



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 16, 2018 – 07:38 am GMT

PDB ID : 2E30  
Title : Solution structure of the cytoplasmic region of Na<sup>+</sup>/H<sup>+</sup> exchanger 1 complexed with essential cofactor calcineurin B homologous protein 1  
Authors : Mishima, M.; Wakabayashi, S.; Kojima, C.  
Deposited on : 2006-11-19

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

<https://www.wwpdb.org/validation/2017/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  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk30686  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

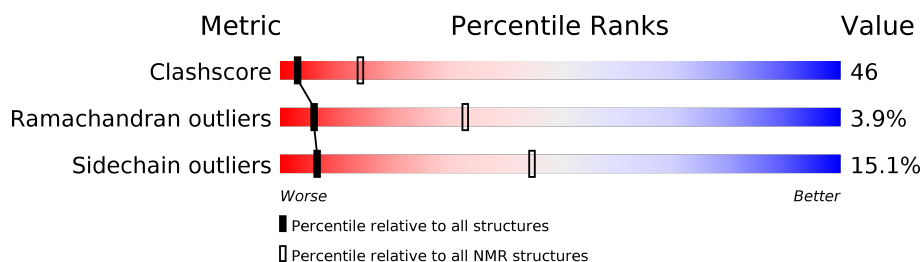
# 1 Overall quality at a glance

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            | 136279                      | 12091                     |
| Ramachandran outliers | 132675                      | 10835                     |
| Sidechain outliers    | 132484                      | 10811                     |

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     | 195    |                  |
| 2   | B     | 43     |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 12 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:11-A:22, A:26-A:39,<br>A:44-A:71, A:75-A:92,<br>A:108-A:191, B:517-B:538<br>(178) | 0.31              | 12           |

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

### 3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3843 atoms, of which 1908 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calcium-binding protein p22.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1   | A     | 195      | Total | C   | H    | N   | O   | S | 0     |
|     |       |          | 3135  | 983 | 1555 | 279 | 313 | 5 |       |

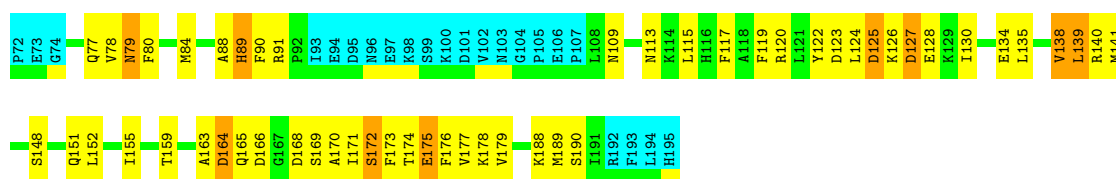
- Molecule 2 is a protein called Sodium/hydrogen exchanger 1.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 2   | B     | 43       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 706   | 221 | 353 | 65 | 66 | 1 |       |

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

| Mol | Chain | Residues | Atoms |    |
|-----|-------|----------|-------|----|
| 3   | A     | 2        | Total | Ca |
|     |       |          | 2     | 2  |



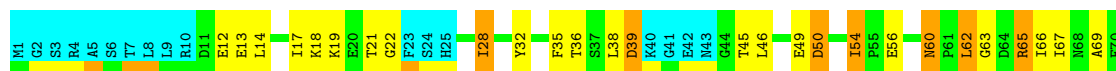


- Molecule 2: Sodium/hydrogen exchanger 1



## 4.2.2 Score per residue for model 2

- Molecule 1: Calcium-binding protein p22

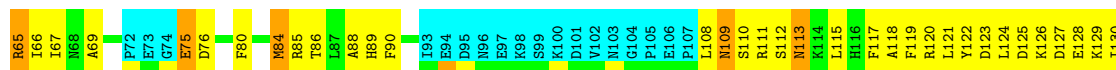


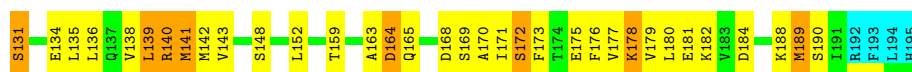
- Molecule 2: Sodium/hydrogen exchanger 1



## 4.2.3 Score per residue for model 3

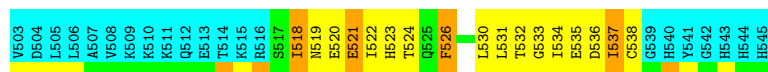
- Molecule 1: Calcium-binding protein p22





### • Molecule 2: Sodium/hydrogen exchanger 1

Chain B: 12% 30% 9% 49%



## 4.2.4 Score per residue for model 4

### • Molecule 1: Calcium-binding protein p22

Chain A: 33% 38% 8% 20%



### • Molecule 2: Sodium/hydrogen exchanger 1

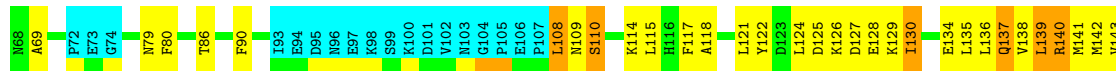
Chain B: 7% 35% 9% 49%



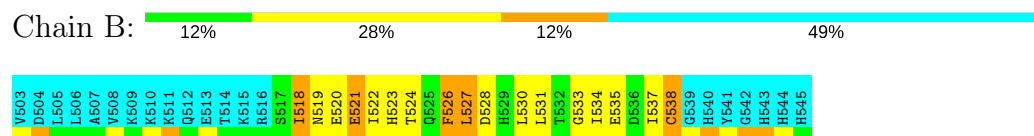
## 4.2.5 Score per residue for model 5

### • Molecule 1: Calcium-binding protein p22

Chain A: 36% 35% 9% 20%

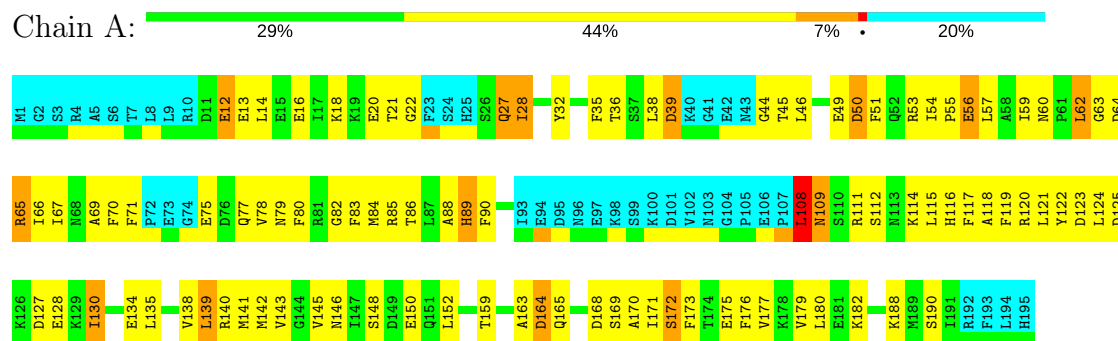


### • Molecule 2: Sodium/hydrogen exchanger 1

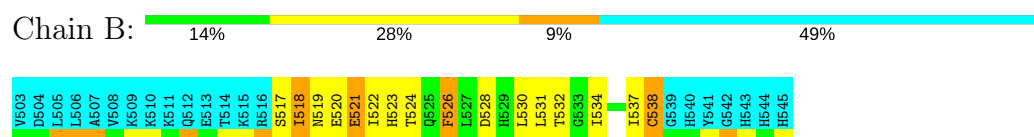


#### 4.2.6 Score per residue for model 6

- Molecule 1: Calcium-binding protein p22



- Molecule 2: Sodium/hydrogen exchanger 1

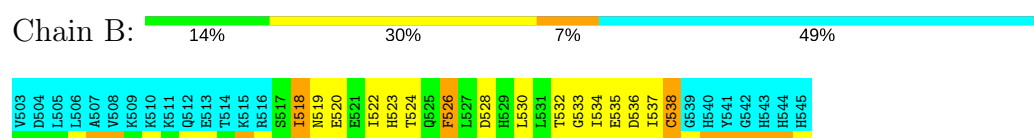


#### 4.2.7 Score per residue for model 7

- Molecule 1: Calcium-binding protein p22

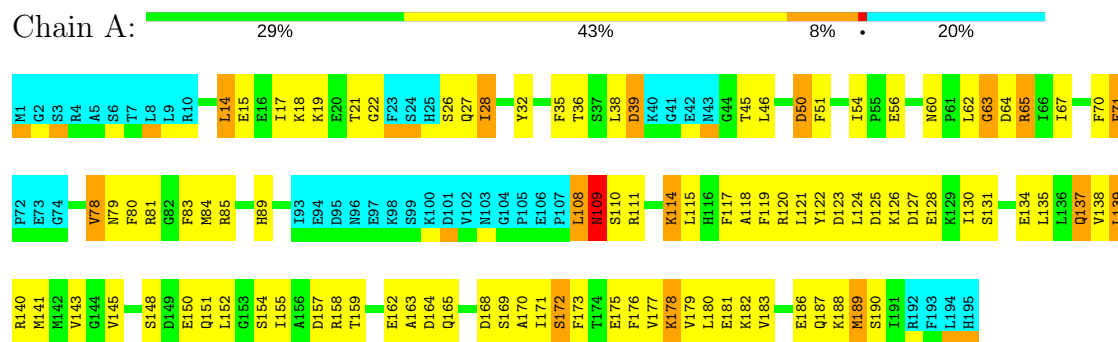


- Molecule 2: Sodium/hydrogen exchanger 1

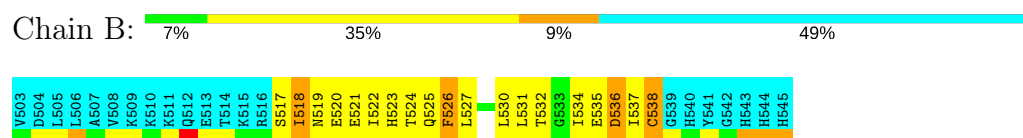


### 4.2.8 Score per residue for model 8

- Molecule 1: Calcium-binding protein p22

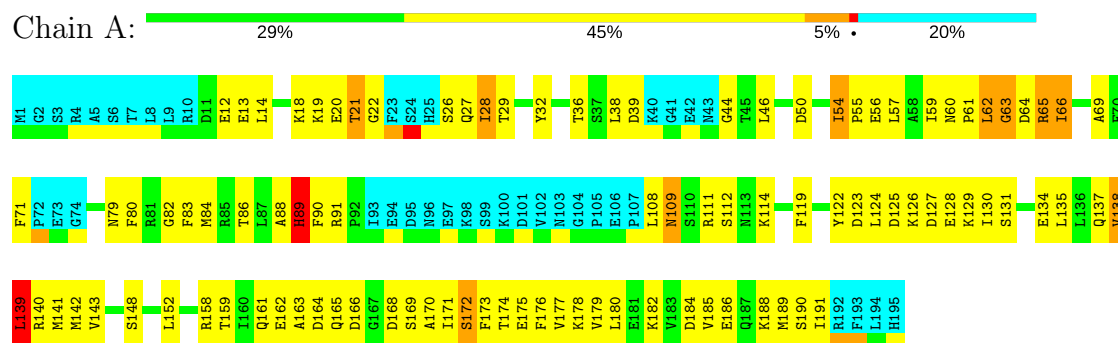


- Molecule 2: Sodium/hydrogen exchanger 1

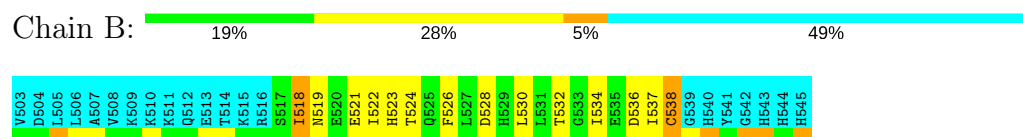


### 4.2.9 Score per residue for model 9

- Molecule 1: Calcium-binding protein p22

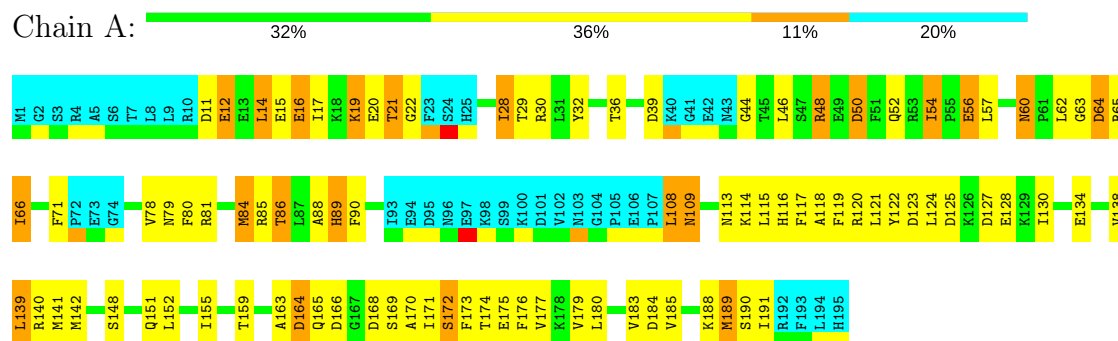


- Molecule 2: Sodium/hydrogen exchanger 1

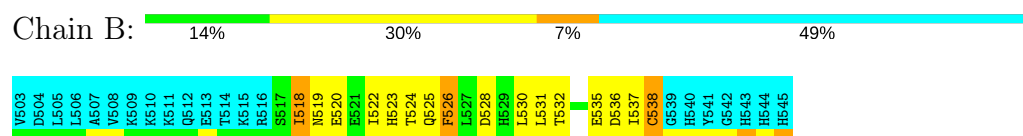


### 4.2.10 Score per residue for model 10

- Molecule 1: Calcium-binding protein p22

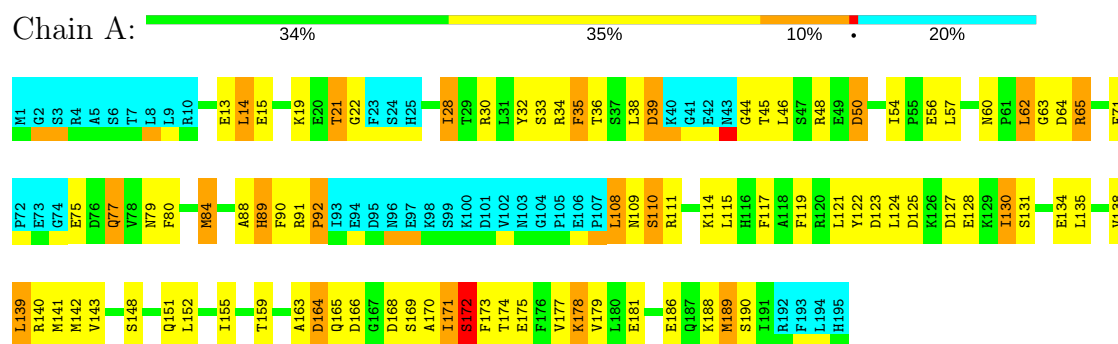


- Molecule 2: Sodium/hydrogen exchanger 1

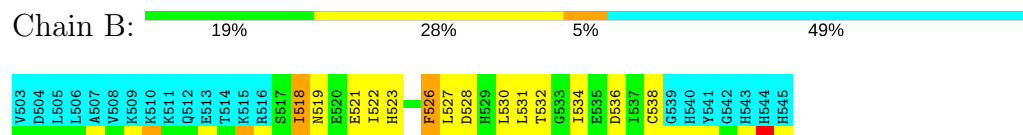


#### 4.2.11 Score per residue for model 11

- Molecule 1: Calcium-binding protein p22

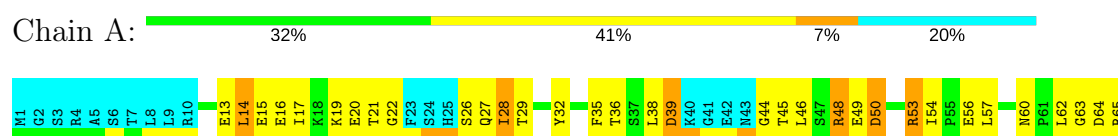


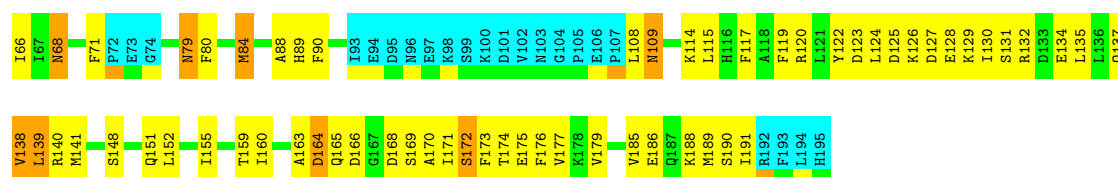
- Molecule 2: Sodium/hydrogen exchanger 1



