



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:51 PM UTC

PDB ID : 6ID2 / pdb\_00006id2  
Title : Crystal structure of H7 hemagglutinin mutant H7-AVTL (P221T) from the influenza virus A/Anhui/1/2013 (H7N9)  
Authors : Gao, G.F.; Xu, Y.; Qi, J.X.  
Deposited on : 2018-09-08  
Resolution : 2.71 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

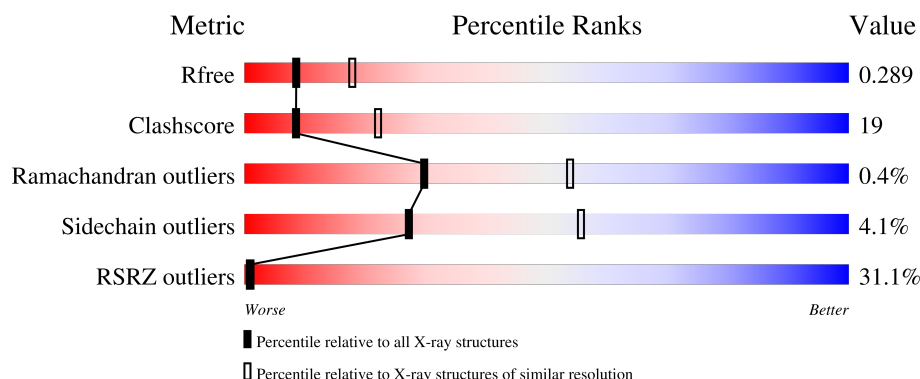
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3538 (2.70-2.70)                                      |
| Clashscore            | 190562                      | 3843 (2.70-2.70)                                      |
| Ramachandran outliers | 187476                      | 3778 (2.70-2.70)                                      |
| Sidechain outliers    | 187428                      | 3778 (2.70-2.70)                                      |
| RSRZ outliers         | 180081                      | 3538 (2.70-2.70)                                      |

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

| Mol | Chain | Length | Quality of chain                                                         |
|-----|-------|--------|--------------------------------------------------------------------------|
| 1   | A     | 321    | <div> <div>30%</div> <div>69%</div> <div>25%</div> <div>...</div> </div> |
| 1   | C     | 321    | <div> <div>18%</div> <div>68%</div> <div>29%</div> <div>..</div> </div>  |
| 1   | E     | 321    | <div> <div>16%</div> <div>74%</div> <div>22%</div> <div>...</div> </div> |
| 1   | G     | 321    | <div> <div>52%</div> <div>69%</div> <div>27%</div> <div>...</div> </div> |
| 1   | I     | 321    | <div> <div>39%</div> <div>73%</div> <div>24%</div> <div>..</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | K     | 321    |                  |
| 2   | B     | 177    |                  |
| 2   | D     | 177    |                  |
| 2   | F     | 177    |                  |
| 2   | H     | 177    |                  |
| 2   | J     | 177    |                  |
| 2   | L     | 177    |                  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22978 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin HA1 chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 314      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2395  | 1487 | 433 | 460 | 15 |         |         |       |
| 1   | C     | 314      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2395  | 1487 | 433 | 460 | 15 |         |         |       |
| 1   | E     | 314      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2395  | 1487 | 433 | 460 | 15 |         |         |       |
| 1   | G     | 316      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2412  | 1497 | 436 | 464 | 15 |         |         |       |
| 1   | I     | 316      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2412  | 1497 | 436 | 464 | 15 |         |         |       |
| 1   | K     | 316      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2412  | 1497 | 436 | 464 | 15 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 212     | THR      | PRO    | engineered mutation | UNP R4NN21 |
| C     | 212     | THR      | PRO    | engineered mutation | UNP R4NN21 |
| E     | 212     | THR      | PRO    | engineered mutation | UNP R4NN21 |
| G     | 212     | THR      | PRO    | engineered mutation | UNP R4NN21 |
| I     | 212     | THR      | PRO    | engineered mutation | UNP R4NN21 |
| K     | 212     | THR      | PRO    | engineered mutation | UNP R4NN21 |

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1328  | 817 | 231 | 273 | 7 |         |         |       |
| 2   | D     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1328  | 817 | 231 | 273 | 7 |         |         |       |
| 2   | F     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1328  | 817 | 231 | 273 | 7 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | H     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1328  | 817 | 231 | 273 | 7 |         |         |       |
| 2   | J     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1328  | 817 | 231 | 273 | 7 |         |         |       |
| 2   | L     | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1328  | 817 | 231 | 273 | 7 |         |         |       |

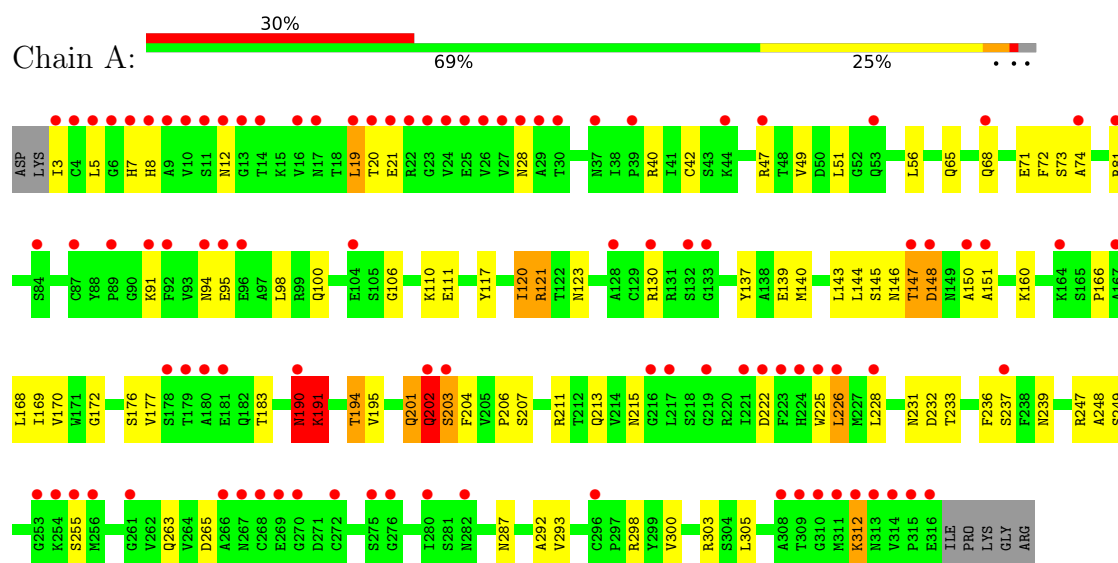
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 69       | Total | O  | 0       | 0       |
|     |       |          | 69    | 69 |         |         |
| 3   | B     | 28       | Total | O  | 0       | 0       |
|     |       |          | 28    | 28 |         |         |
| 3   | C     | 84       | Total | O  | 0       | 0       |
|     |       |          | 84    | 84 |         |         |
| 3   | D     | 29       | Total | O  | 0       | 0       |
|     |       |          | 29    | 29 |         |         |
| 3   | E     | 56       | Total | O  | 0       | 0       |
|     |       |          | 56    | 56 |         |         |
| 3   | F     | 34       | Total | O  | 0       | 0       |
|     |       |          | 34    | 34 |         |         |
| 3   | G     | 34       | Total | O  | 0       | 0       |
|     |       |          | 34    | 34 |         |         |
| 3   | H     | 68       | Total | O  | 0       | 0       |
|     |       |          | 68    | 68 |         |         |
| 3   | I     | 40       | Total | O  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 3   | J     | 58       | Total | O  | 0       | 0       |
|     |       |          | 58    | 58 |         |         |
| 3   | K     | 47       | Total | O  | 0       | 0       |
|     |       |          | 47    | 47 |         |         |
| 3   | L     | 42       | Total | O  | 0       | 0       |
|     |       |          | 42    | 42 |         |         |

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

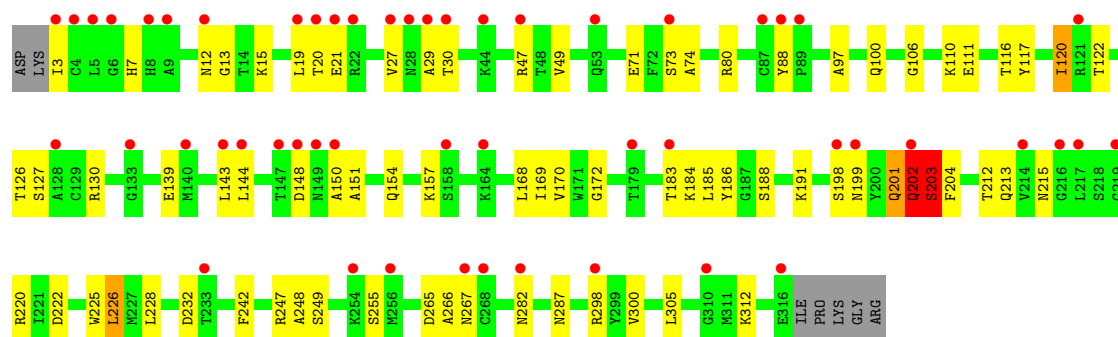
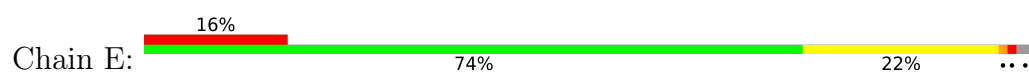
#### • Molecule 1: Hemagglutinin HA1 chain



