     | 2.04        | 3      | 1     |
| 1:A:554:ASP:CG   | 1:A:555:LYS:N    | 0.52     | 2.66        | 4      | 1     |
| 1:A:536:SER:CA   | 1:A:543:TRP:CZ2  | 0.52     | 2.93        | 4      | 5     |
| 1:A:569:LEU:HD11 | 1:A:577:TYR:HE2  | 0.52     | 1.64        | 3      | 3     |
| 1:A:580:ILE:HG21 | 1:A:590:TRP:CE2  | 0.52     | 2.39        | 5      | 4     |
| 1:A:519:PHE:CE2  | 1:A:567:VAL:HB   | 0.52     | 2.38        | 3      | 4     |
| 1:A:581:ARG:CD   | 1:A:589:GLU:OE1  | 0.52     | 2.58        | 2      | 1     |
| 1:A:551:LEU:HG   | 1:A:565:VAL:HG21 | 0.52     | 1.82        | 1      | 3     |
| 1:A:568:THR:O    | 1:A:569:LEU:CD2  | 0.52     | 2.57        | 5      | 2     |
| 1:A:578:LYS:CD   | 1:A:591:GLU:OE2  | 0.52     | 2.58        | 1      | 1     |
| 1:A:537:ILE:HD13 | 1:A:575:PHE:HD1  | 0.52     | 1.61        | 2      | 2     |
| 1:A:610:THR:O    | 1:A:611:VAL:CG2  | 0.52     | 2.56        | 1      | 2     |
| 1:A:552:SER:OG   | 1:A:553:ALA:N    | 0.52     | 2.43        | 2      | 1     |
| 1:A:581:ARG:CG   | 1:A:589:GLU:O    | 0.52     | 2.57        | 3      | 1     |
| 1:A:556:TYR:HB2  | 1:A:562:LEU:N    | 0.52     | 2.20        | 1      | 4     |
| 1:A:521:LEU:O    | 1:A:561:PRO:O    | 0.52     | 2.27        | 5      | 2     |
| 1:A:534:VAL:HG23 | 1:A:540:LEU:O    | 0.51     | 2.06        | 4      | 5     |
| 1:A:515:VAL:HB   | 1:A:600:VAL:HG13 | 0.51     | 1.80        | 2      | 2     |
| 1:A:581:ARG:O    | 1:A:588:VAL:CA   | 0.51     | 2.58        | 4      | 4     |
| 1:A:581:ARG:HG2  | 1:A:615:TRP:CZ3  | 0.51     | 2.41        | 3      | 2     |
| 1:A:515:VAL:CG2  | 1:A:600:VAL:CG1  | 0.51     | 2.80        | 2      | 2     |
| 1:A:579:PHE:CE1  | 1:A:615:TRP:CZ3  | 0.51     | 2.99        | 2      | 2     |
| 1:A:554:ASP:OD1  | 1:A:554:ASP:C    | 0.51     | 2.53        | 1      | 3     |
| 1:A:532:TYR:HB2  | 1:A:580:ILE:CD1  | 0.51     | 2.36        | 3      | 4     |
| 1:A:516:ALA:O    | 1:A:609:ALA:N    | 0.51     | 2.43        | 1      | 4     |
| 1:A:580:ILE:HB   | 1:A:582:ILE:CD1  | 0.51     | 2.31        | 4      | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:521:LEU:CD2  | 1:A:615:TRP:HB2  | 0.51     | 2.36        | 3      | 2     |
| 1:A:581:ARG:NH2  | 1:A:589:GLU:OE2  | 0.51     | 2.44        | 4      | 1     |
| 1:A:575:PHE:CB   | 1:A:577:TYR:CZ   | 0.51     | 2.94        | 5      | 1     |
| 1:A:520:ASP:OD1  | 1:A:520:ASP:N    | 0.51     | 2.43        | 5      | 1     |
| 1:A:534:VAL:CG1  | 1:A:590:TRP:CZ3  | 0.50     | 2.94        | 3      | 2     |
| 1:A:519:PHE:CD1  | 1:A:519:PHE:N    | 0.50     | 2.74        | 3      | 1     |
| 1:A:580:ILE:CG2  | 1:A:590:TRP:CD2  | 0.50     | 2.94        | 5      | 5     |
| 1:A:581:ARG:HA   | 1:A:615:TRP:CZ3  | 0.50     | 2.41        | 3      | 4     |
| 1:A:520:ASP:O    | 1:A:613:ASP:O    | 0.50     | 2.29        | 4      | 4     |
| 1:A:570:PRO:O    | 1:A:571:ALA:CB   | 0.50     | 2.56        | 3      | 1     |
| 1:A:543:TRP:CZ3  | 1:A:578:LYS:CD   | 0.50     | 2.94        | 4      | 1     |
| 1:A:521:LEU:HB2  | 1:A:563:TRP:CG   | 0.50     | 2.42        | 5      | 2     |
| 1:A:519:PHE:CG   | 1:A:533:LEU:CD2  | 0.50     | 2.94        | 3      | 1     |
| 1:A:532:TYR:CD1  | 1:A:582:ILE:HB   | 0.50     | 2.41        | 5      | 1     |
| 1:A:543:TRP:CH2  | 1:A:578:LYS:HG3  | 0.50     | 2.41        | 4      | 2     |
| 1:A:557:THR:HG23 | 1:A:558:SER:N    | 0.50     | 2.22        | 5      | 1     |