#### 4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Calcium-binding protein p22



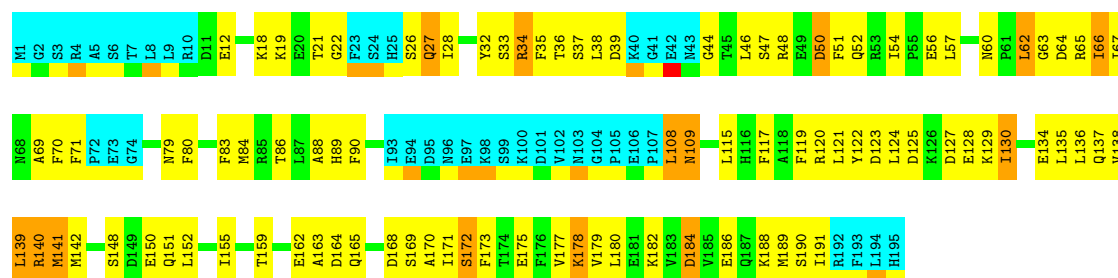


- Molecule 2: Sodium/hydrogen exchanger 1



#### 4.2.13 Score per residue for model 13

- Molecule 1: Calcium-binding protein p22

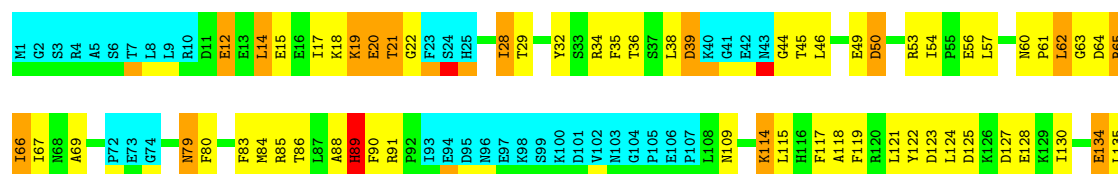


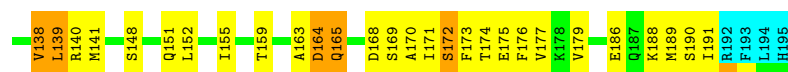
- Molecule 2: Sodium/hydrogen exchanger 1



#### 4.2.14 Score per residue for model 14

- Molecule 1: Calcium-binding protein p22



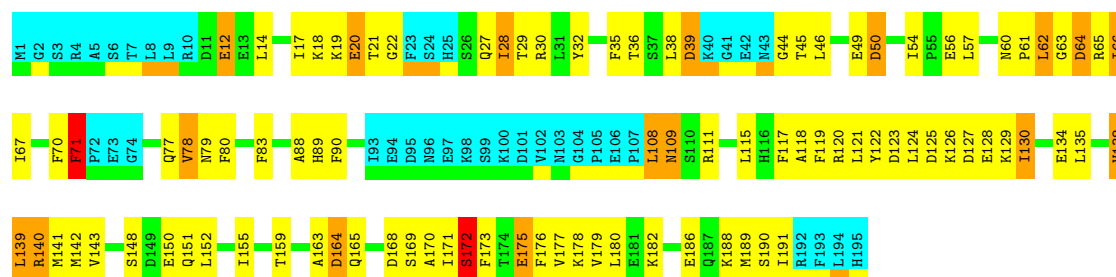


• Molecule 2: Sodium/hydrogen exchanger 1



#### 4.2.15 Score per residue for model 15

• Molecule 1: Calcium-binding protein p22

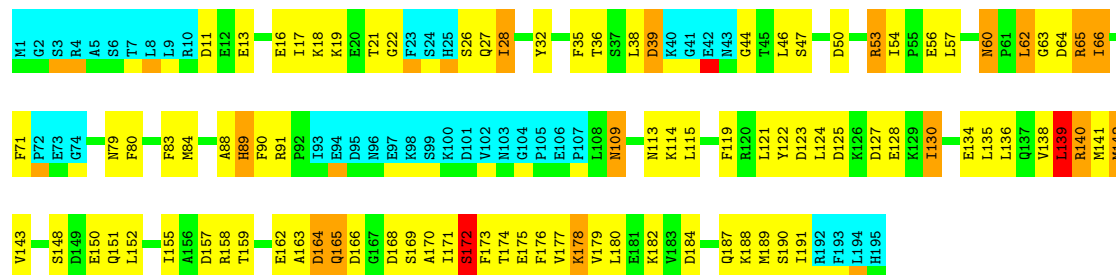


• Molecule 2: Sodium/hydrogen exchanger 1

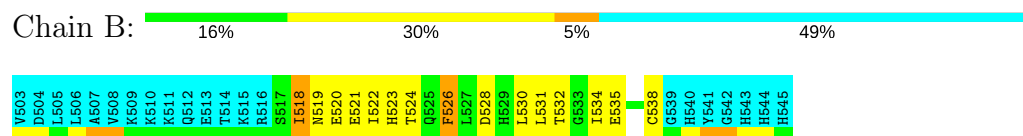


#### 4.2.16 Score per residue for model 16

• Molecule 1: Calcium-binding protein p22

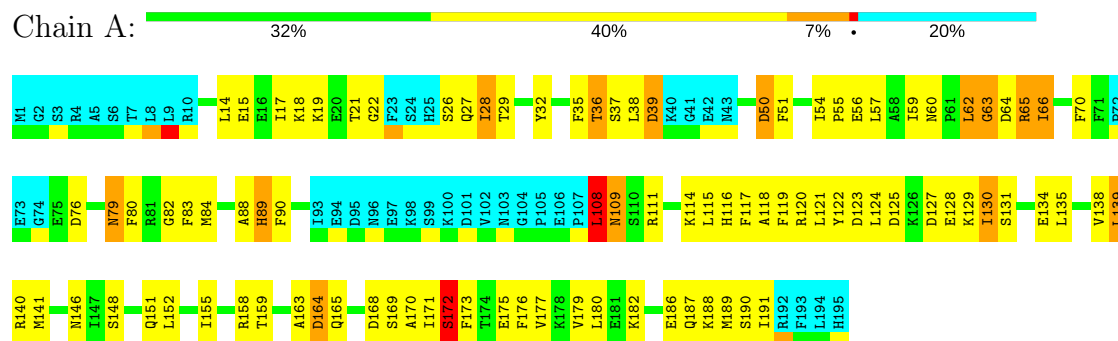


• Molecule 2: Sodium/hydrogen exchanger 1

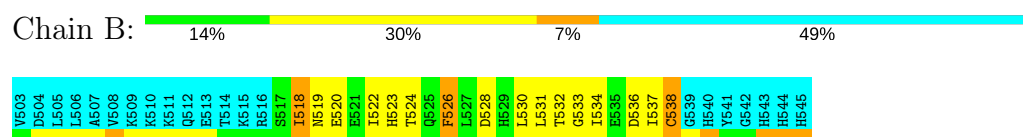


#### 4.2.17 Score per residue for model 17

- Molecule 1: Calcium-binding protein p22

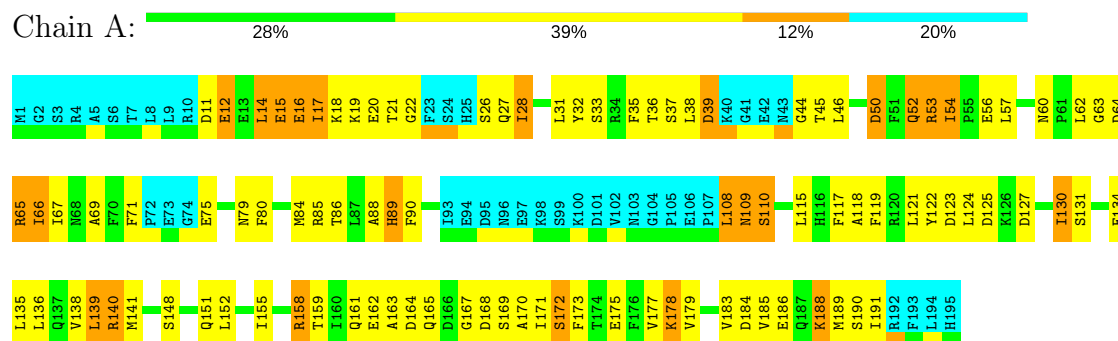


- Molecule 2: Sodium/hydrogen exchanger 1

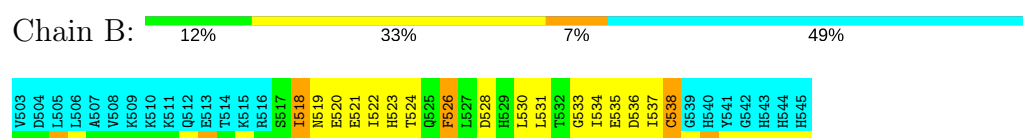


#### 4.2.18 Score per residue for model 18

- Molecule 1: Calcium-binding protein p22

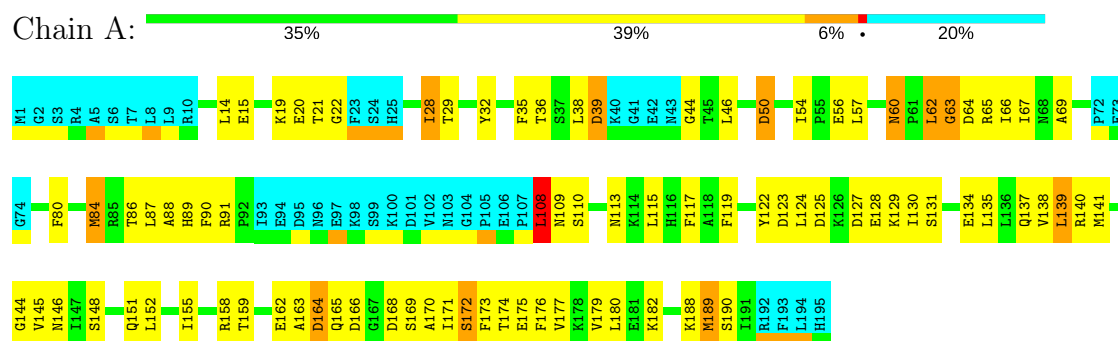


- Molecule 2: Sodium/hydrogen exchanger 1

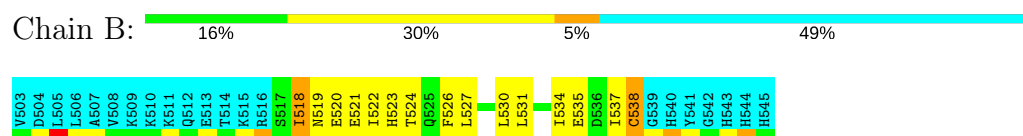


### 4.2.19 Score per residue for model 19

- Molecule 1: Calcium-binding protein p22

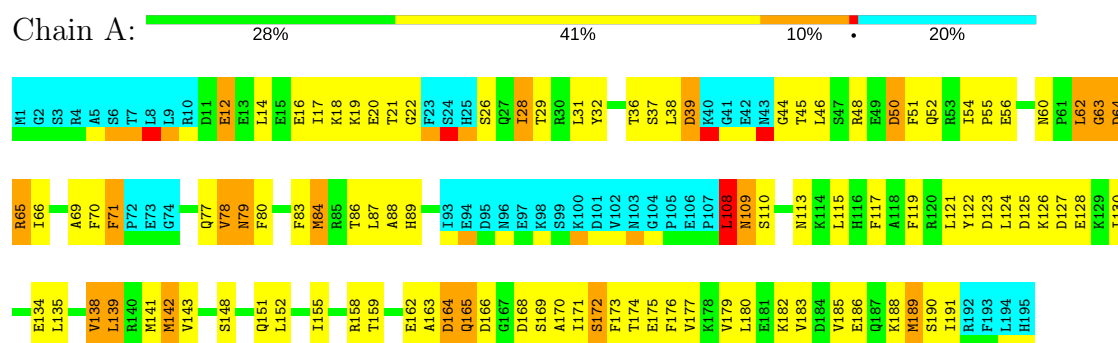


- Molecule 2: Sodium/hydrogen exchanger 1

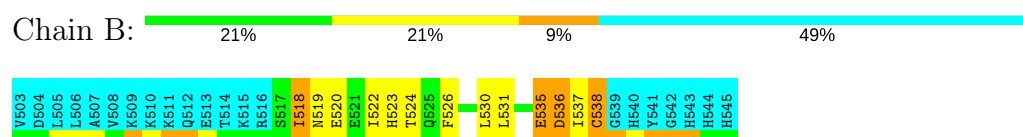


### 4.2.20 Score per residue for model 20

- Molecule 1: Calcium-binding protein p22



- Molecule 2: Sodium/hydrogen exchanger 1



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification | Version |
|---------------|----------------|---------|
| XPLOR-NIH     | refinement     | 2.9.6   |

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:  
CA

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     | 1272  | 1258     | 1256     | 117±9   |
| 2   | B     | 177   | 169      | 167      | 23±5    |
| All | All   | 29020 | 28540    | 28453    | 2624    |