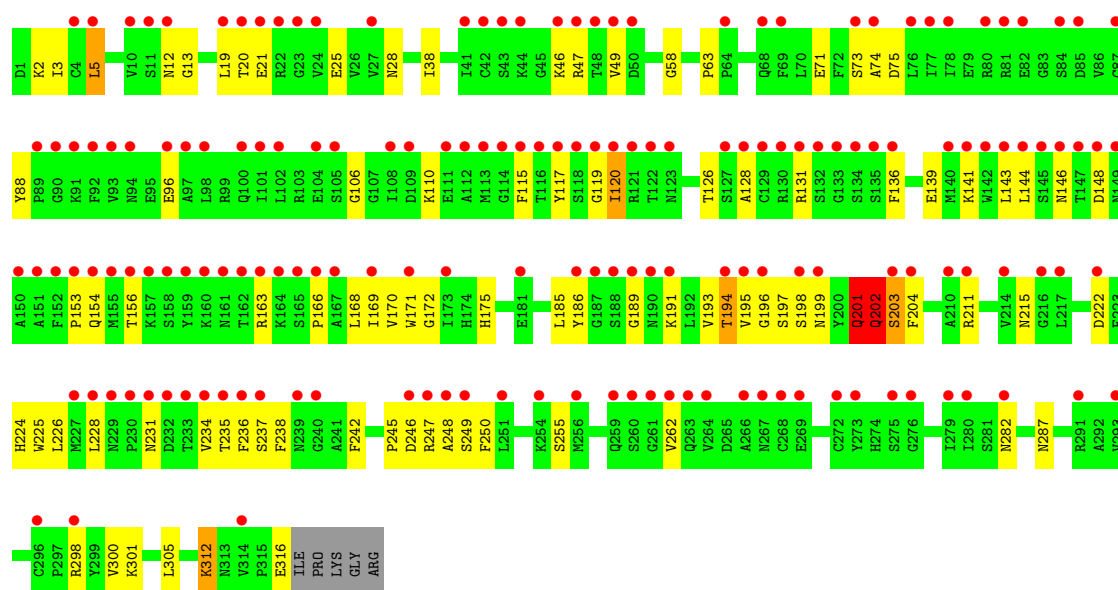
#### • Molecule 1: Hemagglutinin HA1 chain



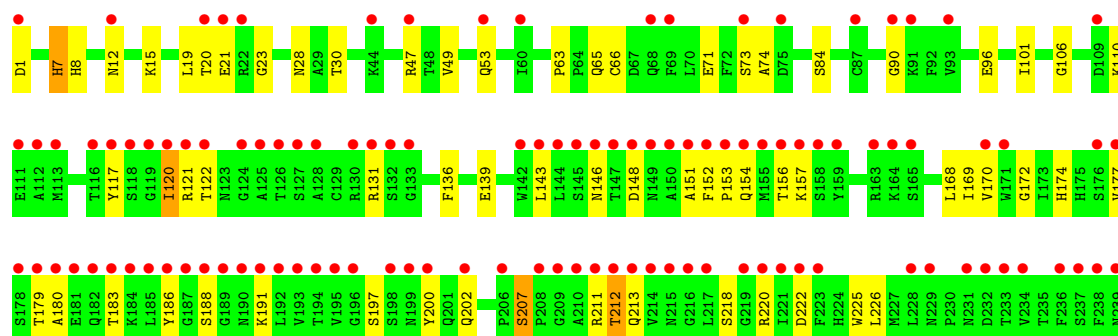
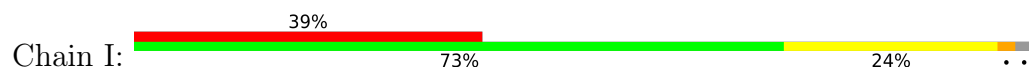
#### • Molecule 1: Hemagglutinin HA1 chain



• Molecule 1: Hemagglutinin HA1 chain

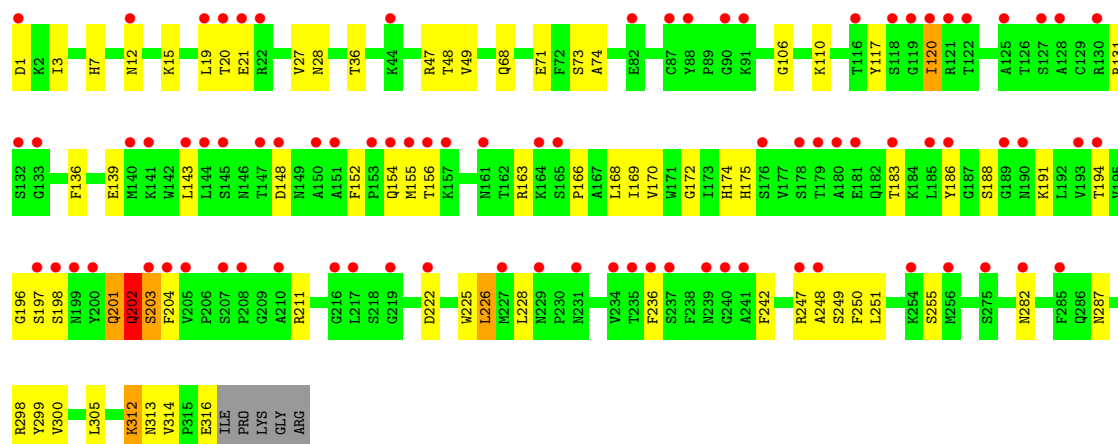
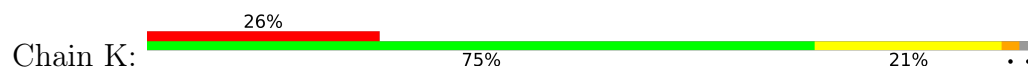