| 1:A:556:TYR:CE1  | 1:A:561:PRO:HB3  | 0.50     | 2.41        | 1      | 5     |
| 1:A:517:VAL:CG1  | 1:A:610:THR:O    | 0.50     | 2.59        | 2      | 1     |
| 1:A:572:GLY:O    | 1:A:573:GLU:CB   | 0.50     | 2.57        | 3      | 3     |
| 1:A:569:LEU:HD13 | 1:A:577:TYR:OH   | 0.50     | 2.07        | 5      | 1     |
| 1:A:549:ILE:HG13 | 1:A:567:VAL:HG21 | 0.50     | 1.83        | 3      | 1     |
| 1:A:569:LEU:HD21 | 1:A:577:TYR:OH   | 0.50     | 2.07        | 1      | 2     |
| 1:A:580:ILE:CG1  | 1:A:582:ILE:HD11 | 0.50     | 2.37        | 3      | 5     |
| 1:A:551:LEU:O    | 1:A:563:TRP:HZ3  | 0.50     | 1.89        | 3      | 1     |
| 1:A:590:TRP:O    | 1:A:591:GLU:O    | 0.50     | 2.30        | 3      | 1     |
| 1:A:531:ILE:O    | 1:A:551:LEU:HB2  | 0.50     | 2.06        | 3      | 4     |
| 1:A:572:GLY:HA2  | 1:A:600:VAL:O    | 0.49     | 2.07        | 5      | 4     |
| 1:A:536:SER:HA   | 1:A:543:TRP:NE1  | 0.49     | 2.21        | 1      | 5     |
| 1:A:540:LEU:HD13 | 1:A:577:TYR:OH   | 0.49     | 2.06        | 1      | 1     |
| 1:A:556:TYR:CD1  | 1:A:561:PRO:HB3  | 0.49     | 2.42        | 2      | 3     |
| 1:A:570:PRO:O    | 1:A:600:VAL:HG11 | 0.49     | 2.07        | 4      | 1     |
| 1:A:578:LYS:CB   | 1:A:591:GLU:HB3  | 0.49     | 2.37        | 1      | 4     |
| 1:A:520:ASP:OD1  | 1:A:612:THR:CG2  | 0.49     | 2.58        | 1      | 1     |
| 1:A:532:TYR:CZ   | 1:A:550:ALA:CB   | 0.49     | 2.89        | 1      | 4     |
| 1:A:517:VAL:CG1  | 1:A:611:VAL:HG23 | 0.49     | 2.37        | 4      | 2     |
| 1:A:524:THR:HG23 | 1:A:524:THR:O    | 0.49     | 2.07        | 1      | 3     |
| 1:A:551:LEU:HG   | 1:A:565:VAL:CG2  | 0.49     | 2.37        | 3      | 5     |
| 1:A:588:VAL:HG23 | 1:A:589:GLU:N    | 0.49     | 2.23        | 2      | 4     |
| 1:A:517:VAL:HG11 | 1:A:611:VAL:HG23 | 0.49     | 1.85        | 5      | 1     |
| 1:A:525:THR:O    | 1:A:556:TYR:OH   | 0.49     | 2.30        | 3      | 4     |
| 1:A:537:ILE:O    | 1:A:538:SER:C    | 0.49     | 2.53        | 4      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:590:TRP:O    | 1:A:591:GLU:C    | 0.49     | 2.55        | 2      | 4     |
| 1:A:578:LYS:CG   | 1:A:595:ASN:HA   | 0.49     | 2.37        | 5      | 1     |
| 1:A:574:SER:O    | 1:A:575:PHE:O    | 0.49     | 2.31        | 2      | 5     |
| 1:A:538:SER:O    | 1:A:539:GLN:C    | 0.49     | 2.56        | 4      | 3     |
| 1:A:591:GLU:C    | 1:A:592:SER:O    | 0.49     | 2.55        | 2      | 5     |
| 1:A:572:GLY:N    | 1:A:600:VAL:O    | 0.49     | 2.45        | 4      | 1     |
| 1:A:523:ALA:HB1  | 1:A:615:TRP:CD1  | 0.49     | 2.43        | 1      | 4     |
| 1:A:578:LYS:HE2  | 1:A:590:TRP:CZ3  | 0.49     | 2.43        | 1      | 1     |
| 1:A:591:GLU:O    | 1:A:592:SER:O    | 0.49     | 2.31        | 1      | 5     |
| 1:A:595:ASN:OD1  | 1:A:595:ASN:N    | 0.49     | 2.46        | 5      | 5     |
| 1:A:525:THR:HG1  | 1:A:615:TRP:CD1  | 0.49     | 2.25        | 3      | 1     |
| 1:A:578:LYS:HG3  | 1:A:591:GLU:CB   | 0.49     | 2.38        | 5      | 1     |
| 1:A:613:ASP:OD1  | 1:A:613:ASP:N    | 0.48     | 2.46        | 1      | 1     |
| 1:A:534:VAL:CG1  | 1:A:578:LYS:HE2  | 0.48     | 2.35        | 1      | 1     |
| 1:A:560:ASP:O    | 1:A:562:LEU:HD13 | 0.48     | 2.08        | 1      | 2     |
| 1:A:581:ARG:CD   | 1:A:589:GLU:CD   | 0.48     | 2.87        | 5      | 1     |