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 46.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:527:LEU:HD13 | 2:B:528:ASP:N    | 0.94     | 1.78        | 5      | 1     |
| 1:A:138:VAL:HG11 | 2:B:526:PHE:CZ   | 0.93     | 1.98        | 8      | 14    |
| 1:A:163:ALA:O    | 1:A:175:GLU:OE1  | 0.88     | 1.92        | 10     | 13    |
| 2:B:527:LEU:O    | 2:B:527:LEU:HD22 | 0.83     | 1.72        | 5      | 1     |
| 1:A:28:ILE:H     | 1:A:28:ILE:HD13  | 0.83     | 1.34        | 7      | 7     |
| 1:A:32:TYR:O     | 1:A:36:THR:HG22  | 0.83     | 1.74        | 13     | 20    |
| 1:A:138:VAL:HG12 | 1:A:142:MET:SD   | 0.82     | 2.15        | 16     | 6     |
| 1:A:130:ILE:N    | 1:A:130:ILE:HD13 | 0.81     | 1.90        | 17     | 9     |
| 1:A:165:GLN:N    | 1:A:175:GLU:OE1  | 0.81     | 2.13        | 8      | 13    |
| 1:A:28:ILE:HD13  | 1:A:28:ILE:H     | 0.81     | 1.34        | 10     | 11    |
| 1:A:130:ILE:HD13 | 1:A:130:ILE:N    | 0.79     | 1.91        | 4      | 11    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:175:GLU:O    | 1:A:179:VAL:HG23 | 0.77     | 1.78        | 1      | 20    |
| 1:A:171:ILE:HG22 | 1:A:172:SER:N    | 0.76     | 1.94        | 20     | 19    |
| 2:B:530:LEU:O    | 2:B:534:ILE:HG22 | 0.75     | 1.81        | 7      | 17    |
| 1:A:28:ILE:N     | 1:A:28:ILE:HD13  | 0.74     | 1.96        | 7      | 6     |
| 1:A:139:LEU:C    | 1:A:139:LEU:HD13 | 0.74     | 2.02        | 16     | 12    |
| 1:A:28:ILE:HD13  | 1:A:28:ILE:N     | 0.74     | 1.97        | 10     | 10    |
| 2:B:520:GLU:O    | 2:B:524:THR:HG23 | 0.74     | 1.83        | 16     | 15    |
| 1:A:139:LEU:HD13 | 1:A:140:ARG:N    | 0.73     | 1.97        | 19     | 18    |
| 1:A:117:PHE:CZ   | 1:A:121:LEU:HD11 | 0.73     | 2.18        | 11     | 5     |
| 1:A:46:LEU:HD22  | 1:A:50:ASP:OD2   | 0.72     | 1.83        | 9      | 3     |
| 1:A:35:PHE:CE2   | 1:A:46:LEU:HD12  | 0.72     | 2.19        | 2      | 2     |
| 1:A:139:LEU:HD13 | 1:A:139:LEU:C    | 0.72     | 2.04        | 15     | 8     |
| 1:A:130:ILE:HG12 | 1:A:171:ILE:O    | 0.71     | 1.85        | 14     | 17    |
| 1:A:122:TYR:CE1  | 2:B:526:PHE:CZ   | 0.70     | 2.78        | 10     | 18    |
| 1:A:122:TYR:CE1  | 2:B:526:PHE:CE2  | 0.70     | 2.80        | 7      | 9     |
| 2:B:518:ILE:O    | 2:B:522:ILE:HG22 | 0.69     | 1.86        | 4      | 20    |
| 2:B:527:LEU:C    | 2:B:527:LEU:HD22 | 0.68     | 2.09        | 5      | 1     |
| 2:B:523:HIS:O    | 2:B:527:LEU:HD23 | 0.68     | 1.88        | 12     | 2     |
| 1:A:35:PHE:CD2   | 1:A:83:PHE:CE1   | 0.68     | 2.82        | 13     | 4     |
| 1:A:51:PHE:CG    | 1:A:70:PHE:CE2   | 0.67     | 2.83        | 8      | 1     |
| 1:A:171:ILE:CG2  | 1:A:172:SER:N    | 0.66     | 2.59        | 10     | 19    |
| 1:A:60:ASN:ND2   | 1:A:63:GLY:H     | 0.66     | 1.87        | 6      | 2     |
| 1:A:136:LEU:HD13 | 1:A:136:LEU:C    | 0.66     | 2.11        | 16     | 1     |
| 1:A:51:PHE:CD1   | 1:A:70:PHE:CE2   | 0.66     | 2.84        | 8      | 2     |
| 1:A:188:LYS:NZ   | 2:B:524:THR:HG22 | 0.66     | 2.05        | 6      | 1     |
| 1:A:124:LEU:HD13 | 1:A:124:LEU:C    | 0.65     | 2.12        | 2      | 12    |
| 1:A:124:LEU:C    | 1:A:124:LEU:HD13 | 0.65     | 2.11        | 15     | 8     |
| 2:B:527:LEU:HD12 | 2:B:527:LEU:C    | 0.65     | 2.11        | 1      | 3     |
| 1:A:48:ARG:NH1   | 1:A:57:LEU:HD13  | 0.65     | 2.06        | 12     | 1     |
| 1:A:163:ALA:O    | 1:A:175:GLU:OE2  | 0.65     | 2.15        | 5      | 7     |
| 1:A:35:PHE:CE1   | 1:A:83:PHE:CD1   | 0.65     | 2.85        | 8      | 3     |
| 1:A:176:PHE:CE1  | 2:B:523:HIS:NE2  | 0.65     | 2.64        | 14     | 14    |
| 2:B:519:ASN:ND2  | 2:B:523:HIS:NE2  | 0.65     | 2.45        | 4      | 1     |
| 1:A:35:PHE:CE2   | 1:A:83:PHE:CD1   | 0.65     | 2.84        | 2      | 2     |
| 1:A:117:PHE:CE2  | 1:A:121:LEU:HD11 | 0.64     | 2.26        | 8      | 4     |
| 1:A:66:ILE:HD12  | 1:A:66:ILE:O     | 0.64     | 1.92        | 1      | 2     |
| 1:A:122:TYR:CE1  | 2:B:526:PHE:CE1  | 0.64     | 2.86        | 1      | 6     |
| 1:A:35:PHE:CE1   | 1:A:46:LEU:HD12  | 0.64     | 2.27        | 8      | 3     |
| 1:A:79:ASN:ND2   | 1:A:79:ASN:H     | 0.64     | 1.90        | 17     | 2     |
| 1:A:171:ILE:HG21 | 1:A:175:GLU:HG2  | 0.63     | 1.68        | 4      | 18    |
| 1:A:46:LEU:HD13  | 1:A:50:ASP:OD2   | 0.63     | 1.93        | 9      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:66:ILE:O     | 1:A:66:ILE:HD12  | 0.63     | 1.93        | 17     | 1     |
| 1:A:51:PHE:CE1   | 1:A:70:PHE:CD2   | 0.63     | 2.86        | 20     | 4     |
| 1:A:122:TYR:CD1  | 2:B:526:PHE:CE2  | 0.63     | 2.86        | 7      | 6     |
| 1:A:116:HIS:NE2  | 1:A:120:ARG:NH1  | 0.63     | 2.46        | 6      | 2     |
| 1:A:137:GLN:NE2  | 1:A:140:ARG:NH1  | 0.63     | 2.47        | 8      | 1     |
| 1:A:65:ARG:CD    | 1:A:65:ARG:N     | 0.63     | 2.62        | 20     | 3     |
| 1:A:89:HIS:CD2   | 1:A:117:PHE:CG   | 0.63     | 2.86        | 1      | 6     |
| 1:A:60:ASN:ND2   | 1:A:63:GLY:N     | 0.63     | 2.46        | 2      | 2     |
| 1:A:170:ALA:C    | 1:A:171:ILE:HD12 | 0.63     | 2.14        | 9      | 9     |
| 1:A:130:ILE:N    | 1:A:130:ILE:CD1  | 0.62     | 2.62        | 4      | 8     |
| 1:A:176:PHE:CE1  | 2:B:523:HIS:CE1  | 0.62     | 2.87        | 19     | 12    |
| 1:A:91:ARG:N     | 1:A:109:ASN:ND2  | 0.62     | 2.47        | 4      | 1     |
| 1:A:116:HIS:CD2  | 1:A:120:ARG:NH1  | 0.62     | 2.67        | 6      | 1     |
| 1:A:137:GLN:NE2  | 1:A:140:ARG:NH2  | 0.62     | 2.47        | 5      | 1     |
| 1:A:119:PHE:CE2  | 1:A:120:ARG:NH2  | 0.62     | 2.67        | 4      | 1     |
| 2:B:519:ASN:ND2  | 2:B:523:HIS:CE1  | 0.62     | 2.67        | 4      | 1     |
| 1:A:168:ASP:N    | 1:A:168:ASP:OD1  | 0.62     | 2.32        | 7      | 10    |
| 1:A:27:GLN:NE2   | 1:A:27:GLN:N     | 0.62     | 2.48        | 13     | 1     |
| 1:A:65:ARG:NH1   | 2:B:534:ILE:N    | 0.62     | 2.48        | 12     | 1     |
| 1:A:57:LEU:HD23  | 1:A:57:LEU:C     | 0.62     | 2.15        | 14     | 3     |
| 1:A:65:ARG:HH21  | 2:B:534:ILE:N    | 0.62     | 1.93        | 5      | 2     |
| 1:A:139:LEU:O    | 1:A:143:VAL:HG22 | 0.62     | 1.95        | 16     | 9     |
| 1:A:188:LYS:HZ3  | 2:B:524:THR:HG22 | 0.62     | 1.55        | 6      | 1     |
| 1:A:116:HIS:CE1  | 1:A:120:ARG:NH1  | 0.61     | 2.68        | 7      | 1     |
| 1:A:57:LEU:C     | 1:A:57:LEU:HD23  | 0.61     | 2.15        | 11     | 8     |
| 1:A:51:PHE:CE2   | 1:A:70:PHE:CD2   | 0.61     | 2.88        | 8      | 1     |
| 1:A:20:GLU:CB    | 1:A:28:ILE:HG21  | 0.61     | 2.23        | 10     | 3     |
| 1:A:60:ASN:ND2   | 1:A:65:ARG:NH1   | 0.61     | 2.47        | 5      | 2     |
| 1:A:57:LEU:HD12  | 1:A:66:ILE:HD11  | 0.61     | 1.72        | 16     | 5     |
| 1:A:65:ARG:NH2   | 2:B:534:ILE:N    | 0.61     | 2.48        | 5      | 3     |
| 1:A:51:PHE:CD1   | 1:A:70:PHE:CZ    | 0.61     | 2.89        | 8      | 1     |
| 1:A:138:VAL:HG11 | 2:B:526:PHE:CE2  | 0.61     | 2.31        | 6      | 13    |
| 2:B:530:LEU:C    | 2:B:530:LEU:HD12 | 0.61     | 2.15        | 12     | 13    |
| 1:A:108:LEU:O    | 1:A:109:ASN:ND2  | 0.60     | 2.34        | 2      | 9     |
| 1:A:176:PHE:CZ   | 2:B:523:HIS:CE1  | 0.60     | 2.88        | 15     | 11    |
| 1:A:81:ARG:NH1   | 1:A:85:ARG:NH1   | 0.60     | 2.49        | 4      | 1     |
| 2:B:519:ASN:O    | 2:B:523:HIS:CG   | 0.60     | 2.55        | 15     | 18    |
| 2:B:534:ILE:HG23 | 2:B:535:GLU:OE1  | 0.60     | 1.96        | 15     | 1     |
| 1:A:60:ASN:ND2   | 1:A:62:LEU:H     | 0.60     | 1.94        | 2      | 2     |
| 1:A:31:LEU:C     | 1:A:31:LEU:HD13  | 0.60     | 2.16        | 20     | 1     |
| 1:A:168:ASP:OD1  | 1:A:168:ASP:N    | 0.60     | 2.35        | 1      | 10    |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:51:PHE:CZ    | 1:A:70:PHE:CG    | 0.60     | 2.90        | 8      | 1     |
| 1:A:80:PHE:CE2   | 1:A:84:MET:SD    | 0.60     | 2.95        | 11     | 6     |
| 1:A:53:ARG:N     | 1:A:53:ARG:NE    | 0.60     | 2.50        | 12     | 1     |
| 1:A:164:ASP:OD2  | 1:A:169:SER:N    | 0.60     | 2.35        | 14     | 20    |
| 1:A:115:LEU:HD22 | 1:A:115:LEU:N    | 0.59     | 2.12        | 1      | 8     |
| 1:A:63:GLY:O     | 1:A:65:ARG:N     | 0.59     | 2.35        | 20     | 9     |
| 1:A:63:GLY:O     | 1:A:66:ILE:N     | 0.59     | 2.35        | 10     | 7     |
| 1:A:176:PHE:CZ   | 2:B:523:HIS:NE2  | 0.59     | 2.70        | 7      | 4     |
| 1:A:139:LEU:O    | 1:A:139:LEU:HD22 | 0.59     | 1.98        | 19     | 12    |
| 1:A:80:PHE:CZ    | 1:A:84:MET:SD    | 0.59     | 2.95        | 19     | 7     |
| 1:A:188:LYS:O    | 1:A:190:SER:N    | 0.59     | 2.35        | 8      | 20    |
| 1:A:140:ARG:NH1  | 1:A:141:MET:SD   | 0.59     | 2.75        | 7      | 1     |
| 2:B:528:ASP:O    | 2:B:532:THR:HG22 | 0.59     | 1.98        | 11     | 10    |
| 1:A:54:ILE:HG22  | 1:A:56:GLU:H     | 0.59     | 1.58        | 7      | 17    |
| 1:A:163:ALA:O    | 1:A:165:GLN:N    | 0.58     | 2.36        | 7      | 15    |
| 1:A:60:ASN:ND2   | 1:A:65:ARG:HH22  | 0.58     | 1.96        | 13     | 2     |
| 1:A:66:ILE:C     | 1:A:66:ILE:HD12  | 0.58     | 2.19        | 17     | 5     |
| 1:A:30:ARG:NH2   | 1:A:34:ARG:NH2   | 0.58     | 2.51        | 11     | 1     |
| 1:A:65:ARG:HE    | 1:A:66:ILE:CG2   | 0.58     | 2.11        | 16     | 1     |
| 1:A:32:TYR:O     | 1:A:36:THR:CG2   | 0.58     | 2.52        | 18     | 16    |
| 2:B:527:LEU:HD13 | 2:B:527:LEU:C    | 0.58     | 2.18        | 5      | 1     |
| 1:A:165:GLN:CB   | 1:A:175:GLU:OE1  | 0.58     | 2.51        | 8      | 12    |
| 1:A:62:LEU:O     | 1:A:64:ASP:N     | 0.58     | 2.36        | 18     | 16    |
| 1:A:51:PHE:CE1   | 1:A:70:PHE:CE2   | 0.58     | 2.91        | 20     | 2     |
| 1:A:125:ASP:N    | 1:A:134:GLU:OE2  | 0.58     | 2.37        | 12     | 8     |
| 1:A:173:PHE:O    | 1:A:177:VAL:HG23 | 0.58     | 1.99        | 1      | 20    |
| 1:A:171:ILE:HG21 | 1:A:175:GLU:CG   | 0.58     | 2.29        | 11     | 17    |
| 1:A:17:ILE:O     | 1:A:21:THR:HG22  | 0.58     | 1.98        | 10     | 2     |
| 2:B:530:LEU:HD12 | 2:B:530:LEU:C    | 0.58     | 2.19        | 6      | 7     |
| 1:A:46:LEU:HD22  | 1:A:50:ASP:CG    | 0.58     | 2.19        | 10     | 4     |
| 1:A:89:HIS:CE1   | 1:A:117:PHE:CB   | 0.58     | 2.87        | 17     | 2     |
| 1:A:28:ILE:H     | 1:A:28:ILE:CD1   | 0.57     | 2.07        | 20     | 5     |
| 1:A:28:ILE:CD1   | 1:A:28:ILE:H     | 0.57     | 2.12        | 19     | 8     |
| 1:A:18:LYS:O     | 1:A:22:GLY:N     | 0.57     | 2.37        | 9      | 7     |
| 1:A:65:ARG:HG2   | 1:A:66:ILE:N     | 0.57     | 2.14        | 14     | 2     |
| 1:A:48:ARG:CD    | 1:A:48:ARG:H     | 0.57     | 2.13        | 10     | 1     |
| 1:A:53:ARG:N     | 1:A:53:ARG:HE    | 0.57     | 1.97        | 12     | 1     |
| 1:A:89:HIS:CE1   | 1:A:113:ASN:HD22 | 0.57     | 2.18        | 19     | 1     |
| 1:A:179:VAL:HG21 | 2:B:519:ASN:CB   | 0.57     | 2.29        | 5      | 1     |
| 1:A:158:ARG:CZ   | 1:A:161:GLN:NE2  | 0.57     | 2.68        | 18     | 1     |
| 1:A:12:GLU:N     | 1:A:12:GLU:OE1   | 0.57     | 2.38        | 15     | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:60:ASN:ND2   | 1:A:65:ARG:HH21  | 0.57     | 1.97        | 9      | 1     |
| 1:A:79:ASN:HD22  | 1:A:79:ASN:N     | 0.56     | 1.96        | 20     | 1     |
| 1:A:89:HIS:ND1   | 1:A:113:ASN:ND2  | 0.56     | 2.52        | 19     | 1     |
| 2:B:519:ASN:O    | 2:B:523:HIS:ND1  | 0.56     | 2.39        | 5      | 4     |
| 1:A:115:LEU:N    | 1:A:115:LEU:HD22 | 0.56     | 2.16        | 12     | 11    |
| 1:A:115:LEU:CD2  | 1:A:115:LEU:N    | 0.56     | 2.68        | 6      | 9     |
| 1:A:70:PHE:O     | 1:A:71:PHE:CD1   | 0.56     | 2.58        | 15     | 2     |
| 1:A:60:ASN:HD22  | 1:A:62:LEU:H     | 0.56     | 1.44        | 2      | 2     |
| 1:A:55:PRO:O     | 1:A:59:ILE:HD12  | 0.56     | 2.00        | 1      | 4     |
| 1:A:35:PHE:CE1   | 1:A:83:PHE:CE1   | 0.56     | 2.94        | 8      | 3     |
| 1:A:27:GLN:NE2   | 1:A:30:ARG:HH21  | 0.56     | 1.99        | 15     | 1     |
| 1:A:35:PHE:CZ    | 1:A:83:PHE:CE1   | 0.56     | 2.93        | 8      | 1     |
| 1:A:53:ARG:NE    | 1:A:53:ARG:N     | 0.56     | 2.54        | 18     | 2     |
| 1:A:122:TYR:CD1  | 1:A:122:TYR:N    | 0.56     | 2.72        | 14     | 6     |
| 1:A:62:LEU:HD22  | 1:A:138:VAL:HG13 | 0.56     | 1.76        | 8      | 2     |
| 1:A:189:MET:CE   | 2:B:527:LEU:HD23 | 0.56     | 2.31        | 5      | 1     |
| 1:A:65:ARG:CG    | 1:A:66:ILE:N     | 0.56     | 2.69        | 14     | 4     |
| 1:A:171:ILE:CG2  | 1:A:175:GLU:HG2  | 0.56     | 2.30        | 4      | 19    |
| 1:A:90:PHE:CD1   | 1:A:90:PHE:N     | 0.56     | 2.74        | 11     | 4     |
| 1:A:139:LEU:HD22 | 1:A:139:LEU:O    | 0.56     | 2.01        | 14     | 6     |
| 1:A:127:ASP:N    | 1:A:127:ASP:OD1  | 0.56     | 2.39        | 1      | 4     |
| 1:A:66:ILE:HD12  | 1:A:66:ILE:C     | 0.56     | 2.21        | 1      | 3     |
| 1:A:79:ASN:N     | 1:A:79:ASN:ND2   | 0.56     | 2.53        | 20     | 2     |
| 1:A:151:GLN:O    | 1:A:155:ILE:HD13 | 0.55     | 2.02        | 17     | 16    |
| 1:A:122:TYR:N    | 1:A:122:TYR:CD1  | 0.55     | 2.73        | 13     | 3     |
| 1:A:175:GLU:OE1  | 1:A:175:GLU:N    | 0.55     | 2.40        | 11     | 4     |
| 1:A:178:LYS:NZ   | 1:A:182:LYS:NZ   | 0.55     | 2.54        | 8      | 1     |
| 1:A:89:HIS:O     | 1:A:109:ASN:ND2  | 0.55     | 2.38        | 1      | 3     |
| 1:A:109:ASN:H    | 1:A:113:ASN:ND2  | 0.55     | 1.99        | 7      | 2     |
| 1:A:62:LEU:C     | 1:A:64:ASP:H     | 0.55     | 2.05        | 9      | 13    |
| 1:A:60:ASN:HD22  | 1:A:62:LEU:N     | 0.55     | 1.99        | 2      | 1     |
| 1:A:65:ARG:HH21  | 2:B:534:ILE:CA   | 0.55     | 2.15        | 5      | 1     |
| 1:A:125:ASP:OD1  | 1:A:125:ASP:N    | 0.55     | 2.39        | 1      | 1     |
| 1:A:71:PHE:CD1   | 1:A:75:GLU:O     | 0.55     | 2.60        | 4      | 3     |
| 1:A:50:ASP:OD1   | 1:A:50:ASP:N     | 0.55     | 2.40        | 14     | 6     |
| 1:A:60:ASN:OD1   | 1:A:65:ARG:NH2   | 0.55     | 2.39        | 19     | 1     |
| 1:A:12:GLU:OE1   | 1:A:12:GLU:N     | 0.55     | 2.40        | 10     | 4     |
| 1:A:125:ASP:OD1  | 1:A:127:ASP:N    | 0.54     | 2.40        | 2      | 13    |