• Molecule 1: Hemagglutinin HA1 chain

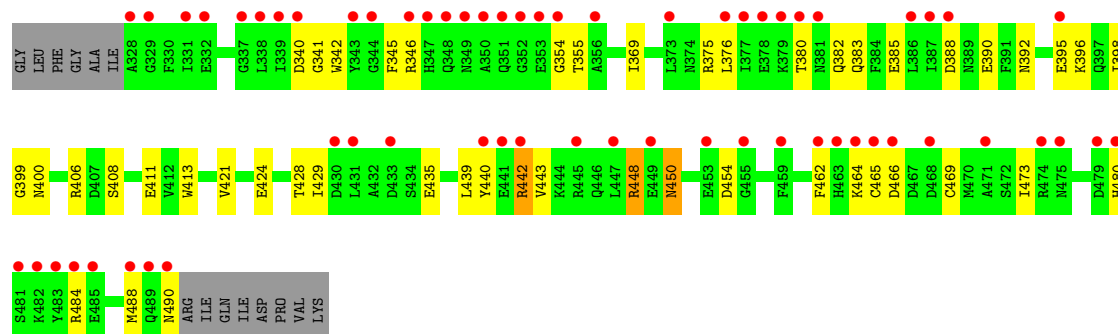




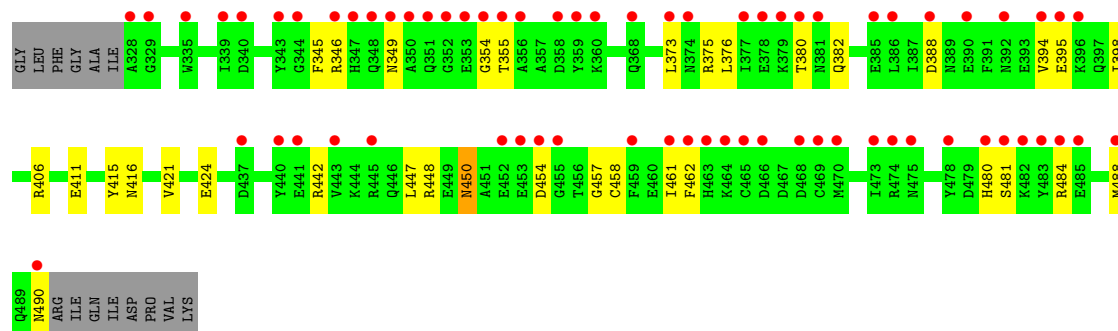
• Molecule 1: Hemagglutinin HA1 chain



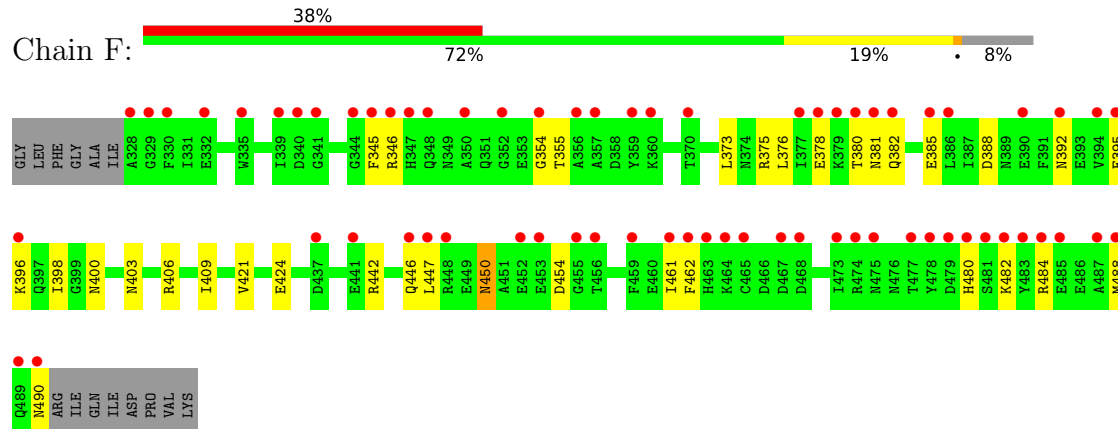
• Molecule 2: Hemagglutinin HA2 chain



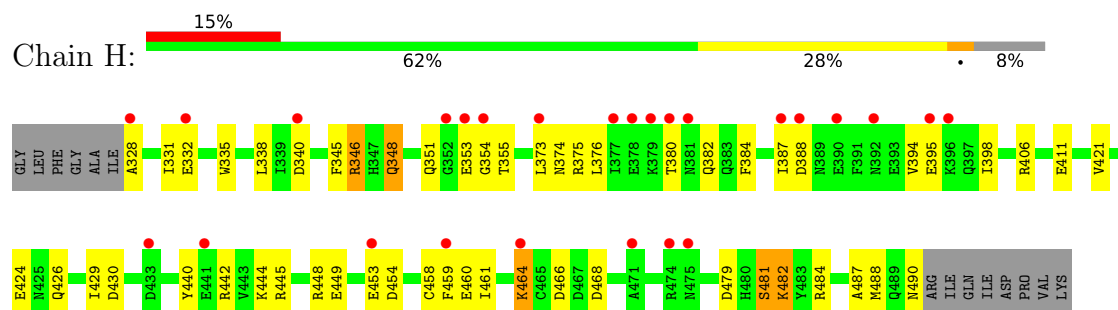
• Molecule 2: Hemagglutinin HA2 chain



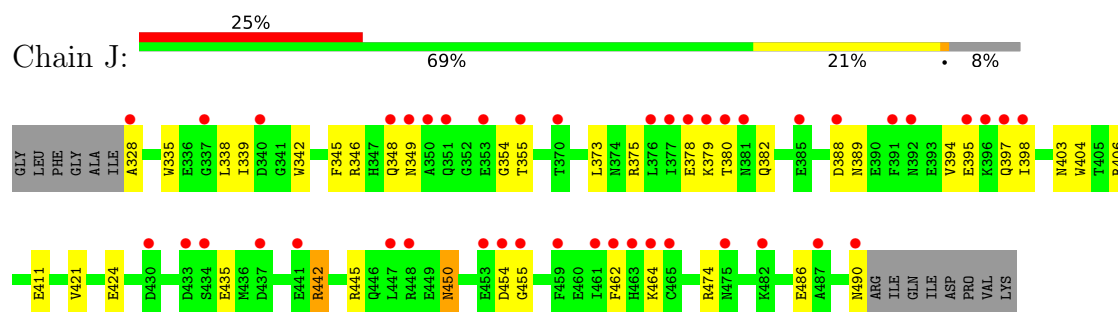
- Molecule 2: Hemagglutinin HA2 chain



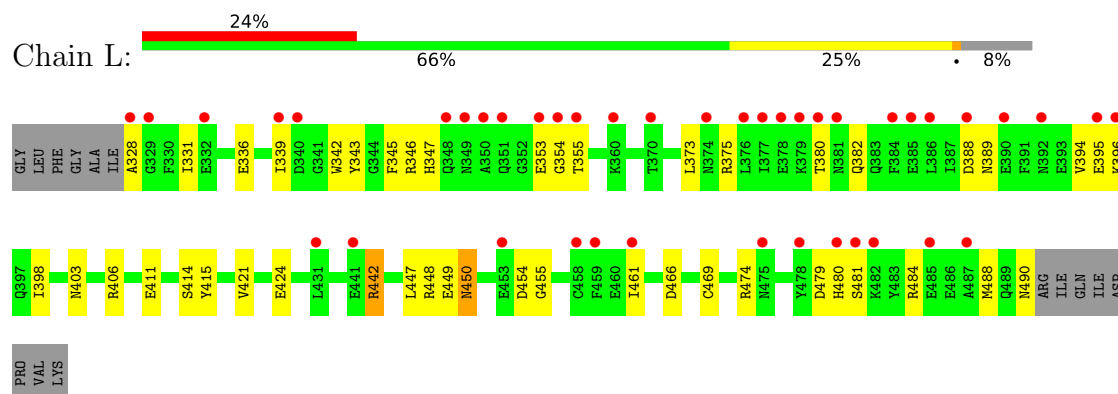
- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



## 4 Data and refinement statistics

| Property                                                                | Value                                                          | Source           |
|-------------------------------------------------------------------------|----------------------------------------------------------------|------------------|
| Space group                                                             | P 3                                                            | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 165.19Å 165.19Å 191.25Å<br>90.00° 90.00° 120.00°               | Depositor        |
| Resolution (Å)                                                          | 47.69 – 2.71<br>47.69 – 2.71                                   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 90.2 (47.69-2.71)<br>90.2 (47.69-2.71)                         | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                                | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.60 (at 2.69Å)                                                | Xtriage          |
| Refinement program                                                      | PHENIX (1.11.1_2575: ???)                                      | Depositor        |
| R, $R_{free}$                                                           | 0.264 , 0.290<br>0.264 , 0.289                                 | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 7125 reflections (4.47%)                                       | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 40.6                                                           | Xtriage          |
| Anisotropy                                                              | 0.084                                                          | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 50.0                                                    | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$    | Xtriage          |
| Estimated twinning fraction                                             | 0.000 for -h,-k,l<br>0.020 for h,-h-k,-l<br>0.012 for -k,-h,-l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.88                                                           | EDS              |
| Total number of atoms                                                   | 22978                                                          | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 58.0                                                           | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7316e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.12         | 0/2440         | 0.73        | 7/3298 (0.2%)   |
| 1   | C     | 0.10         | 0/2440         | 0.31        | 0/3298          |
| 1   | E     | 0.41         | 5/2440 (0.2%)  | 0.38        | 2/3298 (0.1%)   |
| 1   | G     | 0.19         | 0/2457         | 0.41        | 2/3320 (0.1%)   |
| 1   | I     | 0.08         | 0/2457         | 0.27        | 0/3320          |
| 1   | K     | 0.29         | 1/2457 (0.0%)  | 0.42        | 3/3320 (0.1%)   |
| 2   | B     | 0.08         | 0/1351         | 0.23        | 0/1821          |
| 2   | D     | 0.08         | 0/1351         | 0.23        | 0/1821          |
| 2   | F     | 0.08         | 0/1351         | 0.22        | 0/1821          |
| 2   | H     | 0.09         | 0/1351         | 0.25        | 0/1821          |
| 2   | J     | 0.09         | 0/1351         | 0.23        | 0/1821          |
| 2   | L     | 0.08         | 0/1351         | 0.22        | 0/1821          |
| All | All   | 0.19         | 6/22797 (0.0%) | 0.38        | 14/30780 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |
| 1   | E     | 0                   | 1                   |
| 1   | G     | 0                   | 1                   |
| 1   | K     | 0                   | 1                   |
| All | All   | 0                   | 5                   |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | E     | 202 | GLN  | CA-C  | -9.38 | 1.40        | 1.52     |
| 1   | E     | 202 | GLN  | C-O   | -8.08 | 1.13        | 1.24     |
| 1   | E     | 204 | PHE  | C-O   | -6.44 | 1.16        | 1.23     |
| 1   | E     | 203 | SER  | C-O   | -6.26 | 1.16        | 1.24     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | E     | 201 | GLN  | C-O   | -5.54 | 1.17        | 1.23     |
| 1   | K     | 204 | PHE  | CA-C  | -5.24 | 1.46        | 1.52     |