| 1:A:537:ILE:CD1  | 1:A:569:LEU:CD2  | 0.48     | 2.81        | 2      | 1     |
| 1:A:569:LEU:CD2  | 1:A:577:TYR:CZ   | 0.48     | 2.97        | 4      | 1     |
| 1:A:570:PRO:HG2  | 1:A:575:PHE:CE1  | 0.48     | 2.44        | 4      | 1     |
| 1:A:545:THR:OG1  | 1:A:580:ILE:HD12 | 0.48     | 2.09        | 2      | 1     |
| 1:A:578:LYS:HE2  | 1:A:579:PHE:O    | 0.48     | 2.09        | 4      | 1     |
| 1:A:575:PHE:HB2  | 1:A:577:TYR:CZ   | 0.48     | 2.43        | 5      | 1     |
| 1:A:532:TYR:CB   | 1:A:580:ILE:CD1  | 0.48     | 2.92        | 3      | 1     |
| 1:A:575:PHE:CG   | 1:A:577:TYR:OH   | 0.48     | 2.67        | 5      | 1     |
| 1:A:536:SER:O    | 1:A:536:SER:OG   | 0.48     | 2.32        | 4      | 2     |
| 1:A:540:LEU:CD1  | 1:A:577:TYR:CZ   | 0.48     | 2.93        | 1      | 1     |
| 1:A:545:THR:HB   | 1:A:590:TRP:CE2  | 0.48     | 2.44        | 2      | 2     |
| 1:A:572:GLY:O    | 1:A:573:GLU:CD   | 0.48     | 2.57        | 2      | 2     |
| 1:A:521:LEU:HD23 | 1:A:563:TRP:CD1  | 0.48     | 2.44        | 1      | 1     |
| 1:A:554:ASP:CG   | 1:A:564:TYR:OH   | 0.48     | 2.57        | 3      | 1     |
| 1:A:551:LEU:HG   | 1:A:565:VAL:HG23 | 0.47     | 1.84        | 3      | 1     |
| 1:A:593:ASP:O    | 1:A:595:ASN:OD1  | 0.47     | 2.32        | 5      | 5     |
| 1:A:532:TYR:C    | 1:A:580:ILE:HG13 | 0.47     | 2.34        | 3      | 1     |
| 1:A:579:PHE:CD1  | 1:A:579:PHE:C    | 0.47     | 2.92        | 2      | 1     |
| 1:A:534:VAL:HG13 | 1:A:543:TRP:CZ3  | 0.47     | 2.44        | 3      | 2     |
| 1:A:593:ASP:HB2  | 1:A:594:PRO:CD   | 0.47     | 2.40        | 1      | 1     |
| 1:A:563:TRP:O    | 1:A:564:TYR:CD2  | 0.47     | 2.68        | 4      | 2     |
| 1:A:569:LEU:O    | 1:A:600:VAL:CG2  | 0.47     | 2.55        | 2      | 2     |
| 1:A:578:LYS:HB3  | 1:A:591:GLU:HB3  | 0.47     | 1.86        | 2      | 2     |
| 1:A:554:ASP:OD2  | 1:A:564:TYR:OH   | 0.47     | 2.33        | 3      | 1     |
| 1:A:519:PHE:N    | 1:A:565:VAL:O    | 0.47     | 2.48        | 1      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:554:ASP:OD1  | 1:A:555:LYS:N    | 0.47     | 2.48        | 1      | 2     |
| 1:A:555:LYS:O    | 1:A:560:ASP:O    | 0.47     | 2.33        | 3      | 1     |
| 1:A:575:PHE:HB2  | 1:A:577:TYR:OH   | 0.47     | 2.10        | 5      | 1     |
| 1:A:517:VAL:HG22 | 1:A:598:TYR:CE2  | 0.47     | 2.45        | 2      | 1     |
| 1:A:532:TYR:HB2  | 1:A:580:ILE:HD12 | 0.47     | 1.87        | 1      | 3     |
| 1:A:572:GLY:O    | 1:A:573:GLU:HB2  | 0.47     | 2.10        | 3      | 3     |
| 1:A:578:LYS:CG   | 1:A:591:GLU:CB   | 0.47     | 2.93        | 5      | 1     |
| 1:A:521:LEU:CB   | 1:A:563:TRP:CD1  | 0.46     | 2.97        | 5      | 2     |
| 1:A:573:GLU:O    | 1:A:598:TYR:O    | 0.46     | 2.33        | 2      | 3     |
| 1:A:573:GLU:HB2  | 1:A:575:PHE:CE2  | 0.46     | 2.44        | 4      | 1     |
| 1:A:547:ASP:O    | 1:A:548:GLY:O    | 0.46     | 2.33        | 2      | 4     |
| 1:A:587:SER:O    | 1:A:588:VAL:HG12 | 0.46     | 2.11        | 3      | 5     |
| 1:A:524:THR:O    | 1:A:524:THR:HG23 | 0.46     | 2.09        | 4      | 1     |
| 1:A:545:THR:CB   | 1:A:580:ILE:HD13 | 0.46     | 2.40        | 5      | 4     |
| 1:A:578:LYS:HD2  | 1:A:591:GLU:CG   | 0.46     | 2.40        | 1      | 1     |
| 1:A:545:THR:OG1  | 1:A:580:ILE:CD1  | 0.46     | 2.63        | 4      | 2     |
| 1:A:591:GLU:OE2  | 1:A:595:ASN:CG   | 0.46     | 2.58        | 5      | 1     |