| 1:A:122:TYR:HB2  | 1:A:130:ILE:HD12 | 0.54     | 1.77        | 2      | 11    |
| 1:A:116:HIS:CE1  | 1:A:120:ARG:HE   | 0.54     | 2.20        | 17     | 1     |
| 1:A:51:PHE:CZ    | 1:A:70:PHE:CD2   | 0.54     | 2.94        | 20     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:186:GLU:N    | 1:A:186:GLU:OE1  | 0.54     | 2.40        | 20     | 4     |
| 1:A:65:ARG:CD    | 1:A:66:ILE:H     | 0.54     | 2.15        | 14     | 1     |
| 2:B:519:ASN:OD1  | 2:B:523:HIS:NE2  | 0.54     | 2.40        | 12     | 1     |
| 1:A:28:ILE:O     | 1:A:31:LEU:N     | 0.54     | 2.41        | 7      | 1     |
| 2:B:537:ILE:O    | 2:B:538:CYS:SG   | 0.54     | 2.65        | 9      | 4     |
| 1:A:172:SER:O    | 1:A:176:PHE:CD2  | 0.54     | 2.60        | 4      | 12    |
| 1:A:60:ASN:OD1   | 1:A:63:GLY:N     | 0.54     | 2.40        | 20     | 10    |
| 1:A:91:ARG:O     | 1:A:109:ASN:ND2  | 0.54     | 2.40        | 1      | 2     |
| 1:A:20:GLU:HB2   | 1:A:28:ILE:HG21  | 0.54     | 1.78        | 20     | 3     |
| 1:A:175:GLU:N    | 1:A:175:GLU:OE1  | 0.54     | 2.39        | 1      | 3     |
| 1:A:68:ASN:O     | 1:A:120:ARG:NH1  | 0.54     | 2.41        | 1      | 1     |
| 1:A:109:ASN:O    | 1:A:109:ASN:ND2  | 0.54     | 2.40        | 9      | 2     |
| 1:A:85:ARG:O     | 1:A:89:HIS:CD2   | 0.54     | 2.60        | 3      | 1     |
| 1:A:84:MET:O     | 1:A:88:ALA:HB3   | 0.54     | 2.02        | 10     | 17    |
| 1:A:168:ASP:C    | 1:A:170:ALA:N    | 0.54     | 2.57        | 11     | 20    |
| 1:A:171:ILE:HG23 | 1:A:175:GLU:OE2  | 0.54     | 2.03        | 3      | 4     |
| 1:A:91:ARG:N     | 1:A:109:ASN:HD22 | 0.54     | 2.01        | 1      | 1     |
| 1:A:127:ASP:OD1  | 1:A:127:ASP:N    | 0.54     | 2.40        | 10     | 5     |
| 2:B:535:GLU:O    | 2:B:537:ILE:N    | 0.54     | 2.40        | 20     | 8     |
| 1:A:109:ASN:ND2  | 1:A:110:SER:N    | 0.54     | 2.55        | 2      | 1     |
| 1:A:90:PHE:N     | 1:A:90:PHE:CD1   | 0.54     | 2.76        | 10     | 2     |
| 2:B:522:ILE:HG23 | 2:B:523:HIS:N    | 0.54     | 2.17        | 2      | 13    |
| 1:A:129:LYS:NZ   | 1:A:168:ASP:OD2  | 0.54     | 2.40        | 17     | 2     |
| 1:A:91:ARG:NH2   | 1:A:108:LEU:O    | 0.54     | 2.41        | 2      | 1     |
| 1:A:119:PHE:CD1  | 1:A:123:ASP:OD1  | 0.54     | 2.60        | 7      | 1     |
| 1:A:127:ASP:O    | 1:A:128:GLU:CB   | 0.54     | 2.56        | 19     | 19    |
| 1:A:191:ILE:HG23 | 1:A:191:ILE:O    | 0.54     | 2.02        | 14     | 2     |
| 1:A:137:GLN:HE22 | 1:A:140:ARG:HH21 | 0.54     | 1.46        | 5      | 1     |
| 1:A:19:LYS:O     | 1:A:22:GLY:N     | 0.54     | 2.36        | 8      | 6     |
| 1:A:109:ASN:O    | 1:A:114:LYS:NZ   | 0.54     | 2.41        | 4      | 1     |
| 1:A:50:ASP:OD1   | 1:A:51:PHE:N     | 0.54     | 2.40        | 13     | 1     |
| 1:A:56:GLU:O     | 1:A:60:ASN:ND2   | 0.54     | 2.41        | 19     | 3     |
| 1:A:56:GLU:OE2   | 1:A:60:ASN:ND2   | 0.53     | 2.42        | 18     | 4     |
| 1:A:91:ARG:N     | 1:A:109:ASN:OD1  | 0.53     | 2.41        | 9      | 2     |
| 1:A:171:ILE:O    | 1:A:172:SER:CB   | 0.53     | 2.55        | 11     | 1     |
| 1:A:60:ASN:OD1   | 1:A:62:LEU:N     | 0.53     | 2.40        | 20     | 3     |
| 1:A:28:ILE:CD1   | 1:A:28:ILE:N     | 0.53     | 2.68        | 9      | 4     |
| 1:A:119:PHE:CZ   | 1:A:123:ASP:OD2  | 0.53     | 2.62        | 1      | 9     |
| 1:A:85:ARG:O     | 1:A:89:HIS:ND1   | 0.53     | 2.41        | 18     | 4     |
| 1:A:63:GLY:C     | 1:A:65:ARG:N     | 0.53     | 2.61        | 15     | 13    |
| 1:A:171:ILE:CG2  | 1:A:175:GLU:CG   | 0.53     | 2.86        | 11     | 7     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:65:ARG:HH21  | 1:A:138:VAL:CG2  | 0.53     | 2.16        | 15     | 1     |
| 1:A:65:ARG:CG    | 1:A:66:ILE:H     | 0.53     | 2.16        | 7      | 1     |
| 1:A:80:PHE:CD1   | 1:A:80:PHE:O     | 0.53     | 2.62        | 19     | 2     |
| 2:B:519:ASN:O    | 2:B:523:HIS:CD2  | 0.53     | 2.62        | 14     | 10    |
| 2:B:530:LEU:HD12 | 2:B:531:LEU:N    | 0.53     | 2.19        | 16     | 16    |
| 1:A:51:PHE:CD2   | 1:A:70:PHE:CD2   | 0.53     | 2.97        | 8      | 1     |
| 2:B:521:GLU:OE1  | 2:B:522:ILE:N    | 0.53     | 2.42        | 3      | 3     |
| 1:A:16:GLU:OE1   | 1:A:16:GLU:N     | 0.53     | 2.42        | 18     | 2     |
| 1:A:124:LEU:N    | 1:A:134:GLU:OE2  | 0.53     | 2.41        | 7      | 5     |
| 1:A:124:LEU:HD13 | 1:A:124:LEU:O    | 0.53     | 2.04        | 12     | 11    |
| 1:A:172:SER:OG   | 1:A:173:PHE:N    | 0.53     | 2.42        | 5      | 2     |
| 1:A:68:ASN:OD1   | 1:A:126:LYS:NZ   | 0.53     | 2.42        | 12     | 1     |
| 1:A:121:LEU:CD1  | 2:B:530:LEU:HD13 | 0.53     | 2.33        | 4      | 8     |
| 1:A:49:GLU:O     | 1:A:53:ARG:NH1   | 0.53     | 2.42        | 5      | 3     |
| 1:A:60:ASN:HD21  | 1:A:65:ARG:NH1   | 0.53     | 2.02        | 14     | 1     |
| 1:A:89:HIS:O     | 1:A:89:HIS:ND1   | 0.53     | 2.42        | 16     | 1     |
| 1:A:65:ARG:CA    | 1:A:65:ARG:HE    | 0.53     | 2.16        | 20     | 1     |
| 1:A:111:ARG:NH1  | 1:A:186:GLU:OE2  | 0.53     | 2.42        | 15     | 1     |
| 2:B:535:GLU:OE1  | 2:B:536:ASP:N    | 0.53     | 2.41        | 8      | 2     |
| 1:A:28:ILE:N     | 1:A:28:ILE:CD1   | 0.53     | 2.67        | 10     | 4     |
| 1:A:61:PRO:O     | 1:A:141:MET:SD   | 0.53     | 2.67        | 1      | 4     |
| 1:A:118:ALA:O    | 1:A:122:TYR:CD2  | 0.53     | 2.62        | 5      | 4     |
| 1:A:122:TYR:O    | 1:A:124:LEU:N    | 0.52     | 2.41        | 4      | 3     |
| 1:A:108:LEU:O    | 1:A:110:SER:N    | 0.52     | 2.41        | 8      | 1     |
| 1:A:88:ALA:O     | 1:A:90:PHE:N     | 0.52     | 2.42        | 15     | 12    |
| 1:A:150:GLU:CD   | 1:A:150:GLU:H    | 0.52     | 2.08        | 6      | 6     |
| 1:A:89:HIS:O     | 1:A:89:HIS:CG    | 0.52     | 2.62        | 1      | 4     |
| 1:A:110:SER:O    | 1:A:113:ASN:N    | 0.52     | 2.42        | 3      | 1     |
| 2:B:535:GLU:O    | 2:B:538:CYS:SG   | 0.52     | 2.67        | 3      | 1     |
| 1:A:122:TYR:OH   | 2:B:530:LEU:CD2  | 0.52     | 2.58        | 14     | 5     |
| 1:A:150:GLU:H    | 1:A:150:GLU:CD   | 0.52     | 2.08        | 4      | 1     |
| 1:A:137:GLN:OE1  | 1:A:140:ARG:NH1  | 0.52     | 2.42        | 13     | 2     |
| 1:A:50:ASP:N     | 1:A:50:ASP:OD1   | 0.52     | 2.42        | 18     | 7     |
| 1:A:130:ILE:CD1  | 1:A:130:ILE:N    | 0.52     | 2.70        | 18     | 1     |
| 1:A:138:VAL:O    | 1:A:141:MET:N    | 0.52     | 2.42        | 16     | 19    |
| 1:A:124:LEU:N    | 1:A:134:GLU:OE1  | 0.52     | 2.42        | 11     | 4     |
| 1:A:66:ILE:O     | 1:A:69:ALA:HB3   | 0.52     | 2.05        | 4      | 1     |
| 1:A:70:PHE:N     | 1:A:70:PHE:CD1   | 0.52     | 2.72        | 20     | 1     |
| 2:B:520:GLU:OE1  | 2:B:521:GLU:N    | 0.52     | 2.42        | 19     | 3     |
| 1:A:119:PHE:O    | 1:A:123:ASP:N    | 0.52     | 2.42        | 14     | 14    |
| 1:A:54:ILE:CG2   | 1:A:56:GLU:H     | 0.52     | 2.17        | 4      | 9     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:157:ASP:OD1  | 1:A:157:ASP:N    | 0.52     | 2.41        | 8      | 1     |
| 1:A:178:LYS:O    | 1:A:182:LYS:NZ   | 0.52     | 2.43        | 15     | 1     |
| 1:A:124:LEU:O    | 1:A:124:LEU:HD13 | 0.52     | 2.05        | 8      | 9     |
| 1:A:165:GLN:O    | 1:A:165:GLN:NE2  | 0.52     | 2.38        | 14     | 1     |
| 1:A:164:ASP:CG   | 1:A:169:SER:H    | 0.51     | 2.08        | 11     | 17    |
| 1:A:46:LEU:O     | 1:A:78:VAL:HG12  | 0.51     | 2.05        | 8      | 5     |
| 1:A:20:GLU:OE2   | 1:A:84:MET:SD    | 0.51     | 2.68        | 6      | 2     |
| 1:A:137:GLN:O    | 1:A:141:MET:SD   | 0.51     | 2.68        | 7      | 3     |
| 1:A:186:GLU:H    | 1:A:186:GLU:CD   | 0.51     | 2.08        | 7      | 5     |
| 1:A:89:HIS:CG    | 1:A:89:HIS:O     | 0.51     | 2.62        | 7      | 4     |
| 1:A:80:PHE:CD1   | 1:A:80:PHE:C     | 0.51     | 2.84        | 13     | 5     |
| 1:A:57:LEU:O     | 1:A:57:LEU:HD23  | 0.51     | 2.05        | 1      | 6     |
| 1:A:129:LYS:HA   | 1:A:172:SER:OG   | 0.51     | 2.04        | 15     | 1     |
| 1:A:119:PHE:CE1  | 1:A:123:ASP:CG   | 0.51     | 2.83        | 7      | 12    |
| 1:A:125:ASP:N    | 1:A:134:GLU:OE1  | 0.51     | 2.39        | 11     | 5     |
| 1:A:168:ASP:OD1  | 1:A:170:ALA:O    | 0.51     | 2.28        | 2      | 9     |
| 1:A:132:ARG:HA   | 1:A:160:ILE:HD13 | 0.51     | 1.82        | 12     | 1     |
| 1:A:57:LEU:HD23  | 1:A:57:LEU:O     | 0.51     | 2.05        | 9      | 4     |
| 1:A:109:ASN:HD22 | 1:A:110:SER:N    | 0.51     | 2.04        | 2      | 1     |
| 1:A:35:PHE:O     | 1:A:46:LEU:HD11  | 0.51     | 2.06        | 2      | 2     |
| 1:A:186:GLU:OE1  | 1:A:186:GLU:N    | 0.51     | 2.43        | 17     | 3     |
| 1:A:119:PHE:CZ   | 1:A:123:ASP:CG   | 0.51     | 2.84        | 14     | 14    |
| 1:A:163:ALA:HB1  | 2:B:519:ASN:HD21 | 0.51     | 1.66        | 8      | 3     |
| 1:A:127:ASP:O    | 1:A:128:GLU:CG   | 0.51     | 2.59        | 1      | 2     |
| 1:A:108:LEU:O    | 1:A:109:ASN:OD1  | 0.51     | 2.28        | 12     | 2     |
| 1:A:117:PHE:CE1  | 1:A:121:LEU:HD11 | 0.51     | 2.41        | 11     | 1     |
| 1:A:168:ASP:CG   | 1:A:170:ALA:O    | 0.51     | 2.49        | 2      | 19    |
| 1:A:33:SER:OG    | 1:A:34:ARG:NH1   | 0.51     | 2.43        | 11     | 1     |
| 1:A:53:ARG:HE    | 1:A:53:ARG:N     | 0.51     | 2.03        | 18     | 1     |
| 1:A:28:ILE:O     | 1:A:29:THR:C     | 0.51     | 2.48        | 7      | 4     |
| 1:A:139:LEU:CD1  | 1:A:139:LEU:C    | 0.51     | 2.80        | 20     | 10    |
| 1:A:69:ALA:O     | 1:A:86:THR:OG1   | 0.50     | 2.27        | 9      | 12    |
| 1:A:125:ASP:OD2  | 1:A:127:ASP:OD1  | 0.50     | 2.30        | 1      | 1     |
| 1:A:109:ASN:C    | 1:A:109:ASN:ND2  | 0.50     | 2.64        | 2      | 2     |
| 1:A:178:LYS:NZ   | 1:A:181:GLU:OE2  | 0.50     | 2.44        | 11     | 1     |
| 1:A:48:ARG:CD    | 1:A:48:ARG:N     | 0.50     | 2.74        | 10     | 1     |
| 1:A:14:LEU:O     | 1:A:16:GLU:N     | 0.50     | 2.42        | 18     | 1     |
| 1:A:45:THR:HG22  | 1:A:79:ASN:HA    | 0.50     | 1.84        | 7      | 10    |
| 1:A:163:ALA:CB   | 2:B:519:ASN:HD21 | 0.50     | 2.19        | 8      | 2     |
| 1:A:68:ASN:ND2   | 1:A:68:ASN:O     | 0.50     | 2.41        | 12     | 1     |
| 1:A:80:PHE:O     | 1:A:80:PHE:CD1   | 0.50     | 2.64        | 11     | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:48:ARG:NH2   | 1:A:52:GLN:NE2   | 0.50     | 2.59        | 13     | 1     |
| 1:A:115:LEU:N    | 1:A:115:LEU:CD2  | 0.50     | 2.74        | 15     | 9     |
| 1:A:35:PHE:CZ    | 1:A:83:PHE:CD1   | 0.50     | 3.00        | 8      | 1     |
| 1:A:17:ILE:O     | 1:A:20:GLU:N     | 0.50     | 2.44        | 18     | 1     |
| 1:A:137:GLN:O    | 1:A:141:MET:CE   | 0.50     | 2.60        | 4      | 3     |
| 1:A:80:PHE:C     | 1:A:80:PHE:CD1   | 0.50     | 2.85        | 2      | 14    |
| 1:A:163:ALA:HB1  | 2:B:519:ASN:ND2  | 0.50     | 2.22        | 8      | 2     |
| 2:B:521:GLU:CD   | 2:B:522:ILE:N    | 0.50     | 2.66        | 12     | 3     |
| 1:A:109:ASN:H    | 1:A:113:ASN:HD22 | 0.50     | 1.48        | 19     | 1     |
| 1:A:114:LYS:HZ1  | 1:A:185:VAL:HG11 | 0.49     | 1.66        | 12     | 2     |
| 2:B:525:GLN:O    | 2:B:529:HIS:CD2  | 0.49     | 2.64        | 4      | 1     |
| 1:A:165:GLN:OE1  | 1:A:174:THR:CG2  | 0.49     | 2.60        | 14     | 1     |
| 1:A:79:ASN:OD1   | 1:A:79:ASN:N     | 0.49     | 2.43        | 15     | 2     |
| 1:A:65:ARG:CA    | 1:A:65:ARG:NE    | 0.49     | 2.75        | 20     | 1     |
| 1:A:122:TYR:CD1  | 2:B:526:PHE:CZ   | 0.49     | 3.00        | 7      | 5     |
| 1:A:86:THR:O     | 1:A:90:PHE:CE1   | 0.49     | 2.65        | 2      | 2     |
| 1:A:88:ALA:C     | 1:A:90:PHE:N     | 0.49     | 2.65        | 18     | 13    |
| 1:A:121:LEU:HD13 | 2:B:530:LEU:HD13 | 0.49     | 1.83        | 11     | 8     |
| 1:A:138:VAL:O    | 1:A:142:MET:SD   | 0.49     | 2.70        | 20     | 1     |
| 1:A:71:PHE:N     | 1:A:71:PHE:CD1   | 0.49     | 2.81        | 1      | 1     |
| 1:A:173:PHE:O    | 1:A:173:PHE:CD1  | 0.49     | 2.66        | 5      | 2     |
| 1:A:111:ARG:CG   | 1:A:112:SER:N    | 0.49     | 2.75        | 9      | 3     |
| 1:A:165:GLN:N    | 1:A:175:GLU:OE2  | 0.49     | 2.38        | 5      | 5     |
| 1:A:171:ILE:CG2  | 1:A:175:GLU:CD   | 0.49     | 2.80        | 11     | 1     |
| 1:A:175:GLU:O    | 1:A:179:VAL:CG2  | 0.49     | 2.61        | 3      | 15    |
| 2:B:538:CYS:SG   | 2:B:538:CYS:O    | 0.49     | 2.70        | 8      | 1     |
| 1:A:30:ARG:CD    | 1:A:30:ARG:N     | 0.49     | 2.76        | 5      | 1     |
| 1:A:149:ASP:OD1  | 1:A:150:GLU:N    | 0.49     | 2.44        | 7      | 1     |
| 1:A:166:ASP:OD2  | 1:A:174:THR:OG1  | 0.49     | 2.31        | 19     | 9     |
| 1:A:65:ARG:NH1   | 2:B:526:PHE:CE1  | 0.49     | 2.81        | 8      | 1     |
| 1:A:66:ILE:CD1   | 2:B:537:ILE:HD11 | 0.49     | 2.37        | 2      | 1     |
| 1:A:64:ASP:OD1   | 1:A:65:ARG:N     | 0.49     | 2.45        | 9      | 3     |
| 1:A:53:ARG:CA    | 1:A:53:ARG:NE    | 0.49     | 2.75        | 12     | 1     |
| 1:A:17:ILE:CG2   | 1:A:18:LYS:N     | 0.49     | 2.75        | 18     | 1     |
| 1:A:139:LEU:C    | 1:A:139:LEU:CD1  | 0.49     | 2.79        | 5      | 8     |
| 1:A:173:PHE:O    | 1:A:177:VAL:CG2  | 0.49     | 2.61        | 2      | 15    |
| 1:A:65:ARG:NH2   | 2:B:533:GLY:C    | 0.49     | 2.66        | 17     | 2     |
| 1:A:114:LYS:NZ   | 1:A:185:VAL:CG1  | 0.49     | 2.75        | 12     | 3     |
| 1:A:119:PHE:CZ   | 1:A:120:ARG:NH2  | 0.49     | 2.81        | 4      | 1     |
| 1:A:120:ARG:NH2  | 1:A:123:ASP:OD2  | 0.49     | 2.42        | 15     | 2     |
| 1:A:180:LEU:O    | 1:A:182:LYS:N    | 0.49     | 2.46        | 9      | 6     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:136:LEU:O    | 1:A:140:ARG:CG   | 0.49     | 2.61        | 2      | 5     |
| 1:A:49:GLU:CD    | 1:A:49:GLU:H     | 0.49     | 2.11        | 12     | 2     |
| 1:A:29:THR:OG1   | 1:A:30:ARG:NH1   | 0.49     | 2.42        | 5      | 1     |
| 1:A:108:LEU:O    | 1:A:109:ASN:CB   | 0.48     | 2.61        | 12     | 7     |
| 1:A:66:ILE:HD11  | 2:B:537:ILE:HD11 | 0.48     | 1.84        | 2      | 2     |