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 191 | LYS  | N-CA-C  | 25.81  | 148.47      | 111.56   |
| 1   | A     | 191 | LYS  | CB-CA-C | -19.32 | 87.10       | 111.82   |
| 1   | E     | 202 | GLN  | CB-CA-C | -10.42 | 89.68       | 110.42   |
| 1   | G     | 201 | GLN  | CB-CA-C | 9.61   | 131.10      | 110.45   |
| 1   | K     | 201 | GLN  | CB-CA-C | 8.41   | 127.85      | 109.94   |
| 1   | A     | 191 | LYS  | CA-C-N  | 8.30   | 135.52      | 122.74   |
| 1   | A     | 191 | LYS  | C-N-CA  | 8.30   | 135.52      | 122.74   |
| 1   | K     | 201 | GLN  | N-CA-C  | -6.99  | 98.02       | 108.99   |
| 1   | A     | 201 | GLN  | CB-CA-C | -6.54  | 97.39       | 110.42   |
| 1   | A     | 190 | ASN  | CB-CA-C | -6.35  | 99.62       | 110.22   |
| 1   | A     | 190 | ASN  | N-CA-C  | 6.30   | 118.98      | 108.96   |
| 1   | K     | 202 | GLN  | CB-CA-C | -6.21  | 98.07       | 110.42   |
| 1   | G     | 202 | GLN  | CB-CA-C | -6.19  | 98.11       | 110.42   |
| 1   | E     | 202 | GLN  | CA-C-O  | -5.81  | 112.20      | 120.51   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 190 | ASN  | Peptide |
| 1   | A     | 202 | GLN  | Peptide |
| 1   | E     | 202 | GLN  | Peptide |
| 1   | G     | 202 | GLN  | Peptide |
| 1   | K     | 202 | GLN  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2395  | 0        | 2354     | 111     | 0            |
| 1   | C     | 2395  | 0        | 2354     | 118     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | E     | 2395  | 0        | 2354     | 73      | 1            |
| 1   | G     | 2412  | 0        | 2374     | 108     | 0            |
| 1   | I     | 2412  | 0        | 2374     | 88      | 0            |
| 1   | K     | 2412  | 0        | 2374     | 76      | 0            |
| 2   | B     | 1328  | 0        | 1223     | 54      | 0            |
| 2   | D     | 1328  | 0        | 1223     | 33      | 0            |
| 2   | F     | 1328  | 0        | 1223     | 43      | 0            |
| 2   | H     | 1328  | 0        | 1223     | 69      | 0            |
| 2   | J     | 1328  | 0        | 1223     | 47      | 1            |
| 2   | L     | 1328  | 0        | 1223     | 57      | 0            |
| 3   | A     | 69    | 0        | 0        | 57      | 0            |
| 3   | B     | 28    | 0        | 0        | 29      | 0            |
| 3   | C     | 84    | 0        | 0        | 79      | 1            |
| 3   | D     | 29    | 0        | 0        | 23      | 0            |
| 3   | E     | 56    | 0        | 0        | 37      | 0            |
| 3   | F     | 34    | 0        | 0        | 28      | 0            |
| 3   | G     | 34    | 0        | 0        | 52      | 0            |
| 3   | H     | 68    | 0        | 0        | 50      | 0            |
| 3   | I     | 40    | 0        | 0        | 59      | 0            |
| 3   | J     | 58    | 0        | 0        | 32      | 0            |
| 3   | K     | 47    | 0        | 0        | 40      | 1            |
| 3   | L     | 42    | 0        | 0        | 36      | 0            |
| All | All   | 22978 | 0        | 21522    | 833     | 2            |

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 19.

All (833) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|---------------|--------------------------|-------------------|
| 1:K:154:GLN:HG3 | 3:K:404:HOH:O | 1.19                     | 1.33              |
| 1:C:178:SER:HA  | 3:C:404:HOH:O | 1.27                     | 1.31              |
| 1:C:30:THR:HG23 | 3:C:402:HOH:O | 1.20                     | 1.30              |
| 1:A:293:VAL:HA  | 3:A:406:HOH:O | 1.30                     | 1.27              |
| 1:C:121:ARG:HA  | 3:C:407:HOH:O | 1.27                     | 1.26              |
| 1:K:21:GLU:HA   | 3:K:403:HOH:O | 1.26                     | 1.26              |
| 2:L:353:GLU:HB2 | 3:L:507:HOH:O | 1.09                     | 1.25              |
| 1:K:68:GLN:CG   | 3:K:401:HOH:O | 1.88                     | 1.21              |
| 1:I:7:HIS:CE1   | 3:I:403:HOH:O | 1.89                     | 1.20              |
| 2:D:447:LEU:C   | 3:D:501:HOH:O | 1.85                     | 1.19              |
| 1:C:25:GLU:HB2  | 3:C:417:HOH:O | 1.38                     | 1.19              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:C:30:THR:C     | 3:C:402:HOH:O   | 1.86                     | 1.16              |
| 1:C:213:GLN:C    | 3:C:403:HOH:O   | 1.87                     | 1.15              |
| 2:H:445:ARG:HD2  | 3:H:506:HOH:O   | 1.46                     | 1.15              |
| 1:K:197:SER:C    | 3:K:402:HOH:O   | 1.89                     | 1.15              |
| 1:E:202:GLN:O    | 1:E:202:GLN:HG3 | 1.37                     | 1.13              |
| 2:H:346:ARG:NH1  | 2:H:353:GLU:OE2 | 1.81                     | 1.13              |
| 1:C:177:VAL:C    | 3:C:401:HOH:O   | 1.89                     | 1.13              |
| 2:D:448:ARG:N    | 3:D:501:HOH:O   | 1.80                     | 1.13              |
| 1:G:128:ALA:HB1  | 3:G:413:HOH:O   | 1.47                     | 1.13              |
| 1:C:121:ARG:CA   | 3:C:407:HOH:O   | 1.84                     | 1.12              |
| 2:F:447:LEU:HA   | 3:F:506:HOH:O   | 1.49                     | 1.12              |
| 2:F:381:ASN:CA   | 3:F:503:HOH:O   | 1.95                     | 1.11              |
| 2:F:381:ASN:CB   | 3:F:503:HOH:O   | 1.97                     | 1.11              |
| 1:A:303:ARG:NH2  | 3:A:402:HOH:O   | 1.82                     | 1.11              |
| 2:J:328:ALA:N    | 3:J:501:HOH:O   | 1.81                     | 1.11              |
| 1:K:68:GLN:HG3   | 3:K:401:HOH:O   | 1.47                     | 1.11              |
| 2:L:469:CYS:SG   | 3:L:536:HOH:O   | 2.05                     | 1.11              |
| 1:I:8:HIS:NE2    | 3:I:402:HOH:O   | 1.83                     | 1.10              |
| 2:F:447:LEU:HD23 | 3:F:506:HOH:O   | 1.49                     | 1.10              |
| 1:A:68:GLN:CD    | 3:A:403:HOH:O   | 1.94                     | 1.10              |
| 2:D:380:THR:C    | 3:D:505:HOH:O   | 1.94                     | 1.10              |
| 1:K:313:ASN:HA   | 3:K:408:HOH:O   | 1.51                     | 1.10              |
| 1:A:49:VAL:HB    | 3:A:409:HOH:O   | 1.50                     | 1.10              |
| 2:B:346:ARG:NH1  | 3:B:502:HOH:O   | 1.84                     | 1.09              |
| 2:J:349:ASN:CA   | 3:J:502:HOH:O   | 2.00                     | 1.09              |
| 2:B:466:ASP:HB2  | 3:B:501:HOH:O   | 1.52                     | 1.09              |
| 1:E:185:LEU:HA   | 3:E:408:HOH:O   | 1.50                     | 1.09              |
| 1:G:262:VAL:CG2  | 3:G:402:HOH:O   | 1.99                     | 1.08              |
| 2:J:349:ASN:N    | 3:J:502:HOH:O   | 1.84                     | 1.08              |
| 2:L:328:ALA:N    | 3:L:502:HOH:O   | 1.82                     | 1.08              |
| 1:A:201:GLN:O    | 1:A:201:GLN:HG2 | 1.40                     | 1.08              |
| 2:B:466:ASP:CB   | 3:B:501:HOH:O   | 1.99                     | 1.08              |
| 2:D:349:ASN:C    | 3:D:503:HOH:O   | 1.96                     | 1.08              |
| 1:K:21:GLU:CD    | 3:K:405:HOH:O   | 1.94                     | 1.08              |
| 1:K:198:SER:N    | 3:K:402:HOH:O   | 1.87                     | 1.08              |
| 2:L:415:TYR:N    | 3:L:504:HOH:O   | 1.86                     | 1.07              |
| 1:E:198:SER:CA   | 3:E:401:HOH:O   | 2.00                     | 1.07              |
| 2:L:414:SER:C    | 3:L:504:HOH:O   | 1.94                     | 1.07              |
| 1:C:173:ILE:N    | 3:C:410:HOH:O   | 1.88                     | 1.06              |
| 1:G:262:VAL:C    | 3:G:402:HOH:O   | 1.97                     | 1.06              |
| 2:H:487:ALA:N    | 3:H:502:HOH:O   | 1.85                     | 1.06              |