| 1:A:574:SER:O    | 1:A:575:PHE:C    | 0.46     | 2.58        | 1      | 2     |
| 1:A:541:GLY:C    | 1:A:542:ASP:CG   | 0.46     | 2.81        | 4      | 4     |
| 1:A:537:ILE:CG1  | 1:A:539:GLN:HB2  | 0.46     | 2.40        | 4      | 1     |
| 1:A:548:GLY:O    | 1:A:549:ILE:HG13 | 0.46     | 2.11        | 1      | 3     |
| 1:A:588:VAL:CG2  | 1:A:590:TRP:NE1  | 0.46     | 2.79        | 2      | 5     |
| 1:A:541:GLY:O    | 1:A:542:ASP:OD2  | 0.46     | 2.33        | 2      | 4     |
| 1:A:555:LYS:CB   | 1:A:562:LEU:HD21 | 0.46     | 2.41        | 2      | 2     |
| 1:A:557:THR:O    | 1:A:557:THR:HG23 | 0.46     | 2.10        | 3      | 1     |
| 1:A:570:PRO:HG2  | 1:A:575:PHE:CZ   | 0.46     | 2.45        | 4      | 1     |
| 1:A:580:ILE:C    | 1:A:582:ILE:CD1  | 0.46     | 2.89        | 5      | 4     |
| 1:A:533:LEU:N    | 1:A:549:ILE:O    | 0.46     | 2.48        | 3      | 1     |
| 1:A:578:LYS:HB2  | 1:A:591:GLU:HB3  | 0.46     | 1.87        | 4      | 1     |
| 1:A:581:ARG:HD3  | 1:A:589:GLU:OE1  | 0.46     | 2.11        | 2      | 1     |
| 1:A:519:PHE:CZ   | 1:A:567:VAL:HB   | 0.45     | 2.46        | 3      | 4     |
| 1:A:573:GLU:O    | 1:A:599:THR:HA   | 0.45     | 2.11        | 3      | 4     |
| 1:A:581:ARG:CG   | 1:A:589:GLU:HB2  | 0.45     | 2.40        | 1      | 1     |
| 1:A:579:PHE:CE2  | 1:A:615:TRP:CE3  | 0.45     | 3.04        | 5      | 1     |
| 1:A:534:VAL:HG22 | 1:A:535:GLY:N    | 0.45     | 2.25        | 5      | 4     |
| 1:A:521:LEU:HD22 | 1:A:531:ILE:HG21 | 0.45     | 1.87        | 3      | 1     |
| 1:A:536:SER:CB   | 1:A:576:GLU:O    | 0.45     | 2.65        | 4      | 1     |
| 1:A:537:ILE:O    | 1:A:539:GLN:N    | 0.45     | 2.50        | 4      | 1     |
| 1:A:581:ARG:HB3  | 1:A:589:GLU:CB   | 0.45     | 2.42        | 2      | 3     |
| 1:A:520:ASP:CA   | 1:A:564:TYR:HB3  | 0.45     | 2.42        | 3      | 1     |
| 1:A:591:GLU:OE1  | 1:A:592:SER:O    | 0.45     | 2.34        | 3      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:581:ARG:HD2  | 1:A:589:GLU:CD   | 0.45     | 2.36        | 5      | 1     |
| 1:A:556:TYR:CD2  | 1:A:563:TRP:CD1  | 0.45     | 3.05        | 4      | 1     |
| 1:A:571:ALA:HA   | 1:A:600:VAL:CG1  | 0.45     | 2.41        | 4      | 1     |
| 1:A:568:THR:C    | 1:A:569:LEU:HG   | 0.45     | 2.37        | 5      | 1     |
| 1:A:521:LEU:CD1  | 1:A:613:ASP:HB2  | 0.45     | 2.42        | 1      | 1     |
| 1:A:521:LEU:CG   | 1:A:615:TRP:HB2  | 0.45     | 2.42        | 3      | 3     |
| 1:A:535:GLY:HA3  | 1:A:577:TYR:CD1  | 0.45     | 2.47        | 1      | 1     |
| 1:A:575:PHE:O    | 1:A:597:GLU:HB2  | 0.45     | 2.12        | 1      | 2     |
| 1:A:538:SER:O    | 1:A:541:GLY:N    | 0.45     | 2.50        | 3      | 1     |
| 1:A:578:LYS:CG   | 1:A:595:ASN:HB3  | 0.45     | 2.42        | 5      | 1     |
| 1:A:579:PHE:CD2  | 1:A:615:TRP:CE3  | 0.45     | 3.04        | 5      | 1     |
| 1:A:554:ASP:OD1  | 1:A:564:TYR:CE2  | 0.45     | 2.69        | 3      | 1     |
| 1:A:568:THR:O    | 1:A:569:LEU:CG   | 0.45     | 2.65        | 1      | 2     |
| 1:A:521:LEU:HD23 | 1:A:531:ILE:HG12 | 0.45     | 1.88        | 4      | 1     |
| 1:A:520:ASP:HB3  | 1:A:564:TYR:HB3  | 0.44     | 1.89        | 3      | 1     |
| 1:A:534:VAL:C    | 1:A:540:LEU:CD1  | 0.44     | 2.90        | 4      | 1     |
| 1:A:598:TYR:OH   | 1:A:609:ALA:HA   | 0.44     | 2.12        | 4      | 2     |