| 1:A:109:ASN:CG   | 1:A:114:LYS:NZ   | 0.48     | 2.66        | 4      | 1     |
| 1:A:47:SER:N     | 1:A:50:ASP:OD2   | 0.48     | 2.42        | 16     | 1     |
| 1:A:14:LEU:O     | 1:A:15:GLU:C     | 0.48     | 2.52        | 4      | 10    |
| 1:A:89:HIS:CE1   | 1:A:113:ASN:OD1  | 0.48     | 2.65        | 1      | 2     |
| 1:A:89:HIS:CE1   | 1:A:117:PHE:CG   | 0.48     | 3.00        | 17     | 1     |
| 1:A:110:SER:O    | 1:A:114:LYS:N    | 0.48     | 2.43        | 8      | 3     |
| 1:A:171:ILE:N    | 1:A:171:ILE:HD12 | 0.48     | 2.23        | 4      | 4     |
| 2:B:535:GLU:C    | 2:B:537:ILE:N    | 0.48     | 2.66        | 20     | 10    |
| 1:A:79:ASN:ND2   | 1:A:80:PHE:H     | 0.48     | 2.06        | 10     | 1     |
| 1:A:180:LEU:C    | 1:A:182:LYS:N    | 0.48     | 2.67        | 20     | 11    |
| 1:A:184:ASP:N    | 1:A:184:ASP:OD1  | 0.48     | 2.46        | 13     | 3     |
| 1:A:35:PHE:CD2   | 1:A:46:LEU:CD1   | 0.48     | 2.96        | 13     | 1     |
| 1:A:16:GLU:O     | 1:A:28:ILE:CG2   | 0.48     | 2.61        | 20     | 4     |
| 1:A:65:ARG:N     | 1:A:65:ARG:CD    | 0.48     | 2.75        | 15     | 1     |
| 2:B:522:ILE:CG2  | 2:B:523:HIS:N    | 0.48     | 2.77        | 18     | 13    |
| 1:A:85:ARG:HH21  | 1:A:120:ARG:NH1  | 0.48     | 2.06        | 8      | 1     |
| 1:A:138:VAL:O    | 1:A:140:ARG:N    | 0.48     | 2.46        | 16     | 3     |
| 1:A:53:ARG:N     | 1:A:53:ARG:CD    | 0.48     | 2.76        | 12     | 3     |
| 1:A:63:GLY:O     | 1:A:64:ASP:C     | 0.48     | 2.51        | 20     | 7     |
| 1:A:168:ASP:O    | 1:A:170:ALA:N    | 0.48     | 2.47        | 11     | 4     |
| 1:A:129:LYS:CE   | 1:A:168:ASP:OD2  | 0.48     | 2.62        | 4      | 3     |
| 1:A:174:THR:HG22 | 1:A:175:GLU:N    | 0.48     | 2.23        | 20     | 3     |
| 1:A:71:PHE:CE2   | 1:A:77:GLN:O     | 0.48     | 2.66        | 20     | 1     |
| 1:A:123:ASP:OD1  | 1:A:130:ILE:CD1  | 0.48     | 2.62        | 7      | 1     |
| 1:A:34:ARG:O     | 1:A:37:SER:OG    | 0.48     | 2.27        | 7      | 1     |
| 1:A:62:LEU:C     | 1:A:64:ASP:N     | 0.48     | 2.67        | 9      | 10    |
| 1:A:115:LEU:H    | 1:A:115:LEU:CD2  | 0.48     | 2.21        | 11     | 3     |
| 1:A:186:GLU:OE2  | 1:A:186:GLU:N    | 0.48     | 2.44        | 9      | 1     |
| 1:A:114:LYS:NZ   | 1:A:185:VAL:HG11 | 0.48     | 2.24        | 7      | 1     |
| 1:A:173:PHE:CD1  | 1:A:173:PHE:O    | 0.48     | 2.66        | 7      | 2     |
| 1:A:79:ASN:N     | 1:A:79:ASN:OD1   | 0.48     | 2.46        | 7      | 3     |
| 2:B:520:GLU:O    | 2:B:524:THR:CG2  | 0.48     | 2.62        | 7      | 3     |
| 1:A:79:ASN:CG    | 1:A:80:PHE:N     | 0.48     | 2.67        | 9      | 4     |
| 1:A:111:ARG:CZ   | 1:A:186:GLU:OE2  | 0.48     | 2.62        | 8      | 1     |
| 1:A:56:GLU:OE1   | 2:B:536:ASP:CB   | 0.48     | 2.62        | 20     | 1     |
| 1:A:129:LYS:CA   | 1:A:172:SER:OG   | 0.48     | 2.62        | 15     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:39:ASP:OD2   | 1:A:45:THR:O     | 0.48     | 2.31        | 15     | 6     |
| 1:A:18:LYS:NZ    | 1:A:191:ILE:O    | 0.47     | 2.42        | 4      | 3     |
| 1:A:150:GLU:OE1  | 1:A:150:GLU:N    | 0.47     | 2.42        | 8      | 1     |
| 1:A:17:ILE:HD12  | 1:A:20:GLU:HB3   | 0.47     | 1.85        | 7      | 2     |
| 1:A:35:PHE:CE2   | 1:A:83:PHE:CE1   | 0.47     | 3.02        | 2      | 3     |
| 1:A:108:LEU:HD23 | 1:A:109:ASN:N    | 0.47     | 2.24        | 3      | 5     |
| 1:A:38:LEU:O     | 1:A:39:ASP:O     | 0.47     | 2.32        | 19     | 5     |
| 1:A:117:PHE:O    | 1:A:119:PHE:N    | 0.47     | 2.47        | 8      | 2     |
| 1:A:12:GLU:CD    | 1:A:12:GLU:H     | 0.47     | 2.13        | 3      | 3     |
| 2:B:521:GLU:H    | 2:B:521:GLU:CD   | 0.47     | 2.12        | 6      | 1     |
| 1:A:71:PHE:O     | 1:A:120:ARG:NH2  | 0.47     | 2.42        | 13     | 1     |
| 1:A:65:ARG:NH1   | 2:B:526:PHE:CZ   | 0.47     | 2.83        | 8      | 1     |
| 1:A:149:ASP:OD1  | 1:A:149:ASP:N    | 0.47     | 2.48        | 7      | 1     |
| 1:A:186:GLU:CD   | 1:A:186:GLU:H    | 0.47     | 2.11        | 13     | 4     |
| 1:A:154:SER:O    | 1:A:157:ASP:OD1  | 0.47     | 2.33        | 8      | 1     |
| 1:A:53:ARG:NE    | 1:A:53:ARG:CA    | 0.47     | 2.77        | 18     | 2     |
| 1:A:116:HIS:CD2  | 1:A:120:ARG:HE   | 0.47     | 2.27        | 10     | 1     |
| 1:A:178:LYS:CD   | 1:A:178:LYS:C    | 0.47     | 2.83        | 18     | 3     |
| 1:A:178:LYS:C    | 1:A:178:LYS:CD   | 0.47     | 2.83        | 13     | 4     |
| 1:A:125:ASP:OD1  | 1:A:127:ASP:OD1  | 0.47     | 2.33        | 19     | 9     |
| 1:A:115:LEU:HD12 | 1:A:172:SER:O    | 0.47     | 2.10        | 2      | 1     |
| 1:A:49:GLU:O     | 1:A:53:ARG:CZ    | 0.47     | 2.62        | 6      | 2     |
| 1:A:91:ARG:H     | 1:A:109:ASN:ND2  | 0.47     | 2.08        | 4      | 1     |
| 1:A:65:ARG:N     | 1:A:65:ARG:NE    | 0.47     | 2.63        | 20     | 2     |
| 1:A:19:LYS:CD    | 1:A:19:LYS:N     | 0.47     | 2.77        | 15     | 4     |
| 1:A:88:ALA:C     | 1:A:90:PHE:H     | 0.47     | 2.13        | 14     | 13    |
| 1:A:191:ILE:CG2  | 1:A:191:ILE:O    | 0.47     | 2.62        | 14     | 2     |
| 1:A:178:LYS:NZ   | 1:A:181:GLU:CD   | 0.47     | 2.68        | 11     | 1     |
| 1:A:13:GLU:OE1   | 2:B:538:CYS:SG   | 0.47     | 2.72        | 4      | 1     |
| 1:A:150:GLU:N    | 1:A:150:GLU:OE2  | 0.47     | 2.44        | 4      | 2     |
| 1:A:130:ILE:HD11 | 1:A:172:SER:OG   | 0.47     | 2.10        | 20     | 1     |
| 1:A:183:VAL:O    | 1:A:185:VAL:N    | 0.47     | 2.48        | 20     | 2     |
| 1:A:48:ARG:NH1   | 1:A:57:LEU:CD1   | 0.47     | 2.78        | 12     | 1     |
| 1:A:124:LEU:CD1  | 1:A:124:LEU:C    | 0.47     | 2.83        | 15     | 9     |
| 2:B:537:ILE:O    | 2:B:538:CYS:C    | 0.47     | 2.53        | 18     | 12    |
| 1:A:130:ILE:CG1  | 1:A:171:ILE:O    | 0.47     | 2.59        | 14     | 3     |
| 2:B:528:ASP:O    | 2:B:532:THR:HG23 | 0.47     | 2.10        | 10     | 1     |
| 1:A:173:PHE:CD1  | 1:A:173:PHE:C    | 0.47     | 2.87        | 20     | 2     |
| 1:A:136:LEU:CD1  | 1:A:136:LEU:C    | 0.47     | 2.83        | 16     | 1     |
| 1:A:53:ARG:CD    | 1:A:53:ARG:N     | 0.47     | 2.76        | 18     | 2     |
| 1:A:60:ASN:HD21  | 1:A:65:ARG:NH2   | 0.47     | 2.08        | 9      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:52:GLN:CD    | 1:A:57:LEU:HD22  | 0.46     | 2.30        | 7      | 3     |
| 2:B:537:ILE:C    | 2:B:538:CYS:SG   | 0.46     | 2.93        | 17     | 1     |
| 1:A:140:ARG:CG   | 1:A:141:MET:N    | 0.46     | 2.77        | 10     | 6     |
| 1:A:119:PHE:CE1  | 1:A:123:ASP:OD1  | 0.46     | 2.68        | 7      | 1     |
| 1:A:138:VAL:O    | 1:A:139:LEU:C    | 0.46     | 2.53        | 4      | 19    |
| 1:A:138:VAL:C    | 1:A:142:MET:SD   | 0.46     | 2.93        | 15     | 7     |
| 1:A:124:LEU:C    | 1:A:124:LEU:CD1  | 0.46     | 2.84        | 2      | 9     |
| 1:A:16:GLU:OE1   | 1:A:27:GLN:O     | 0.46     | 2.34        | 12     | 2     |
| 1:A:27:GLN:NE2   | 1:A:30:ARG:NH2   | 0.46     | 2.63        | 15     | 1     |
| 1:A:13:GLU:O     | 2:B:538:CYS:SG   | 0.46     | 2.73        | 7      | 1     |
| 1:A:189:MET:N    | 1:A:189:MET:SD   | 0.46     | 2.86        | 17     | 1     |
| 1:A:63:GLY:O     | 1:A:67:ILE:HD12  | 0.46     | 2.11        | 8      | 1     |
| 1:A:27:GLN:NE2   | 1:A:27:GLN:H     | 0.46     | 2.06        | 13     | 1     |
| 1:A:60:ASN:ND2   | 1:A:65:ARG:NH2   | 0.46     | 2.63        | 13     | 1     |
| 1:A:122:TYR:CE1  | 2:B:526:PHE:CD2  | 0.46     | 3.04        | 7      | 2     |
| 1:A:127:ASP:OD1  | 1:A:129:LYS:O    | 0.46     | 2.34        | 3      | 7     |
| 1:A:127:ASP:OD2  | 1:A:131:SER:OG   | 0.46     | 2.34        | 12     | 4     |
| 1:A:16:GLU:OE1   | 1:A:16:GLU:CA    | 0.46     | 2.63        | 18     | 1     |
| 1:A:117:PHE:C    | 1:A:119:PHE:N    | 0.46     | 2.67        | 8      | 4     |
| 1:A:127:ASP:OD1  | 1:A:129:LYS:N    | 0.46     | 2.48        | 5      | 4     |
| 1:A:138:VAL:HG11 | 2:B:526:PHE:CE1  | 0.46     | 2.42        | 8      | 3     |
| 1:A:34:ARG:N     | 1:A:34:ARG:CD    | 0.46     | 2.78        | 13     | 2     |
| 1:A:168:ASP:OD2  | 1:A:170:ALA:O    | 0.46     | 2.33        | 12     | 14    |
| 1:A:137:GLN:HE22 | 1:A:140:ARG:NH2  | 0.46     | 2.04        | 5      | 1     |
| 1:A:62:LEU:HD11  | 1:A:65:ARG:NH2   | 0.46     | 2.26        | 6      | 1     |
| 2:B:521:GLU:CG   | 2:B:522:ILE:N    | 0.46     | 2.79        | 13     | 6     |
| 1:A:125:ASP:OD1  | 1:A:127:ASP:OD2  | 0.46     | 2.33        | 4      | 2     |
| 1:A:65:ARG:NE    | 1:A:121:LEU:O    | 0.46     | 2.49        | 3      | 2     |
| 1:A:111:ARG:CG   | 1:A:112:SER:H    | 0.46     | 2.23        | 9      | 2     |
| 1:A:171:ILE:O    | 1:A:172:SER:OG   | 0.46     | 2.34        | 15     | 1     |
| 1:A:165:GLN:HE21 | 1:A:165:GLN:C    | 0.46     | 2.12        | 14     | 1     |
| 1:A:115:LEU:H    | 1:A:115:LEU:HD22 | 0.46     | 1.71        | 10     | 1     |
| 1:A:182:LYS:CB   | 1:A:182:LYS:NZ   | 0.46     | 2.79        | 19     | 1     |
| 1:A:65:ARG:HG3   | 1:A:66:ILE:N     | 0.45     | 2.26        | 13     | 2     |
| 1:A:178:LYS:HZ2  | 1:A:182:LYS:NZ   | 0.45     | 2.08        | 8      | 1     |
| 1:A:115:LEU:HD22 | 1:A:115:LEU:H    | 0.45     | 1.71        | 11     | 1     |
| 1:A:57:LEU:HD21  | 1:A:66:ILE:HD11  | 0.45     | 1.88        | 15     | 1     |
| 1:A:119:PHE:CE1  | 1:A:123:ASP:OD2  | 0.45     | 2.69        | 7      | 1     |
| 1:A:191:ILE:O    | 1:A:191:ILE:CG2  | 0.45     | 2.64        | 17     | 3     |
| 1:A:118:ALA:HB1  | 1:A:122:TYR:CE2  | 0.45     | 2.46        | 5      | 3     |
| 1:A:122:TYR:CB   | 1:A:130:ILE:HD12 | 0.45     | 2.40        | 11     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:A:126:LYS:NZ  | 1:A:126:LYS:CB   | 0.45     | 2.79        | 15     | 1     |
| 1:A:171:ILE:C   | 1:A:172:SER:OG   | 0.45     | 2.55        | 15     | 1     |
| 1:A:64:ASP:HA   | 1:A:67:ILE:HD12  | 0.45     | 1.89        | 19     | 9     |
| 2:B:527:LEU:C   | 2:B:527:LEU:CD1  | 0.45     | 2.84        | 13     | 1     |
| 1:A:108:LEU:C   | 1:A:110:SER:N    | 0.45     | 2.67        | 8      | 1     |
| 1:A:79:ASN:ND2  | 1:A:79:ASN:N     | 0.45     | 2.64        | 17     | 1     |
| 1:A:79:ASN:ND2  | 1:A:81:ARG:CG    | 0.45     | 2.79        | 8      | 1     |
| 1:A:165:GLN:NE2 | 1:A:165:GLN:C    | 0.45     | 2.70        | 14     | 1     |
| 1:A:65:ARG:CD   | 1:A:65:ARG:H     | 0.45     | 2.25        | 20     | 1     |
| 1:A:125:ASP:OD2 | 1:A:134:GLU:OE2  | 0.45     | 2.35        | 11     | 5     |
| 1:A:118:ALA:HA  | 1:A:121:LEU:HD12 | 0.45     | 1.88        | 18     | 4     |
| 1:A:19:LYS:C    | 1:A:21:THR:N     | 0.45     | 2.69        | 9      | 4     |
| 1:A:131:SER:N   | 1:A:134:GLU:OE1  | 0.45     | 2.45        | 3      | 1     |
| 1:A:191:ILE:O   | 1:A:191:ILE:HG23 | 0.45     | 2.11        | 17     | 7     |
| 2:B:521:GLU:O   | 2:B:524:THR:OG1  | 0.45     | 2.35        | 2      | 7     |
| 1:A:35:PHE:CE2  | 1:A:46:LEU:CD1   | 0.45     | 3.00        | 12     | 3     |
| 1:A:163:ALA:O   | 1:A:175:GLU:CD   | 0.45     | 2.53        | 9      | 3     |
| 1:A:26:SER:O    | 1:A:29:THR:N     | 0.45     | 2.50        | 17     | 1     |
| 1:A:76:ASP:N    | 1:A:76:ASP:OD1   | 0.45     | 2.50        | 17     | 1     |
| 1:A:145:VAL:O   | 1:A:146:ASN:OD1  | 0.45     | 2.35        | 19     | 2     |
| 1:A:109:ASN:OD1 | 1:A:109:ASN:C    | 0.45     | 2.55        | 12     | 2     |
| 1:A:48:ARG:CZ   | 1:A:57:LEU:HD13  | 0.45     | 2.41        | 12     | 1     |
| 1:A:60:ASN:CG   | 1:A:65:ARG:HH12  | 0.45     | 2.15        | 7      | 2     |
| 1:A:12:GLU:H    | 1:A:12:GLU:CD    | 0.45     | 2.14        | 5      | 4     |
| 1:A:186:GLU:N   | 1:A:186:GLU:CD   | 0.45     | 2.69        | 15     | 1     |
| 1:A:47:SER:OG   | 1:A:48:ARG:N     | 0.45     | 2.49        | 13     | 2     |
| 1:A:89:HIS:NE2  | 1:A:117:PHE:CB   | 0.45     | 2.80        | 12     | 2     |
| 1:A:108:LEU:C   | 1:A:110:SER:H    | 0.45     | 2.15        | 8      | 5     |
| 1:A:116:HIS:NE2 | 1:A:120:ARG:NE   | 0.45     | 2.65        | 10     | 2     |
| 1:A:27:GLN:HE22 | 1:A:30:ARG:NH2   | 0.45     | 2.10        | 15     | 1     |
| 1:A:109:ASN:O   | 1:A:109:ASN:OD1  | 0.45     | 2.34        | 13     | 2     |
| 1:A:91:ARG:O    | 1:A:109:ASN:OD1  | 0.45     | 2.35        | 16     | 6     |
| 1:A:60:ASN:HD21 | 1:A:65:ARG:HH21  | 0.45     | 1.55        | 9      | 1     |
| 1:A:125:ASP:C   | 1:A:125:ASP:OD1  | 0.44     | 2.56        | 6      | 11    |
| 2:B:517:SER:O   | 2:B:520:GLU:N    | 0.44     | 2.49        | 4      | 2     |
| 1:A:166:ASP:OD1 | 1:A:174:THR:OG1  | 0.44     | 2.36        | 19     | 6     |
| 1:A:90:PHE:O    | 1:A:189:MET:O    | 0.44     | 2.35        | 10     | 2     |
| 1:A:35:PHE:CD1  | 1:A:83:PHE:CE1   | 0.44     | 3.04        | 15     | 2     |
| 1:A:56:GLU:O    | 1:A:60:ASN:OD1   | 0.44     | 2.36        | 18     | 4     |
| 1:A:122:TYR:CZ  | 2:B:526:PHE:CD2  | 0.44     | 3.05        | 8      | 1     |
| 1:A:126:LYS:CD  | 1:A:126:LYS:N    | 0.44     | 2.80        | 20     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:91:ARG:O     | 1:A:92:PRO:O     | 0.44     | 2.35        | 11     | 1     |
| 1:A:39:ASP:HB2   | 1:A:46:LEU:HD23  | 0.44     | 1.88        | 10     | 2     |
| 1:A:108:LEU:O    | 1:A:109:ASN:CG   | 0.44     | 2.56        | 3      | 8     |
| 1:A:183:VAL:O    | 1:A:184:ASP:C    | 0.44     | 2.56        | 10     | 1     |
| 1:A:179:VAL:HG21 | 2:B:519:ASN:HB2  | 0.44     | 1.89        | 5      | 2     |
| 1:A:48:ARG:NH1   | 1:A:71:PHE:CD2   | 0.44     | 2.85        | 11     | 1     |
| 1:A:168:ASP:O    | 1:A:169:SER:C    | 0.44     | 2.53        | 11     | 16    |
| 1:A:173:PHE:C    | 1:A:173:PHE:CD1  | 0.44     | 2.90        | 5      | 3     |
| 1:A:12:GLU:O     | 1:A:16:GLU:OE2   | 0.44     | 2.36        | 18     | 2     |
| 1:A:21:THR:OG1   | 1:A:90:PHE:O     | 0.44     | 2.36        | 11     | 1     |
| 1:A:165:GLN:OE1  | 1:A:165:GLN:O    | 0.44     | 2.36        | 16     | 1     |
| 1:A:35:PHE:CD1   | 1:A:46:LEU:CD1   | 0.44     | 3.01        | 7      | 2     |
| 2:B:527:LEU:CD1  | 2:B:527:LEU:C    | 0.44     | 2.82        | 1      | 2     |
| 1:A:19:LYS:C     | 1:A:22:GLY:H     | 0.44     | 2.16        | 20     | 3     |
| 1:A:16:GLU:O     | 1:A:28:ILE:HG23  | 0.44     | 2.12        | 10     | 1     |