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| Atom-1           | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|----------------|--------------------------|-------------------|
| 1:I:7:HIS:CG     | 3:I:403:HOH:O  | 2.08                     | 1.06              |
| 1:G:47:ARG:N     | 3:G:406:HOH:O  | 1.88                     | 1.06              |
| 1:E:198:SER:HA   | 3:E:401:HOH:O  | 1.55                     | 1.06              |
| 2:J:404:TRP:NE1  | 3:J:504:HOH:O  | 1.87                     | 1.06              |
| 1:K:68:GLN:NE2   | 3:K:401:HOH:O  | 1.84                     | 1.06              |
| 1:K:155:MET:N    | 3:K:404:HOH:O  | 1.88                     | 1.06              |
| 2:L:484:ARG:NH2  | 3:L:505:HOH:O  | 1.87                     | 1.06              |
| 2:L:343:TYR:CD2  | 3:L:509:HOH:O  | 2.09                     | 1.05              |
| 2:F:381:ASN:HB3  | 3:F:503:HOH:O  | 1.53                     | 1.05              |
| 2:L:343:TYR:CG   | 3:L:509:HOH:O  | 2.08                     | 1.05              |
| 1:E:150:ALA:C    | 3:E:404:HOH:O  | 1.98                     | 1.05              |
| 1:I:153:PRO:C    | 3:I:404:HOH:O  | 1.98                     | 1.05              |
| 2:L:484:ARG:NH1  | 3:L:508:HOH:O  | 1.89                     | 1.05              |
| 2:F:381:ASN:N    | 3:F:503:HOH:O  | 1.90                     | 1.04              |
| 2:F:482:LYS:CB   | 3:F:502:HOH:O  | 2.02                     | 1.04              |
| 2:H:375:ARG:NH2  | 3:H:503:HOH:O  | 1.87                     | 1.03              |
| 1:C:220:ARG:NE   | 3:C:412:HOH:O  | 1.90                     | 1.03              |
| 1:E:202:GLN:O    | 1:E:202:GLN:CG | 1.94                     | 1.03              |
| 1:G:312:LYS:NZ   | 3:G:405:HOH:O  | 1.87                     | 1.03              |
| 2:L:415:TYR:CA   | 3:L:504:HOH:O  | 2.06                     | 1.03              |
| 1:K:203:SER:N    | 3:K:407:HOH:O  | 1.90                     | 1.02              |
| 2:L:442:ARG:CZ   | 3:L:511:HOH:O  | 2.05                     | 1.02              |
| 1:G:46:LYS:CA    | 3:G:406:HOH:O  | 2.07                     | 1.02              |
| 1:C:122:THR:N    | 3:C:407:HOH:O  | 1.84                     | 1.02              |
| 2:F:406:ARG:NH2  | 3:F:504:HOH:O  | 1.92                     | 1.01              |
| 1:C:30:THR:CG2   | 3:C:402:HOH:O  | 1.84                     | 1.01              |
| 1:A:81:ARG:N     | 3:A:407:HOH:O  | 1.90                     | 1.01              |
| 1:A:98:LEU:HB3   | 3:A:410:HOH:O  | 1.61                     | 1.01              |
| 1:I:7:HIS:ND1    | 3:I:403:HOH:O  | 1.84                     | 1.00              |
| 1:I:8:HIS:CD2    | 3:I:402:HOH:O  | 2.11                     | 1.00              |
| 2:B:466:ASP:OD2  | 3:B:501:HOH:O  | 1.80                     | 1.00              |
| 2:D:380:THR:HG22 | 3:D:505:HOH:O  | 1.60                     | 0.99              |
| 2:H:338:LEU:HD12 | 3:H:512:HOH:O  | 1.60                     | 0.99              |
| 2:L:343:TYR:CA   | 3:L:509:HOH:O  | 2.09                     | 0.99              |
| 2:F:406:ARG:NE   | 3:F:504:HOH:O  | 1.95                     | 0.99              |
| 1:A:98:LEU:CB    | 3:A:410:HOH:O  | 2.10                     | 0.99              |
| 2:L:415:TYR:HA   | 3:L:504:HOH:O  | 1.58                     | 0.99              |
| 1:G:312:LYS:CE   | 3:G:405:HOH:O  | 2.11                     | 0.98              |
| 2:J:389:ASN:N    | 3:J:505:HOH:O  | 1.92                     | 0.98              |
| 1:G:316:GLU:CD   | 3:G:407:HOH:O  | 2.06                     | 0.98              |
| 1:A:49:VAL:CA    | 3:A:409:HOH:O  | 2.10                     | 0.98              |