| 1:A:536:SER:O    | 1:A:537:ILE:HG23 | 0.44     | 2.11        | 5      | 1     |
| 1:A:578:LYS:CD   | 1:A:591:GLU:HB3  | 0.44     | 2.43        | 5      | 1     |
| 1:A:553:ALA:HB1  | 1:A:556:TYR:CD2  | 0.44     | 2.46        | 4      | 1     |
| 1:A:514:ALA:HA   | 1:A:570:PRO:HA   | 0.44     | 1.89        | 3      | 2     |
| 1:A:549:ILE:CD1  | 1:A:567:VAL:HG22 | 0.44     | 2.36        | 2      | 1     |
| 1:A:551:LEU:HA   | 1:A:565:VAL:HG23 | 0.44     | 1.87        | 3      | 1     |
| 1:A:537:ILE:HG12 | 1:A:577:TYR:OH   | 0.44     | 2.12        | 4      | 1     |
| 1:A:536:SER:O    | 1:A:537:ILE:CG2  | 0.44     | 2.65        | 5      | 1     |
| 1:A:557:THR:HG23 | 1:A:558:SER:H    | 0.44     | 1.73        | 1      | 2     |
| 1:A:575:PHE:O    | 1:A:597:GLU:HA   | 0.44     | 2.12        | 1      | 2     |
| 1:A:524:THR:HA   | 1:A:556:TYR:CZ   | 0.44     | 2.47        | 4      | 1     |
| 1:A:578:LYS:HE3  | 1:A:591:GLU:CB   | 0.44     | 2.43        | 4      | 1     |
| 1:A:517:VAL:CB   | 1:A:609:ALA:HB3  | 0.44     | 2.42        | 1      | 1     |
| 1:A:535:GLY:HA2  | 1:A:577:TYR:HB3  | 0.44     | 1.90        | 3      | 2     |
| 1:A:598:TYR:HB2  | 1:A:611:VAL:CG2  | 0.44     | 2.42        | 2      | 1     |
| 1:A:514:ALA:CB   | 1:A:570:PRO:HA   | 0.44     | 2.43        | 3      | 1     |
| 1:A:533:LEU:HD12 | 1:A:578:LYS:C    | 0.44     | 2.35        | 4      | 1     |
| 1:A:544:GLU:HB3  | 1:A:547:ASP:OD2  | 0.44     | 2.13        | 1      | 1     |
| 1:A:522:THR:HA   | 1:A:561:PRO:O    | 0.44     | 2.13        | 2      | 1     |
| 1:A:581:ARG:HB3  | 1:A:589:GLU:HB2  | 0.44     | 1.90        | 2      | 3     |
| 1:A:580:ILE:HG22 | 1:A:590:TRP:NE1  | 0.44     | 2.25        | 3      | 1     |
| 1:A:536:SER:HB3  | 1:A:576:GLU:O    | 0.44     | 2.12        | 4      | 2     |
| 1:A:581:ARG:O    | 1:A:588:VAL:CB   | 0.44     | 2.66        | 4      | 1     |
| 1:A:514:ALA:HA   | 1:A:570:PRO:CA   | 0.43     | 2.42        | 1      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:534:VAL:C    | 1:A:540:LEU:HD23 | 0.43     | 2.38        | 1      | 1     |
| 1:A:533:LEU:CD1  | 1:A:578:LYS:O    | 0.43     | 2.66        | 2      | 1     |
| 1:A:536:SER:HA   | 1:A:543:TRP:CZ2  | 0.43     | 2.48        | 3      | 4     |
| 1:A:578:LYS:CD   | 1:A:595:ASN:HA   | 0.43     | 2.43        | 2      | 1     |
| 1:A:514:ALA:HA   | 1:A:569:LEU:O    | 0.43     | 2.13        | 4      | 1     |
| 1:A:557:THR:OG1  | 1:A:558:SER:N    | 0.43     | 2.49        | 4      | 1     |
| 1:A:575:PHE:O    | 1:A:597:GLU:CB   | 0.43     | 2.66        | 1      | 1     |
| 1:A:517:VAL:CG1  | 1:A:610:THR:C    | 0.43     | 2.91        | 2      | 1     |
| 1:A:514:ALA:HB2  | 1:A:570:PRO:CB   | 0.43     | 2.42        | 3      | 1     |
| 1:A:572:GLY:HA2  | 1:A:600:VAL:HB   | 0.43     | 1.90        | 5      | 1     |
| 1:A:556:TYR:CD1  | 1:A:561:PRO:CA   | 0.43     | 3.01        | 1      | 2     |
| 1:A:583:GLU:C    | 1:A:585:ASP:N    | 0.43     | 2.75        | 2      | 2     |
| 1:A:556:TYR:HB2  | 1:A:562:LEU:O    | 0.43     | 2.13        | 1      | 1     |
| 1:A:562:LEU:O    | 1:A:562:LEU:CD2  | 0.43     | 2.52        | 4      | 3     |
| 1:A:575:PHE:O    | 1:A:597:GLU:CA   | 0.43     | 2.66        | 1      | 1     |
| 1:A:534:VAL:HG21 | 1:A:543:TRP:C    | 0.43     | 2.37        | 3      | 4     |
| 1:A:549:ILE:HG21 | 1:A:567:VAL:CG2  | 0.43     | 2.42        | 3      | 1     |