| 1:A:178:LYS:CD   | 1:A:178:LYS:O    | 0.44     | 2.66        | 3      | 3     |
| 1:A:79:ASN:H     | 1:A:79:ASN:ND2   | 0.44     | 2.09        | 1      | 1     |
| 1:A:114:LYS:HZ3  | 1:A:186:GLU:HA   | 0.44     | 1.71        | 14     | 1     |
| 1:A:57:LEU:CD1   | 1:A:66:ILE:HD11  | 0.44     | 2.42        | 12     | 1     |
| 1:A:79:ASN:OD1   | 1:A:80:PHE:N     | 0.44     | 2.50        | 13     | 1     |
| 2:B:536:ASP:OD1  | 2:B:536:ASP:O    | 0.44     | 2.35        | 9      | 2     |
| 1:A:125:ASP:OD2  | 1:A:134:GLU:OE1  | 0.44     | 2.36        | 12     | 5     |
| 2:B:533:GLY:O    | 2:B:536:ASP:OD1  | 0.44     | 2.36        | 1      | 1     |
| 1:A:109:ASN:O    | 1:A:110:SER:O    | 0.44     | 2.36        | 18     | 3     |
| 1:A:89:HIS:O     | 1:A:109:ASN:OD1  | 0.43     | 2.35        | 16     | 2     |
| 1:A:33:SER:O     | 1:A:37:SER:OG    | 0.43     | 2.35        | 18     | 2     |
| 1:A:168:ASP:O    | 1:A:169:SER:OG   | 0.43     | 2.35        | 14     | 1     |
| 1:A:163:ALA:HB2  | 2:B:518:ILE:HD12 | 0.43     | 1.89        | 20     | 1     |
| 1:A:68:ASN:OD1   | 1:A:120:ARG:O    | 0.43     | 2.36        | 12     | 1     |
| 2:B:530:LEU:C    | 2:B:530:LEU:CD1  | 0.43     | 2.84        | 12     | 4     |
| 1:A:122:TYR:OH   | 2:B:526:PHE:CD1  | 0.43     | 2.64        | 1      | 1     |
| 1:A:20:GLU:OE1   | 1:A:20:GLU:O     | 0.43     | 2.37        | 14     | 2     |
| 1:A:26:SER:O     | 1:A:27:GLN:C     | 0.43     | 2.56        | 13     | 6     |
| 1:A:37:SER:C     | 1:A:39:ASP:N     | 0.43     | 2.70        | 17     | 3     |
| 1:A:51:PHE:CE1   | 1:A:70:PHE:CZ    | 0.43     | 3.07        | 8      | 1     |
| 1:A:109:ASN:CG   | 1:A:114:LYS:HZ1  | 0.43     | 2.15        | 4      | 1     |
| 1:A:126:LYS:C    | 1:A:128:GLU:H    | 0.43     | 2.16        | 7      | 1     |
| 1:A:57:LEU:C     | 1:A:57:LEU:CD2   | 0.43     | 2.86        | 11     | 6     |
| 1:A:13:GLU:CD    | 2:B:538:CYS:SG   | 0.43     | 2.96        | 11     | 1     |
| 1:A:26:SER:O     | 1:A:28:ILE:N     | 0.43     | 2.50        | 9      | 1     |
| 1:A:139:LEU:HD22 | 1:A:139:LEU:C    | 0.43     | 2.32        | 19     | 1     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:87:LEU:HD22  | 2:B:538:CYS:SG  | 0.43     | 2.54        | 19     | 1     |
| 1:A:184:ASP:O    | 1:A:186:GLU:N   | 0.43     | 2.52        | 18     | 1     |
| 2:B:519:ASN:OD1  | 2:B:520:GLU:N   | 0.43     | 2.52        | 16     | 2     |
| 1:A:115:LEU:CD2  | 1:A:115:LEU:H   | 0.43     | 2.27        | 18     | 3     |
| 1:A:11:ASP:O     | 1:A:15:GLU:OE1  | 0.43     | 2.37        | 18     | 1     |
| 1:A:75:GLU:CD    | 1:A:76:ASP:H    | 0.43     | 2.17        | 3      | 1     |
| 1:A:37:SER:O     | 1:A:39:ASP:N    | 0.43     | 2.52        | 17     | 1     |
| 1:A:157:ASP:OD1  | 1:A:158:ARG:N   | 0.43     | 2.52        | 8      | 1     |
| 1:A:130:ILE:HD13 | 1:A:130:ILE:H   | 0.43     | 1.72        | 4      | 1     |
| 1:A:183:VAL:O    | 1:A:184:ASP:OD1 | 0.43     | 2.36        | 10     | 1     |
| 1:A:65:ARG:HH12  | 2:B:533:GLY:C   | 0.43     | 2.17        | 12     | 1     |
| 1:A:184:ASP:C    | 1:A:186:GLU:N   | 0.43     | 2.72        | 18     | 1     |
| 1:A:52:GLN:NE2   | 1:A:57:LEU:CD2  | 0.43     | 2.81        | 18     | 1     |
| 1:A:189:MET:SD   | 1:A:189:MET:N   | 0.43     | 2.91        | 13     | 1     |
| 1:A:60:ASN:CG    | 1:A:65:ARG:HH22 | 0.43     | 2.17        | 13     | 1     |
| 2:B:532:THR:O    | 2:B:536:ASP:OD2 | 0.43     | 2.37        | 12     | 4     |
| 1:A:122:TYR:CZ   | 2:B:526:PHE:CE1 | 0.43     | 3.07        | 1      | 1     |
| 1:A:79:ASN:CG    | 1:A:80:PHE:H    | 0.43     | 2.17        | 10     | 3     |
| 1:A:158:ARG:O    | 1:A:162:GLU:OE1 | 0.43     | 2.37        | 16     | 3     |
| 1:A:29:THR:HG23  | 1:A:30:ARG:N    | 0.43     | 2.29        | 7      | 2     |
| 1:A:17:ILE:HG23  | 1:A:18:LYS:N    | 0.43     | 2.29        | 14     | 6     |
| 1:A:180:LEU:O    | 1:A:183:VAL:O   | 0.43     | 2.37        | 8      | 1     |
| 1:A:178:LYS:O    | 1:A:181:GLU:CG  | 0.43     | 2.66        | 4      | 3     |
| 1:A:56:GLU:OE1   | 2:B:536:ASP:OD2 | 0.43     | 2.37        | 1      | 1     |
| 1:A:65:ARG:NE    | 1:A:66:ILE:CG2  | 0.43     | 2.81        | 16     | 1     |
| 2:B:517:SER:O    | 2:B:521:GLU:OE2 | 0.43     | 2.37        | 6      | 1     |
| 1:A:140:ARG:CD   | 1:A:140:ARG:C   | 0.43     | 2.87        | 15     | 1     |
| 1:A:163:ALA:CB   | 2:B:519:ASN:ND2 | 0.43     | 2.81        | 8      | 1     |
| 1:A:122:TYR:O    | 1:A:134:GLU:OE1 | 0.43     | 2.37        | 14     | 1     |
| 2:B:530:LEU:CD1  | 2:B:530:LEU:C   | 0.43     | 2.87        | 9      | 2     |
| 2:B:524:THR:O    | 2:B:528:ASP:OD2 | 0.43     | 2.37        | 13     | 2     |
| 1:A:89:HIS:ND1   | 1:A:117:PHE:CG  | 0.43     | 2.87        | 17     | 1     |
| 2:B:536:ASP:OD1  | 2:B:537:ILE:N   | 0.43     | 2.52        | 1      | 1     |
| 1:A:109:ASN:OD1  | 1:A:109:ASN:O   | 0.43     | 2.37        | 6      | 3     |
| 1:A:127:ASP:OD1  | 1:A:127:ASP:C   | 0.43     | 2.56        | 11     | 1     |
| 1:A:125:ASP:OD1  | 1:A:125:ASP:C   | 0.43     | 2.57        | 9      | 5     |
| 1:A:56:GLU:OE1   | 1:A:57:LEU:N    | 0.43     | 2.52        | 16     | 1     |
| 1:A:89:HIS:O     | 1:A:109:ASN:CG  | 0.43     | 2.57        | 9      | 1     |
| 1:A:75:GLU:OE2   | 1:A:77:GLN:O    | 0.42     | 2.37        | 11     | 1     |
| 1:A:158:ARG:HH21 | 1:A:161:GLN:CD  | 0.42     | 2.16        | 9      | 1     |
| 1:A:125:ASP:OD1  | 1:A:134:GLU:OE2 | 0.42     | 2.37        | 1      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:13:GLU:OE1   | 2:B:538:CYS:O    | 0.42     | 2.37        | 16     | 1     |
| 1:A:180:LEU:O    | 1:A:184:ASP:N    | 0.42     | 2.40        | 10     | 1     |
| 1:A:169:SER:O    | 1:A:169:SER:OG   | 0.42     | 2.37        | 19     | 1     |
| 1:A:85:ARG:O     | 1:A:89:HIS:CG    | 0.42     | 2.72        | 3      | 1     |
| 1:A:57:LEU:CD2   | 1:A:57:LEU:C     | 0.42     | 2.87        | 7      | 3     |
| 2:B:523:HIS:O    | 2:B:524:THR:C    | 0.42     | 2.56        | 5      | 2     |
| 1:A:149:ASP:CG   | 1:A:150:GLU:N    | 0.42     | 2.72        | 7      | 1     |
| 1:A:180:LEU:C    | 1:A:182:LYS:H    | 0.42     | 2.17        | 15     | 9     |
| 1:A:127:ASP:OD2  | 1:A:129:LYS:O    | 0.42     | 2.38        | 19     | 2     |
| 1:A:78:VAL:HG13  | 1:A:78:VAL:O     | 0.42     | 2.14        | 10     | 1     |
| 1:A:65:ARG:NH2   | 2:B:534:ILE:CA   | 0.42     | 2.83        | 5      | 1     |
| 1:A:56:GLU:OE1   | 1:A:60:ASN:OD1   | 0.42     | 2.37        | 10     | 1     |
| 1:A:63:GLY:C     | 1:A:65:ARG:H     | 0.42     | 2.18        | 15     | 1     |
| 1:A:26:SER:C     | 1:A:28:ILE:N     | 0.42     | 2.73        | 9      | 1     |
| 1:A:56:GLU:OE2   | 2:B:533:GLY:O    | 0.42     | 2.37        | 12     | 3     |
| 1:A:89:HIS:CE1   | 1:A:113:ASN:ND2  | 0.42     | 2.87        | 19     | 1     |
| 1:A:117:PHE:O    | 1:A:118:ALA:C    | 0.42     | 2.58        | 6      | 7     |
| 1:A:111:ARG:O    | 1:A:114:LYS:N    | 0.42     | 2.53        | 11     | 2     |
| 1:A:115:LEU:O    | 1:A:119:PHE:CB   | 0.42     | 2.68        | 10     | 4     |
| 2:B:527:LEU:HD12 | 2:B:528:ASP:N    | 0.42     | 2.30        | 13     | 3     |
| 1:A:35:PHE:CG    | 1:A:83:PHE:CE1   | 0.42     | 3.08        | 17     | 1     |
| 1:A:57:LEU:HD12  | 1:A:66:ILE:CD1   | 0.42     | 2.44        | 16     | 1     |
| 1:A:48:ARG:HH12  | 1:A:57:LEU:HD13  | 0.42     | 1.72        | 12     | 1     |
| 1:A:140:ARG:O    | 1:A:144:GLY:N    | 0.42     | 2.50        | 19     | 1     |
| 1:A:65:ARG:HH21  | 2:B:533:GLY:C    | 0.42     | 2.18        | 7      | 2     |
| 1:A:84:MET:O     | 1:A:88:ALA:CB    | 0.42     | 2.68        | 18     | 3     |
| 1:A:89:HIS:CD2   | 1:A:117:PHE:CD1  | 0.42     | 3.08        | 1      | 1     |
| 1:A:11:ASP:N     | 1:A:11:ASP:OD1   | 0.42     | 2.49        | 16     | 2     |
| 1:A:65:ARG:NH1   | 1:A:121:LEU:O    | 0.42     | 2.52        | 10     | 1     |
| 2:B:520:GLU:OE1  | 2:B:521:GLU:OE1  | 0.42     | 2.37        | 6      | 1     |
| 1:A:46:LEU:CD1   | 1:A:50:ASP:OD2   | 0.42     | 2.67        | 9      | 1     |
| 1:A:59:ILE:HG22  | 1:A:59:ILE:O     | 0.42     | 2.15        | 17     | 1     |
| 2:B:535:GLU:CD   | 2:B:535:GLU:O    | 0.42     | 2.58        | 2      | 2     |
| 1:A:110:SER:O    | 1:A:111:ARG:C    | 0.42     | 2.57        | 3      | 1     |
| 1:A:19:LYS:O     | 1:A:20:GLU:C     | 0.42     | 2.58        | 14     | 4     |
| 1:A:122:TYR:CZ   | 2:B:526:PHE:CE2  | 0.41     | 3.08        | 8      | 1     |
| 1:A:191:ILE:HD12 | 2:B:535:GLU:OE1  | 0.41     | 2.15        | 5      | 1     |
| 1:A:45:THR:HG22  | 1:A:79:ASN:CA    | 0.41     | 2.45        | 18     | 1     |
| 1:A:47:SER:O     | 1:A:50:ASP:OD1   | 0.41     | 2.37        | 3      | 1     |
| 1:A:155:ILE:HD12 | 1:A:158:ARG:HH21 | 0.41     | 1.75        | 17     | 1     |
| 1:A:60:ASN:CG    | 1:A:65:ARG:HH21  | 0.41     | 2.17        | 2      | 1     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:119:PHE:C    | 1:A:121:LEU:N   | 0.41     | 2.72        | 11     | 1     |
| 1:A:114:LYS:HZ1  | 1:A:185:VAL:CG1 | 0.41     | 2.27        | 12     | 1     |
| 1:A:163:ALA:HB1  | 2:B:519:ASN:OD1 | 0.41     | 2.14        | 18     | 1     |
| 1:A:63:GLY:O     | 1:A:66:ILE:HG13 | 0.41     | 2.14        | 20     | 1     |
| 1:A:17:ILE:O     | 1:A:18:LYS:C    | 0.41     | 2.58        | 14     | 6     |
| 1:A:51:PHE:CE1   | 1:A:70:PHE:CE1  | 0.41     | 3.08        | 8      | 1     |
| 1:A:165:GLN:C    | 1:A:167:GLY:N   | 0.41     | 2.74        | 2      | 2     |
| 1:A:126:LYS:N    | 1:A:126:LYS:CD  | 0.41     | 2.83        | 4      | 1     |
| 1:A:138:VAL:CG1  | 1:A:142:MET:SD  | 0.41     | 3.00        | 15     | 1     |
| 1:A:13:GLU:OE2   | 2:B:538:CYS:SG  | 0.41     | 2.70        | 5      | 1     |
| 2:B:532:THR:O    | 2:B:536:ASP:OD1 | 0.41     | 2.38        | 3      | 1     |
| 1:A:149:ASP:CG   | 1:A:150:GLU:H   | 0.41     | 2.16        | 7      | 1     |
| 1:A:178:LYS:O    | 1:A:178:LYS:CD  | 0.41     | 2.68        | 7      | 1     |
| 2:B:536:ASP:O    | 2:B:538:CYS:SG  | 0.41     | 2.70        | 17     | 1     |
| 1:A:83:PHE:CZ    | 1:A:87:LEU:CD1  | 0.41     | 3.04        | 20     | 1     |
| 1:A:173:PHE:O    | 1:A:173:PHE:CD2 | 0.41     | 2.74        | 15     | 1     |
| 1:A:49:GLU:OE2   | 1:A:49:GLU:O    | 0.41     | 2.38        | 15     | 1     |
| 1:A:35:PHE:CE1   | 1:A:46:LEU:CD1  | 0.41     | 3.03        | 14     | 2     |
| 1:A:85:ARG:NH2   | 1:A:120:ARG:NH1 | 0.41     | 2.69        | 3      | 1     |
| 1:A:126:LYS:C    | 1:A:128:GLU:N   | 0.41     | 2.74        | 7      | 1     |
| 1:A:56:GLU:O     | 1:A:60:ASN:CG   | 0.41     | 2.60        | 7      | 3     |
| 2:B:532:THR:O    | 2:B:536:ASP:CG  | 0.41     | 2.59        | 7      | 1     |
| 1:A:82:GLY:O     | 1:A:83:PHE:C    | 0.41     | 2.59        | 17     | 3     |
| 1:A:37:SER:C     | 1:A:39:ASP:H    | 0.41     | 2.19        | 17     | 1     |
| 1:A:15:GLU:OE1   | 1:A:19:LYS:NZ   | 0.41     | 2.43        | 19     | 2     |
| 1:A:109:ASN:HD21 | 1:A:189:MET:CB  | 0.41     | 2.28        | 11     | 1     |
| 1:A:63:GLY:O     | 1:A:66:ILE:CG2  | 0.41     | 2.69        | 4      | 1     |
| 1:A:125:ASP:CG   | 1:A:134:GLU:OE2 | 0.41     | 2.59        | 14     | 1     |
| 2:B:535:GLU:C    | 2:B:537:ILE:H   | 0.41     | 2.19        | 20     | 2     |
| 1:A:38:LEU:CB    | 1:A:50:ASP:OD1  | 0.41     | 2.69        | 9      | 1     |
| 1:A:129:LYS:HZ3  | 1:A:170:ALA:HB3 | 0.41     | 1.76        | 12     | 1     |
| 1:A:66:ILE:HG23  | 1:A:67:ILE:N    | 0.41     | 2.31        | 2      | 1     |
| 1:A:166:ASP:CG   | 1:A:174:THR:OG1 | 0.41     | 2.59        | 20     | 3     |
| 1:A:21:THR:OG1   | 1:A:90:PHE:C    | 0.41     | 2.59        | 10     | 1     |
| 1:A:48:ARG:HH12  | 1:A:52:GLN:CD   | 0.41     | 2.17        | 20     | 1     |
| 1:A:31:LEU:HD13  | 1:A:31:LEU:O    | 0.40     | 2.16        | 20     | 1     |
| 1:A:172:SER:O    | 1:A:176:PHE:CG  | 0.40     | 2.74        | 3      | 1     |
| 2:B:525:GLN:O    | 2:B:526:PHE:C   | 0.40     | 2.59        | 8      | 2     |
| 1:A:13:GLU:O     | 1:A:17:ILE:HG22 | 0.40     | 2.17        | 1      | 1     |
| 1:A:125:ASP:OD2  | 1:A:134:GLU:CG  | 0.40     | 2.69        | 4      | 1     |
| 1:A:56:GLU:CD    | 1:A:60:ASN:ND2  | 0.40     | 2.74        | 12     | 1     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:36:THR:HA    | 1:A:46:LEU:HD21 | 0.40     | 1.93        | 7      | 1     |
| 2:B:522:ILE:HG23 | 2:B:523:HIS:ND1 | 0.40     | 2.31        | 1      | 1     |
| 1:A:119:PHE:CE2  | 1:A:120:ARG:CZ  | 0.40     | 3.03        | 4      | 1     |
| 1:A:136:LEU:O    | 1:A:137:GLN:C   | 0.40     | 2.60        | 4      | 1     |
| 1:A:114:LYS:HZ2  | 1:A:185:VAL:HB  | 0.40     | 1.76        | 10     | 1     |
| 1:A:81:ARG:CG    | 1:A:85:ARG:HH22 | 0.40     | 2.30        | 10     | 1     |
| 1:A:125:ASP:OD1  | 1:A:127:ASP:CG  | 0.40     | 2.60        | 20     | 1     |
| 1:A:19:LYS:O     | 1:A:21:THR:N    | 0.40     | 2.54        | 9      | 1     |
| 1:A:91:ARG:O     | 1:A:109:ASN:CG  | 0.40     | 2.60        | 19     | 1     |
| 1:A:68:ASN:CB    | 1:A:120:ARG:O   | 0.40     | 2.70        | 7      | 1     |
| 1:A:108:LEU:C    | 1:A:109:ASN:ND2 | 0.40     | 2.75        | 17     | 1     |
| 1:A:143:VAL:C    | 1:A:145:VAL:N   | 0.40     | 2.75        | 8      | 1     |
| 2:B:526:PHE:O    | 2:B:527:LEU:C   | 0.40     | 2.59        | 5      | 3     |
| 1:A:125:ASP:OD1  | 1:A:134:GLU:CD  | 0.40     | 2.60        | 1      | 1     |
| 2:B:520:GLU:O    | 2:B:521:GLU:C   | 0.40     | 2.58        | 5      | 1     |
| 2:B:534:ILE:CG2  | 2:B:535:GLU:OE1 | 0.40     | 2.69        | 15     | 1     |
| 1:A:49:GLU:N     | 1:A:49:GLU:CD   | 0.40     | 2.73        | 12     | 1     |
| 1:A:19:LYS:N     | 1:A:19:LYS:CD   | 0.40     | 2.83        | 11     | 1     |
| 1:A:184:ASP:OD1  | 1:A:184:ASP:O   | 0.40     | 2.39        | 16     | 1     |
| 1:A:20:GLU:O     | 1:A:88:ALA:CB   | 0.40     | 2.69        | 9      | 1     |
| 1:A:14:LEU:C     | 1:A:16:GLU:N    | 0.40     | 2.75        | 18     | 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     | 156/195 (80%)   | 124±3 (79±2%) | 26±3 (17±2%) | 6±2 (4±1%) | 6           | 34 |
| 2   | B     | 22/43 (51%)     | 18±1 (82±6%)  | 3±1 (14±7%)  | 1±1 (4±3%) | 5           | 30 |
| All | All   | 3560/4760 (75%) | 2839 (80%)    | 582 (16%)    | 139 (4%)   | 6           | 33 |