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| Atom-1          | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|---------------|--------------------------|-------------------|
| 1:C:176:SER:O   | 3:C:401:HOH:O | 1.81                     | 0.98              |
| 1:A:49:VAL:CB   | 3:A:409:HOH:O | 2.09                     | 0.97              |
| 2:L:490:ASN:O   | 3:L:501:HOH:O | 1.81                     | 0.97              |
| 1:A:71:GLU:OE1  | 3:A:401:HOH:O | 1.81                     | 0.97              |
| 1:G:154:GLN:O   | 3:G:403:HOH:O | 1.82                     | 0.97              |
| 2:H:351:GLN:HB2 | 3:H:508:HOH:O | 1.64                     | 0.96              |
| 1:C:58:GLY:N    | 3:C:414:HOH:O | 1.97                     | 0.96              |
| 1:K:154:GLN:C   | 3:K:404:HOH:O | 2.09                     | 0.96              |
| 1:A:121:ARG:NH1 | 1:A:145:SER:O | 1.98                     | 0.96              |
| 1:I:23:GLY:O    | 3:I:401:HOH:O | 1.82                     | 0.96              |
| 1:C:209:GLY:O   | 3:C:404:HOH:O | 1.83                     | 0.96              |
| 2:H:482:LYS:O   | 3:H:501:HOH:O | 1.83                     | 0.96              |
| 1:E:30:THR:HA   | 3:E:406:HOH:O | 1.66                     | 0.96              |
| 2:H:484:ARG:O   | 3:H:502:HOH:O | 1.84                     | 0.96              |
| 2:J:474:ARG:O   | 3:J:503:HOH:O | 1.84                     | 0.96              |
| 1:C:71:GLU:OE1  | 3:C:405:HOH:O | 1.83                     | 0.95              |
| 2:J:349:ASN:HB3 | 3:J:502:HOH:O | 1.65                     | 0.95              |
| 1:A:98:LEU:N    | 3:A:410:HOH:O | 1.92                     | 0.95              |
| 1:G:58:GLY:HA3  | 3:G:433:HOH:O | 1.64                     | 0.95              |
| 1:A:111:GLU:OE1 | 3:A:404:HOH:O | 1.84                     | 0.95              |
| 1:E:265:ASP:OD1 | 3:E:402:HOH:O | 1.84                     | 0.95              |
| 1:E:185:LEU:CA  | 3:E:408:HOH:O | 2.09                     | 0.95              |
| 2:J:348:GLN:HG3 | 3:J:514:HOH:O | 1.65                     | 0.94              |
| 1:E:198:SER:O   | 3:E:401:HOH:O | 1.83                     | 0.94              |
| 2:L:343:TYR:HA  | 3:L:509:HOH:O | 1.68                     | 0.94              |
| 1:G:262:VAL:CA  | 3:G:402:HOH:O | 2.13                     | 0.94              |
| 2:J:404:TRP:CE2 | 3:J:504:HOH:O | 2.16                     | 0.94              |
| 1:A:94:ASN:ND2  | 3:A:414:HOH:O | 1.99                     | 0.94              |
| 1:G:262:VAL:O   | 3:G:402:HOH:O | 1.81                     | 0.94              |
| 1:E:265:ASP:CG  | 3:E:402:HOH:O | 2.09                     | 0.94              |
| 1:I:151:ALA:CA  | 3:I:411:HOH:O | 2.15                     | 0.94              |
| 2:F:378:GLU:O   | 3:F:501:HOH:O | 1.84                     | 0.93              |
| 1:G:316:GLU:O   | 3:G:404:HOH:O | 1.86                     | 0.93              |
| 2:D:490:ASN:O   | 3:D:502:HOH:O | 1.86                     | 0.93              |
| 1:I:316:GLU:O   | 3:I:405:HOH:O | 1.87                     | 0.93              |
| 1:C:178:SER:CA  | 3:C:404:HOH:O | 1.95                     | 0.93              |
| 1:I:152:PHE:O   | 3:I:404:HOH:O | 1.86                     | 0.92              |
| 2:F:482:LYS:C   | 3:F:502:HOH:O | 2.11                     | 0.92              |
| 2:J:348:GLN:C   | 3:J:502:HOH:O | 2.10                     | 0.92              |
| 1:C:213:GLN:N   | 3:C:403:HOH:O | 2.03                     | 0.92              |
| 1:A:293:VAL:CA  | 3:A:406:HOH:O | 1.91                     | 0.92              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:F:403:ASN:ND2 | 3:F:505:HOH:O   | 1.98                     | 0.92              |
| 1:G:231:ASN:ND2 | 3:G:409:HOH:O   | 2.00                     | 0.91              |
| 2:F:482:LYS:O   | 3:F:502:HOH:O   | 1.89                     | 0.91              |
| 1:I:8:HIS:CE1   | 3:I:402:HOH:O   | 2.19                     | 0.91              |
| 2:J:445:ARG:HD2 | 3:J:527:HOH:O   | 1.71                     | 0.91              |
| 1:K:20:THR:O    | 3:K:403:HOH:O   | 1.88                     | 0.91              |
| 2:H:351:GLN:CB  | 3:H:508:HOH:O   | 2.16                     | 0.91              |
| 1:I:157:LYS:N   | 3:I:409:HOH:O   | 2.04                     | 0.91              |
| 2:L:480:HIS:O   | 3:L:506:HOH:O   | 1.87                     | 0.91              |
| 2:D:349:ASN:O   | 3:D:503:HOH:O   | 1.87                     | 0.90              |
| 1:C:250:PHE:O   | 3:C:409:HOH:O   | 1.87                     | 0.90              |
| 2:J:464:LYS:CB  | 3:J:509:HOH:O   | 2.17                     | 0.90              |
| 1:I:121:ARG:C   | 3:I:413:HOH:O   | 2.14                     | 0.90              |
| 1:E:111:GLU:OE1 | 3:E:403:HOH:O   | 1.87                     | 0.90              |
| 1:G:46:LYS:HA   | 3:G:406:HOH:O   | 1.71                     | 0.90              |
| 1:G:146:ASN:ND2 | 3:G:411:HOH:O   | 2.04                     | 0.90              |
| 1:A:110:LYS:NZ  | 1:A:139:GLU:OE2 | 2.04                     | 0.90              |
| 1:C:250:PHE:N   | 3:C:409:HOH:O   | 1.97                     | 0.90              |
| 1:E:202:GLN:HA  | 1:E:203:SER:HB2 | 1.53                     | 0.90              |
| 1:C:203:SER:N   | 3:C:408:HOH:O   | 1.85                     | 0.89              |
| 1:G:312:LYS:HE2 | 3:G:405:HOH:O   | 1.68                     | 0.89              |
| 1:A:292:ALA:O   | 3:A:406:HOH:O   | 1.89                     | 0.89              |
| 1:C:30:THR:O    | 3:C:402:HOH:O   | 1.82                     | 0.89              |
| 1:K:21:GLU:OE2  | 3:K:405:HOH:O   | 1.89                     | 0.89              |
| 2:L:353:GLU:OE1 | 3:L:507:HOH:O   | 1.87                     | 0.89              |
| 2:H:382:GLN:C   | 3:H:507:HOH:O   | 2.16                     | 0.89              |
| 2:L:403:ASN:ND2 | 3:L:503:HOH:O   | 1.86                     | 0.89              |
| 2:D:457:GLY:O   | 3:D:504:HOH:O   | 1.89                     | 0.89              |
| 2:L:442:ARG:NH2 | 3:L:511:HOH:O   | 2.05                     | 0.89              |
| 1:K:314:VAL:N   | 3:K:408:HOH:O   | 1.92                     | 0.89              |
| 1:I:152:PHE:N   | 3:I:411:HOH:O   | 2.06                     | 0.88              |
| 2:H:375:ARG:NE  | 3:H:503:HOH:O   | 2.05                     | 0.88              |
| 2:B:392:ASN:OD1 | 3:B:505:HOH:O   | 1.91                     | 0.88              |
| 2:B:435:GLU:O   | 3:B:504:HOH:O   | 1.90                     | 0.88              |
| 2:B:465:CYS:HA  | 3:B:503:HOH:O   | 1.73                     | 0.88              |
| 2:B:480:HIS:O   | 3:B:506:HOH:O   | 1.92                     | 0.88              |
| 1:I:7:HIS:CD2   | 3:I:403:HOH:O   | 2.24                     | 0.88              |
| 1:C:177:VAL:O   | 3:C:404:HOH:O   | 1.89                     | 0.88              |
| 2:L:342:TRP:O   | 3:L:509:HOH:O   | 1.89                     | 0.88              |
| 1:C:213:GLN:O   | 3:C:403:HOH:O   | 1.83                     | 0.88              |
| 1:A:49:VAL:O    | 3:A:409:HOH:O   | 1.91                     | 0.88              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:B:464:LYS:O   | 3:B:503:HOH:O   | 1.90                     | 0.88              |
| 1:K:313:ASN:CA  | 3:K:408:HOH:O   | 2.12                     | 0.88              |
| 2:J:349:ASN:CB  | 3:J:502:HOH:O   | 2.16                     | 0.87              |
| 2:J:378:GLU:O   | 3:J:506:HOH:O   | 1.93                     | 0.87              |
| 1:G:201:GLN:O   | 1:G:202:GLN:HG2 | 1.74                     | 0.87              |
| 1:E:185:LEU:C   | 3:E:408:HOH:O   | 2.16                     | 0.87              |
| 1:A:201:GLN:O   | 1:A:201:GLN:CG  | 2.20                     | 0.86              |
| 1:C:202:GLN:N   | 3:C:408:HOH:O   | 2.02                     | 0.86              |
| 2:B:466:ASP:CG  | 3:B:501:HOH:O   | 2.11                     | 0.86              |