| 1:A:581:ARG:NE   | 1:A:589:GLU:O    | 0.43     | 2.52        | 3      | 1     |
| 1:A:572:GLY:HA2  | 1:A:600:VAL:CB   | 0.43     | 2.44        | 5      | 1     |
| 1:A:521:LEU:CD2  | 1:A:531:ILE:CG1  | 0.43     | 2.97        | 5      | 2     |
| 1:A:535:GLY:HA2  | 1:A:577:TYR:CB   | 0.43     | 2.43        | 2      | 1     |
| 1:A:539:GLN:HA   | 1:A:539:GLN:NE2  | 0.43     | 2.29        | 2      | 1     |
| 1:A:611:VAL:HG12 | 1:A:613:ASP:OD2  | 0.43     | 2.14        | 3      | 1     |
| 1:A:577:TYR:OH   | 1:A:611:VAL:CG2  | 0.43     | 2.56        | 2      | 1     |
| 1:A:578:LYS:CE   | 1:A:579:PHE:O    | 0.43     | 2.65        | 4      | 1     |
| 1:A:545:THR:HB   | 1:A:580:ILE:HD13 | 0.43     | 1.91        | 1      | 1     |
| 1:A:548:GLY:C    | 1:A:549:ILE:HG13 | 0.43     | 2.39        | 5      | 1     |
| 1:A:573:GLU:O    | 1:A:575:PHE:CD2  | 0.43     | 2.72        | 1      | 2     |
| 1:A:521:LEU:CD1  | 1:A:613:ASP:HB3  | 0.42     | 2.44        | 4      | 1     |
| 1:A:532:TYR:HA   | 1:A:550:ALA:HA   | 0.42     | 1.91        | 2      | 4     |
| 1:A:598:TYR:CE1  | 1:A:610:THR:O    | 0.42     | 2.72        | 2      | 1     |
| 1:A:579:PHE:O    | 1:A:590:TRP:HB3  | 0.42     | 2.14        | 3      | 1     |
| 1:A:523:ALA:O    | 1:A:556:TYR:CE2  | 0.42     | 2.72        | 4      | 1     |
| 1:A:560:ASP:OD1  | 1:A:562:LEU:HD12 | 0.42     | 2.14        | 4      | 1     |
| 1:A:572:GLY:CA   | 1:A:600:VAL:O    | 0.42     | 2.67        | 4      | 1     |
| 1:A:536:SER:C    | 1:A:537:ILE:HG23 | 0.42     | 2.40        | 5      | 1     |
| 1:A:561:PRO:O    | 1:A:562:LEU:HD23 | 0.42     | 2.14        | 5      | 1     |
| 1:A:543:TRP:CZ3  | 1:A:578:LYS:CE   | 0.42     | 3.02        | 1      | 1     |
| 1:A:568:THR:O    | 1:A:569:LEU:HG   | 0.42     | 2.13        | 1      | 2     |
| 1:A:598:TYR:OH   | 1:A:609:ALA:HB1  | 0.42     | 2.11        | 3      | 1     |
| 1:A:556:TYR:HA   | 1:A:561:PRO:HA   | 0.42     | 1.91        | 3      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:556:TYR:CD2  | 1:A:563:TRP:NE1  | 0.42     | 2.87        | 3      | 1     |
| 1:A:519:PHE:O    | 1:A:564:TYR:HB3  | 0.42     | 2.13        | 4      | 1     |
| 1:A:589:GLU:C    | 1:A:590:TRP:CD1  | 0.42     | 2.97        | 5      | 4     |
| 1:A:538:SER:O    | 1:A:540:LEU:N    | 0.42     | 2.53        | 3      | 1     |
| 1:A:559:SER:O    | 1:A:561:PRO:HD3  | 0.42     | 2.15        | 5      | 1     |
| 1:A:517:VAL:HG21 | 1:A:598:TYR:CD2  | 0.42     | 2.50        | 2      | 1     |
| 1:A:569:LEU:O    | 1:A:600:VAL:HG11 | 0.42     | 2.15        | 2      | 1     |
| 1:A:523:ALA:CB   | 1:A:615:TRP:CD1  | 0.42     | 3.03        | 1      | 1     |
| 1:A:532:TYR:CD2  | 1:A:550:ALA:N    | 0.42     | 2.88        | 2      | 3     |
| 1:A:576:GLU:HG2  | 1:A:596:ARG:O    | 0.42     | 2.15        | 3      | 1     |
| 1:A:537:ILE:HD11 | 1:A:577:TYR:OH   | 0.42     | 2.14        | 4      | 1     |
| 1:A:598:TYR:OH   | 1:A:609:ALA:CA   | 0.42     | 2.68        | 5      | 1     |
| 1:A:611:VAL:HG12 | 1:A:613:ASP:OD1  | 0.42     | 2.15        | 2      | 1     |
| 1:A:540:LEU:N    | 1:A:540:LEU:CD1  | 0.41     | 2.82        | 1      | 1     |
| 1:A:517:VAL:CG2  | 1:A:598:TYR:CD2  | 0.41     | 3.02        | 2      | 1     |
| 1:A:556:TYR:CD1  | 1:A:557:THR:N    | 0.41     | 2.88        | 4      | 1     |
| 1:A:611:VAL:O    | 1:A:611:VAL:HG12 | 0.41     | 2.13        | 1      | 1     |
| 1:A:574:SER:HA   | 1:A:598:TYR:O    | 0.41     | 2.14        | 3      | 1     |