All 22 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     | 172 | SER  | 18             |
| 1   | A     | 189 | MET  | 16             |
| 1   | A     | 39  | ASP  | 15             |
| 1   | A     | 164 | ASP  | 15             |
| 2   | B     | 538 | CYS  | 12             |
| 1   | A     | 44  | GLY  | 11             |
| 1   | A     | 108 | LEU  | 10             |
| 1   | A     | 63  | GLY  | 8              |
| 1   | A     | 89  | HIS  | 8              |
| 2   | B     | 536 | ASP  | 6              |
| 1   | A     | 110 | SER  | 4              |
| 1   | A     | 131 | SER  | 3              |
| 1   | A     | 64  | ASP  | 3              |
| 1   | A     | 139 | LEU  | 2              |
| 1   | A     | 15  | GLU  | 1              |
| 1   | A     | 109 | ASN  | 1              |
| 1   | A     | 123 | ASP  | 1              |
| 1   | A     | 71  | PHE  | 1              |
| 1   | A     | 184 | ASP  | 1              |
| 1   | A     | 55  | PRO  | 1              |
| 2   | B     | 537 | ILE  | 1              |
| 1   | A     | 92  | PRO  | 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     | 142/176 (81%)   | 120±3 (84±2%) | 22±3 (16±2%) | 6           | 44 |
| 2   | B     | 21/39 (54%)     | 19±1 (88±4%)  | 3±1 (12±4%)  | 9           | 52 |
| All | All   | 3260/4300 (76%) | 2769 (85%)    | 491 (15%)    | 6           | 45 |