| 1:C:162:THR:OG1 | 3:C:413:HOH:O   | 1.92                     | 0.85              |
| 1:G:201:GLN:O   | 1:G:202:GLN:CG  | 2.24                     | 0.85              |
| 2:H:430:ASP:OD1 | 3:H:504:HOH:O   | 1.93                     | 0.85              |
| 1:G:262:VAL:N   | 3:G:402:HOH:O   | 2.10                     | 0.85              |
| 1:E:150:ALA:O   | 3:E:404:HOH:O   | 1.91                     | 0.85              |
| 1:C:55:GLY:O    | 3:C:414:HOH:O   | 1.94                     | 0.84              |
| 1:C:71:GLU:CD   | 3:C:405:HOH:O   | 2.18                     | 0.84              |
| 1:G:316:GLU:OE2 | 3:G:407:HOH:O   | 1.95                     | 0.84              |
| 2:J:464:LYS:CA  | 3:J:509:HOH:O   | 2.25                     | 0.84              |
| 1:I:122:THR:CA  | 3:I:413:HOH:O   | 2.26                     | 0.84              |
| 1:A:151:ALA:O   | 3:A:411:HOH:O   | 1.96                     | 0.83              |
| 1:A:65:GLN:O    | 3:A:412:HOH:O   | 1.96                     | 0.83              |
| 2:H:444:LYS:O   | 3:H:505:HOH:O   | 1.95                     | 0.83              |
| 1:E:143:LEU:O   | 3:E:405:HOH:O   | 1.96                     | 0.83              |
| 1:I:84:SER:HB3  | 3:I:414:HOH:O   | 1.79                     | 0.83              |
| 2:J:380:THR:N   | 3:J:511:HOH:O   | 2.10                     | 0.83              |
| 1:K:202:GLN:C   | 3:K:407:HOH:O   | 2.20                     | 0.83              |
| 1:A:263:GLN:HB2 | 3:A:418:HOH:O   | 1.79                     | 0.83              |
| 2:B:340:ASP:O   | 3:B:507:HOH:O   | 1.95                     | 0.82              |
| 1:E:29:ALA:O    | 3:E:406:HOH:O   | 1.97                     | 0.82              |
| 2:J:464:LYS:HB2 | 3:J:509:HOH:O   | 1.78                     | 0.82              |
| 1:E:265:ASP:C   | 3:E:402:HOH:O   | 2.22                     | 0.82              |
| 1:C:250:PHE:CA  | 3:C:409:HOH:O   | 2.28                     | 0.82              |
| 2:L:484:ARG:HG2 | 3:L:510:HOH:O   | 1.79                     | 0.82              |
| 2:H:445:ARG:NH1 | 3:H:506:HOH:O   | 1.96                     | 0.82              |
| 2:L:342:TRP:C   | 3:L:509:HOH:O   | 2.22                     | 0.82              |
| 2:H:395:GLU:CG  | 3:H:511:HOH:O   | 2.28                     | 0.82              |
| 1:I:122:THR:N   | 3:I:413:HOH:O   | 2.12                     | 0.81              |
| 1:C:56:LEU:C    | 3:C:414:HOH:O   | 2.22                     | 0.81              |
| 1:K:251:LEU:N   | 3:K:410:HOH:O   | 2.05                     | 0.81              |
| 1:C:30:THR:OG1  | 3:C:418:HOH:O   | 1.99                     | 0.81              |
| 1:K:312:LYS:O   | 3:K:408:HOH:O   | 1.97                     | 0.81              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:F:480:HIS:C    | 3:F:508:HOH:O   | 2.24                     | 0.81              |
| 1:C:188:SER:O    | 3:C:419:HOH:O   | 1.99                     | 0.81              |
| 2:H:382:GLN:O    | 3:H:507:HOH:O   | 1.98                     | 0.81              |
| 3:G:414:HOH:O    | 2:H:464:LYS:HG3 | 1.80                     | 0.80              |
| 2:H:375:ARG:CZ   | 3:H:503:HOH:O   | 2.20                     | 0.80              |
| 1:C:25:GLU:OE1   | 3:C:417:HOH:O   | 1.99                     | 0.80              |
| 1:K:27:VAL:O     | 3:K:409:HOH:O   | 1.97                     | 0.80              |
| 2:H:351:GLN:OE1  | 3:H:508:HOH:O   | 1.99                     | 0.80              |
| 1:C:119:GLY:O    | 3:C:415:HOH:O   | 1.97                     | 0.80              |
| 2:H:490:ASN:O    | 3:H:509:HOH:O   | 1.99                     | 0.80              |
| 2:H:374:ASN:OD1  | 3:H:510:HOH:O   | 2.00                     | 0.80              |
| 1:C:232:ASP:OD2  | 3:C:416:HOH:O   | 1.98                     | 0.79              |
| 2:H:395:GLU:OE2  | 3:H:511:HOH:O   | 2.01                     | 0.79              |
| 1:A:190:ASN:HA   | 1:A:191:LYS:HB2 | 1.62                     | 0.79              |
| 1:G:215:ASN:O    | 3:G:410:HOH:O   | 2.00                     | 0.79              |
| 2:H:488:MET:N    | 3:H:502:HOH:O   | 1.97                     | 0.79              |
| 1:I:151:ALA:HA   | 3:I:411:HOH:O   | 1.76                     | 0.79              |
| 1:C:56:LEU:CB    | 3:C:406:HOH:O   | 2.30                     | 0.79              |
| 1:C:178:SER:N    | 3:C:401:HOH:O   | 2.07                     | 0.79              |
| 2:L:450:ASN:OD1  | 3:L:510:HOH:O   | 2.00                     | 0.79              |
| 1:K:27:VAL:C     | 3:K:409:HOH:O   | 2.24                     | 0.79              |
| 2:J:486:GLU:OE2  | 3:J:507:HOH:O   | 2.01                     | 0.79              |
| 1:G:154:GLN:C    | 3:G:403:HOH:O   | 2.21                     | 0.78              |
| 1:I:312:LYS:O    | 3:I:407:HOH:O   | 2.00                     | 0.78              |
| 1:A:95:GLU:O     | 3:A:410:HOH:O   | 2.01                     | 0.78              |
| 1:G:222:ASP:OD1  | 1:K:201:GLN:NE2 | 2.17                     | 0.78              |
| 1:I:180:ALA:N    | 3:I:415:HOH:O   | 2.17                     | 0.78              |
| 1:A:147:THR:HG23 | 1:A:150:ALA:HB2 | 1.63                     | 0.77              |
| 1:A:49:VAL:N     | 3:A:409:HOH:O   | 2.10                     | 0.77              |
| 1:C:173:ILE:O    | 3:C:410:HOH:O   | 2.01                     | 0.77              |
| 1:C:149:ASN:ND2  | 3:C:423:HOH:O   | 2.18                     | 0.77              |
| 2:H:375:ARG:NH2  | 2:H:424:GLU:OE2 | 2.17                     | 0.77              |
| 1:I:291:ARG:NH2  | 3:I:406:HOH:O   | 1.89                     | 0.77              |
| 2:B:399:GLY:HA2  | 3:B:508:HOH:O   | 1.83                     | 0.76              |
| 1:A:123:ASN:OD1  | 3:A:415:HOH:O   | 2.02                     | 0.76              |
| 2:B:399:GLY:O    | 3:B:508:HOH:O   | 2.03                     | 0.76              |
| 1:E:154:GLN:NE2  | 3:E:413:HOH:O   | 2.19                     | 0.76              |
| 1:G:25:GLU:OE2   | 3:G:408:HOH:O   | 2.03                     | 0.76              |
| 1:C:147:THR:HB   | 3:C:432:HOH:O   | 1.87                     | 0.75              |
| 2:F:447:LEU:CA   | 3:F:506:HOH:O   | 2.18                     | 0.75              |
| 1:I:207:SER:O    | 1:I:211:ARG:NH2 | 2.18                     | 0.75              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:K:27:VAL:HG12  | 3:K:409:HOH:O   | 1.84                     | 0.75              |
| 2:J:338:LEU:O    | 3:J:508:HOH:O   | 2.04                     | 0.75              |
| 1:I:151:ALA:C    | 3:I:411:HOH:O   | 2.30                     | 0.75              |
| 1:E:298:ARG:HD3  | 3:E:420:HOH:O   | 1.87                     | 0.75              |
| 1:G:119:GLY:C    | 3:G:411:HOH:O   | 2.29                     | 0.75              |
| 1:I:157:LYS:C    | 3:I:409:HOH:O   | 2.30                     | 0.75              |
| 1:C:5:LEU:HD23   | 3:D:504:HOH:O   | 1.85                     | 0.74              |
| 1:G:153:PRO:C    | 3:G:403:HOH:O   | 2.29                     | 0.74              |
| 2:B:399:GLY:CA   | 3:B:508:HOH:O   | 2.35                     | 0.74              |
| 1:I:30:THR:OG1   | 3:I:408:HOH:O   | 2.04                     | 0.74              |
| 1:I:156:THR:HG22 | 3:I:409:HOH:O   | 1.87                     | 0.74              |
| 2:B:375:ARG:NH2  | 2:B:424:GLU:OE2 | 2.20                     | 0.74              |
| 1:G:202:GLN:HA   | 1:G:203:SER:HB3 | 1.67                     | 0.74              |
| 1:K:152:PHE:HB3  | 3:K:420:HOH:O   | 1.87                     | 0.74              |
| 2:D:380:THR:O    | 3:D:505:HOH:O   | 1.93                     | 0.74              |
| 1:E:184:LYS:O    | 3:E:408:HOH:O   | 2.04                     | 0.74              |
| 2:B:480:HIS:HB2  | 3:B:506:HOH:O   | 1.88                     | 0.74              |
| 1:G:262:VAL:HG23 | 3:G:402:HOH:O   | 1.75                     | 0.74              |
| 1:K:202:GLN:HA   | 1:K:203:SER:HB3 | 1.70                     | 0.74              |