| 1:A:521:LEU:CD1  | 1:A:613:ASP:C    | 0.41     | 2.92        | 4      | 1     |
| 1:A:578:LYS:HG2  | 1:A:595:ASN:HA   | 0.41     | 1.91        | 5      | 1     |
| 1:A:517:VAL:HG12 | 1:A:610:THR:C    | 0.41     | 2.40        | 2      | 1     |
| 1:A:572:GLY:HA2  | 1:A:600:VAL:CG1  | 0.41     | 2.46        | 3      | 1     |
| 1:A:557:THR:C    | 1:A:558:SER:OG   | 0.41     | 2.61        | 3      | 1     |
| 1:A:514:ALA:HA   | 1:A:570:PRO:HB3  | 0.41     | 1.92        | 5      | 1     |
| 1:A:537:ILE:HG13 | 1:A:539:GLN:HB2  | 0.41     | 1.91        | 1      | 2     |
| 1:A:578:LYS:HD3  | 1:A:591:GLU:OE2  | 0.41     | 2.15        | 1      | 1     |
| 1:A:519:PHE:CD1  | 1:A:611:VAL:HB   | 0.41     | 2.50        | 5      | 1     |
| 1:A:515:VAL:CG1  | 1:A:608:THR:C    | 0.41     | 2.94        | 3      | 1     |
| 1:A:533:LEU:CD1  | 1:A:534:VAL:O    | 0.41     | 2.68        | 3      | 1     |
| 1:A:569:LEU:HD22 | 1:A:577:TYR:OH   | 0.41     | 2.14        | 4      | 1     |
| 1:A:581:ARG:CB   | 1:A:615:TRP:CH2  | 0.41     | 3.04        | 4      | 1     |
| 1:A:534:VAL:CG2  | 1:A:543:TRP:HA   | 0.41     | 2.46        | 5      | 1     |
| 1:A:537:ILE:C    | 1:A:539:GLN:N    | 0.41     | 2.79        | 4      | 1     |
| 1:A:534:VAL:C    | 1:A:540:LEU:HB3  | 0.41     | 2.40        | 5      | 1     |
| 1:A:562:LEU:HD22 | 1:A:562:LEU:C    | 0.41     | 2.38        | 1      | 1     |
| 1:A:578:LYS:HD2  | 1:A:591:GLU:HB3  | 0.41     | 1.93        | 5      | 2     |
| 1:A:581:ARG:CG   | 1:A:615:TRP:CH2  | 0.41     | 3.04        | 1      | 1     |
| 1:A:538:SER:HA   | 1:A:542:ASP:OD1  | 0.41     | 2.16        | 2      | 1     |
| 1:A:538:SER:OG   | 1:A:542:ASP:OD1  | 0.41     | 2.33        | 2      | 1     |
| 1:A:538:SER:C    | 1:A:540:LEU:N    | 0.41     | 2.74        | 3      | 1     |
| 1:A:564:TYR:C    | 1:A:565:VAL:CG2  | 0.41     | 2.94        | 4      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:520:ASP:HA   | 1:A:564:TYR:HB3  | 0.41     | 1.92        | 3      | 1     |
| 1:A:545:THR:HG21 | 1:A:588:VAL:CG2  | 0.41     | 2.46        | 3      | 1     |
| 1:A:517:VAL:HA   | 1:A:609:ALA:CB   | 0.40     | 2.42        | 2      | 1     |
| 1:A:521:LEU:N    | 1:A:563:TRP:H    | 0.40     | 2.15        | 2      | 1     |
| 1:A:577:TYR:CZ   | 1:A:611:VAL:HG21 | 0.40     | 2.47        | 3      | 1     |
| 1:A:533:LEU:HB3  | 1:A:551:LEU:HD11 | 0.40     | 1.93        | 5      | 1     |
| 1:A:610:THR:HG22 | 1:A:611:VAL:N    | 0.40     | 2.31        | 2      | 1     |
| 1:A:514:ALA:CA   | 1:A:570:PRO:HA   | 0.40     | 2.46        | 3      | 1     |
| 1:A:535:GLY:HA3  | 1:A:577:TYR:HB3  | 0.40     | 1.93        | 3      | 1     |
| 1:A:545:THR:OG1  | 1:A:588:VAL:HG21 | 0.40     | 2.16        | 3      | 1     |
| 1:A:573:GLU:O    | 1:A:575:PHE:CD1  | 0.40     | 2.74        | 5      | 1     |
| 1:A:575:PHE:CE1  | 1:A:600:VAL:CG2  | 0.40     | 3.04        | 5      | 1     |
| 1:A:554:ASP:OD1  | 1:A:564:TYR:OH   | 0.40     | 2.39        | 3      | 1     |
| 1:A:588:VAL:O    | 1:A:589:GLU:HG2  | 0.40     | 2.17        | 3      | 1     |
| 1:A:517:VAL:O    | 1:A:566:THR:HA   | 0.40     | 2.16        | 4      | 1     |
| 1:A:541:GLY:C    | 1:A:542:ASP:OD2  | 0.40     | 2.65        | 2      | 1     |
| 1:A:588:VAL:HG23 | 1:A:589:GLU:O    | 0.40     | 2.17        | 2      | 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     | 96/108 (89%)  | 67±3 (69±3%) | 21±3 (22±4%) | 9±1 (9±1%) | <b>1</b>    | <b>11</b> |