All 87 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     | 28  | ILE  | 20             |
| 1   | A     | 159 | THR  | 20             |
| 1   | A     | 139 | LEU  | 20             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 152 | LEU  | 20             |
| 1   | A     | 21  | THR  | 20             |
| 2   | B     | 518 | ILE  | 20             |
| 1   | A     | 135 | LEU  | 19             |
| 1   | A     | 148 | SER  | 19             |
| 1   | A     | 14  | LEU  | 17             |
| 1   | A     | 50  | ASP  | 16             |
| 1   | A     | 62  | LEU  | 16             |
| 1   | A     | 109 | ASN  | 15             |
| 2   | B     | 526 | PHE  | 15             |
| 1   | A     | 66  | ILE  | 14             |
| 1   | A     | 65  | ARG  | 13             |
| 1   | A     | 12  | GLU  | 12             |
| 1   | A     | 178 | LYS  | 10             |
| 1   | A     | 130 | ILE  | 10             |
| 1   | A     | 138 | VAL  | 8              |
| 1   | A     | 189 | MET  | 8              |
| 1   | A     | 108 | LEU  | 8              |
| 1   | A     | 35  | PHE  | 8              |
| 1   | A     | 84  | MET  | 7              |
| 1   | A     | 89  | HIS  | 7              |
| 1   | A     | 172 | SER  | 7              |
| 1   | A     | 54  | ILE  | 7              |
| 1   | A     | 162 | GLU  | 6              |
| 1   | A     | 140 | ARG  | 6              |
| 1   | A     | 53  | ARG  | 5              |
| 1   | A     | 142 | MET  | 5              |
| 1   | A     | 79  | ASN  | 5              |
| 1   | A     | 126 | LYS  | 5              |
| 1   | A     | 187 | GLN  | 4              |
| 1   | A     | 114 | LYS  | 4              |
| 1   | A     | 71  | PHE  | 4              |
| 1   | A     | 77  | GLN  | 4              |
| 1   | A     | 141 | MET  | 4              |
| 1   | A     | 78  | VAL  | 4              |
| 1   | A     | 60  | ASN  | 4              |
| 1   | A     | 16  | GLU  | 4              |
| 2   | B     | 521 | GLU  | 4              |
| 1   | A     | 19  | LYS  | 3              |
| 1   | A     | 137 | GLN  | 3              |
| 2   | B     | 535 | GLU  | 3              |
| 1   | A     | 113 | ASN  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 56  | GLU  | 3              |
| 1   | A     | 165 | GLN  | 3              |
| 1   | A     | 175 | GLU  | 2              |
| 1   | A     | 52  | GLN  | 2              |
| 2   | B     | 519 | ASN  | 2              |
| 1   | A     | 146 | ASN  | 2              |
| 1   | A     | 20  | GLU  | 2              |
| 2   | B     | 528 | ASP  | 2              |
| 1   | A     | 27  | GLN  | 2              |
| 1   | A     | 48  | ARG  | 2              |
| 2   | B     | 530 | LEU  | 2              |
| 1   | A     | 45  | THR  | 1              |
| 1   | A     | 166 | ASP  | 1              |
| 1   | A     | 125 | ASP  | 1              |
| 1   | A     | 30  | ARG  | 1              |
| 1   | A     | 68  | ASN  | 1              |
| 1   | A     | 111 | ARG  | 1              |
| 1   | A     | 75  | GLU  | 1              |
| 1   | A     | 36  | THR  | 1              |
| 1   | A     | 131 | SER  | 1              |
| 1   | A     | 188 | LYS  | 1              |
| 1   | A     | 123 | ASP  | 1              |
| 1   | A     | 120 | ARG  | 1              |
| 1   | A     | 158 | ARG  | 1              |
| 1   | A     | 191 | ILE  | 1              |
| 1   | A     | 17  | ILE  | 1              |
| 2   | B     | 523 | HIS  | 1              |
| 1   | A     | 184 | ASP  | 1              |
| 1   | A     | 47  | SER  | 1              |
| 1   | A     | 171 | ILE  | 1              |
| 1   | A     | 128 | GLU  | 1              |
| 1   | A     | 134 | GLU  | 1              |
| 1   | A     | 86  | THR  | 1              |
| 1   | A     | 34  | ARG  | 1              |
| 2   | B     | 527 | LEU  | 1              |
| 1   | A     | 127 | ASP  | 1              |
| 1   | A     | 91  | ARG  | 1              |
| 1   | A     | 31  | LEU  | 1              |
| 1   | A     | 64  | ASP  | 1              |
| 1   | A     | 81  | ARG  | 1              |
| 1   | A     | 157 | ASP  | 1              |
| 1   | A     | 129 | LYS  | 1              |

### 6.3.3 RNA [i](#)

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

### 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