| All | All   | 480/540 (89%) | 333 (69%)    | 104 (22%)    | 43 (9%)    | <b>1</b>    | <b>11</b> |

All 15 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 543 | TRP  | 5              |
| 1   | A     | 548 | GLY  | 5              |
| 1   | A     | 575 | PHE  | 5              |
| 1   | A     | 592 | SER  | 5              |
| 1   | A     | 572 | GLY  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 591 | GLU  | 3              |
| 1   | A     | 611 | VAL  | 3              |
| 1   | A     | 601 | PRO  | 3              |
| 1   | A     | 595 | ASN  | 2              |
| 1   | A     | 559 | SER  | 2              |
| 1   | A     | 573 | GLU  | 2              |
| 1   | A     | 564 | TYR  | 2              |
| 1   | A     | 538 | SER  | 1              |
| 1   | A     | 525 | THR  | 1              |
| 1   | A     | 557 | THR  | 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     | 85/94 (90%)   | 57±3 (67±4%) | 28±3 (33±4%) | 1           | 13 |
| All | All   | 425/470 (90%) | 286 (67%)    | 139 (33%)    | 1           | 13 |

All 47 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   | A     | 518 | THR  | 5              |
| 1   | A     | 520 | ASP  | 5              |
| 1   | A     | 521 | LEU  | 5              |
| 1   | A     | 522 | THR  | 5              |
| 1   | A     | 545 | THR  | 5              |
| 1   | A     | 546 | SER  | 5              |
| 1   | A     | 562 | LEU  | 5              |
| 1   | A     | 568 | THR  | 5              |
| 1   | A     | 580 | ILE  | 5              |
| 1   | A     | 588 | VAL  | 5              |
| 1   | A     | 595 | ASN  | 5              |
| 1   | A     | 599 | THR  | 5              |
| 1   | A     | 612 | THR  | 5              |
| 1   | A     | 554 | ASP  | 4              |
| 1   | A     | 555 | LYS  | 4              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 573 | GLU  | 4              |
| 1   | A     | 578 | LYS  | 4              |
| 1   | A     | 582 | ILE  | 4              |
| 1   | A     | 529 | GLU  | 3              |
| 1   | A     | 556 | TYR  | 3              |
| 1   | A     | 557 | THR  | 3              |
| 1   | A     | 564 | TYR  | 3              |
| 1   | A     | 566 | THR  | 3              |
| 1   | A     | 596 | ARG  | 3              |
| 1   | A     | 608 | THR  | 3              |
| 1   | A     | 576 | GLU  | 2              |
| 1   | A     | 613 | ASP  | 2              |
| 1   | A     | 517 | VAL  | 2              |
| 1   | A     | 540 | LEU  | 2              |
| 1   | A     | 559 | SER  | 2              |
| 1   | A     | 577 | TYR  | 2              |
| 1   | A     | 583 | GLU  | 2              |
| 1   | A     | 611 | VAL  | 2              |
| 1   | A     | 558 | SER  | 2              |
| 1   | A     | 591 | GLU  | 2              |
| 1   | A     | 538 | SER  | 2              |
| 1   | A     | 560 | ASP  | 1              |
| 1   | A     | 533 | LEU  | 1              |
| 1   | A     | 584 | SER  | 1              |
| 1   | A     | 585 | ASP  | 1              |
| 1   | A     | 590 | TRP  | 1              |
| 1   | A     | 597 | GLU  | 1              |
| 1   | A     | 537 | ILE  | 1              |
| 1   | A     | 539 | GLN  | 1              |
| 1   | A     | 581 | ARG  | 1              |
| 1   | A     | 593 | ASP  | 1              |
| 1   | A     | 616 | ARG  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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