| 1:K:299:TYR:OH   | 3:K:406:HOH:O   | 1.89                     | 0.74              |
| 1:A:68:GLN:OE1   | 3:A:403:HOH:O   | 1.99                     | 0.73              |
| 2:F:482:LYS:HB3  | 3:F:502:HOH:O   | 1.75                     | 0.73              |
| 1:A:176:SER:OG   | 3:A:416:HOH:O   | 2.06                     | 0.73              |
| 1:E:80:ARG:O     | 3:E:409:HOH:O   | 2.05                     | 0.73              |
| 1:K:21:GLU:CA    | 3:K:403:HOH:O   | 2.04                     | 0.73              |
| 1:C:109:ASP:O    | 3:C:409:HOH:O   | 2.06                     | 0.73              |
| 1:C:202:GLN:CA   | 3:C:408:HOH:O   | 2.35                     | 0.73              |
| 1:A:71:GLU:CD    | 3:A:401:HOH:O   | 2.30                     | 0.73              |
| 1:I:180:ALA:CA   | 3:I:415:HOH:O   | 2.37                     | 0.73              |
| 1:K:21:GLU:CG    | 3:K:405:HOH:O   | 2.31                     | 0.73              |
| 2:D:416:ASN:ND2  | 3:D:507:HOH:O   | 2.14                     | 0.72              |
| 1:G:5:LEU:HD11   | 2:H:440:TYR:HA  | 1.70                     | 0.72              |
| 1:A:42:CYS:O     | 3:A:417:HOH:O   | 2.06                     | 0.72              |
| 2:J:375:ARG:NH2  | 2:J:424:GLU:OE2 | 2.23                     | 0.72              |
| 2:B:390:GLU:OE2  | 3:B:509:HOH:O   | 2.07                     | 0.72              |
| 1:I:316:GLU:OE1  | 3:I:410:HOH:O   | 2.06                     | 0.72              |
| 2:J:464:LYS:O    | 3:J:509:HOH:O   | 2.07                     | 0.72              |
| 1:E:202:GLN:CA   | 1:E:203:SER:HB2 | 2.18                     | 0.72              |
| 2:H:487:ALA:CA   | 3:H:502:HOH:O   | 2.30                     | 0.71              |
| 1:I:90:GLY:N     | 3:I:416:HOH:O   | 2.22                     | 0.71              |
| 2:F:446:GLN:O    | 3:F:506:HOH:O   | 2.08                     | 0.71              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:K:312:LYS:NZ  | 3:K:413:HOH:O    | 2.23                     | 0.71              |
| 1:C:110:LYS:N   | 3:C:405:HOH:O    | 2.13                     | 0.71              |
| 2:B:375:ARG:NH1 | 3:B:510:HOH:O    | 2.23                     | 0.71              |
| 1:A:202:GLN:O   | 1:A:204:PHE:CE1  | 2.44                     | 0.70              |
| 1:A:117:TYR:HB3 | 1:A:120:ILE:HD11 | 1.71                     | 0.70              |
| 2:L:375:ARG:NH2 | 2:L:424:GLU:OE2  | 2.24                     | 0.70              |
| 2:B:465:CYS:CA  | 3:B:503:HOH:O    | 2.37                     | 0.70              |
| 1:A:263:GLN:OE1 | 3:A:418:HOH:O    | 2.09                     | 0.70              |
| 2:F:406:ARG:CZ  | 3:F:504:HOH:O    | 2.18                     | 0.70              |
| 2:F:482:LYS:HB2 | 3:F:502:HOH:O    | 1.77                     | 0.70              |
| 2:L:484:ARG:CZ  | 3:L:505:HOH:O    | 2.28                     | 0.70              |
| 1:C:157:LYS:HD3 | 3:C:427:HOH:O    | 1.92                     | 0.70              |
| 2:F:375:ARG:NH2 | 2:F:424:GLU:OE2  | 2.25                     | 0.70              |
| 2:H:338:LEU:CD1 | 3:H:512:HOH:O    | 2.29                     | 0.70              |
| 1:I:28:ASN:ND2  | 3:I:418:HOH:O    | 2.24                     | 0.69              |
| 2:D:447:LEU:CA  | 3:D:501:HOH:O    | 2.27                     | 0.69              |
| 1:E:222:ASP:OD2 | 3:E:411:HOH:O    | 2.10                     | 0.69              |
| 2:J:339:ILE:HA  | 3:J:508:HOH:O    | 1.91                     | 0.69              |
| 1:A:231:ASN:ND2 | 3:A:405:HOH:O    | 1.87                     | 0.69              |
| 2:J:395:GLU:OE2 | 3:J:510:HOH:O    | 2.09                     | 0.69              |
| 1:K:21:GLU:CB   | 3:K:405:HOH:O    | 2.39                     | 0.69              |
| 1:C:56:LEU:N    | 3:C:406:HOH:O    | 1.83                     | 0.69              |
| 1:A:191:LYS:H   | 1:A:239:ASN:HD21 | 1.41                     | 0.69              |
| 1:E:27:VAL:O    | 3:E:412:HOH:O    | 2.11                     | 0.69              |
| 1:I:96:GLU:OE1  | 3:I:412:HOH:O    | 2.09                     | 0.69              |
| 2:D:380:THR:CB  | 3:D:505:HOH:O    | 2.41                     | 0.69              |
| 1:G:250:PHE:HA  | 3:G:416:HOH:O    | 1.93                     | 0.68              |
| 2:D:375:ARG:NH2 | 2:D:424:GLU:OE2  | 2.26                     | 0.68              |
| 2:J:464:LYS:N   | 3:J:509:HOH:O    | 2.26                     | 0.68              |
| 1:A:146:ASN:N   | 3:A:413:HOH:O    | 1.98                     | 0.68              |
| 1:E:266:ALA:N   | 3:E:402:HOH:O    | 2.27                     | 0.68              |
| 1:G:117:TYR:HB3 | 1:G:120:ILE:HD11 | 1.76                     | 0.68              |
| 2:B:466:ASP:N   | 3:B:503:HOH:O    | 2.24                     | 0.68              |
| 2:H:426:GLN:NE2 | 3:H:519:HOH:O    | 2.26                     | 0.67              |
| 2:J:403:ASN:ND2 | 3:J:515:HOH:O    | 2.28                     | 0.67              |
| 2:L:479:ASP:OD1 | 3:L:512:HOH:O    | 2.12                     | 0.67              |
| 2:H:375:ARG:NH1 | 3:H:520:HOH:O    | 2.27                     | 0.67              |
| 2:H:460:GLU:OE2 | 3:H:514:HOH:O    | 2.13                     | 0.67              |
| 1:C:222:ASP:O   | 3:C:410:HOH:O    | 2.12                     | 0.67              |
| 1:K:202:GLN:HG2 | 1:K:203:SER:OG   | 1.94                     | 0.67              |
| 1:I:316:GLU:CD  | 3:I:410:HOH:O    | 2.38                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:202:GLN:HA   | 1:K:203:SER:CB   | 2.24                     | 0.67              |
| 1:A:91:LYS:NZ    | 3:A:424:HOH:O    | 2.28                     | 0.67              |
| 1:C:177:VAL:CA   | 3:C:401:HOH:O    | 2.34                     | 0.67              |
| 1:C:313:ASN:HA   | 3:C:429:HOH:O    | 1.95                     | 0.67              |
| 1:A:143:LEU:O    | 3:A:419:HOH:O    | 2.13                     | 0.66              |
| 1:A:110:LYS:N    | 3:A:401:HOH:O    | 2.25                     | 0.66              |
| 1:C:207:SER:O    | 1:C:211:ARG:NH2  | 2.29                     | 0.66              |
| 1:G:46:LYS:CB    | 3:G:406:HOH:O    | 2.42                     | 0.66              |
| 1:G:144:LEU:HD22 | 1:G:185:LEU:HB3  | 1.78                     | 0.66              |
| 1:I:53:GLN:O     | 3:I:414:HOH:O    | 2.13                     | 0.66              |
| 2:L:469:CYS:CB   | 3:L:536:HOH:O    | 2.38                     | 0.66              |
| 1:I:291:ARG:NH1  | 3:I:406:HOH:O    | 2.27                     | 0.66              |
| 1:E:185:LEU:O    | 3:E:408:HOH:O    | 2.12                     | 0.66              |
| 1:I:117:TYR:HB3  | 1:I:120:ILE:HD11 | 1.78                     | 0.66              |
| 1:C:21:GLU:CD    | 3:C:422:HOH:O    | 2.39                     | 0.66              |
| 1:K:117:TYR:HB3  | 1:K:120:ILE:HD11 | 1.77                     | 0.66              |
| 1:C:3:ILE:HG22   | 2:D:461:ILE:HD11 | 1.78                     | 0.65              |
| 1:G:71:GLU:OE2   | 1:G:247:ARG:NH2  | 2.29                     | 0.65              |
| 1:G:316:GLU:C    | 3:G:404:HOH:O    | 2.36                     | 0.65              |
| 1:E:117:TYR:HB3  | 1:E:120:ILE:HD11 | 1.79                     | 0.65              |
| 1:I:298:ARG:NH1  | 3:I:420:HOH:O    | 2.29                     | 0.65              |
| 1:I:316:GLU:OE2  | 3:I:410:HOH:O    | 2.15                     | 0.65              |
| 2:L:331:ILE:O    | 3:L:513:HOH:O    | 2.14                     | 0.65              |
| 1:A:68:GLN:N     | 3:A:403:HOH:O    | 1.84                     | 0.65              |
| 2:D:346:ARG:HA   | 2:D:354:GLY:O    | 1.96                     | 0.65              |
| 1:A:201:GLN:NE2  | 3:A:423:HOH:O    | 2.27                     | 0.65              |
| 1:C:272:CYS:HA   | 3:C:436:HOH:O    | 1.96                     | 0.65              |
| 1:I:154:GLN:N    | 3:I:404:HOH:O    | 2.17                     | 0.64              |
| 2:B:341:GLY:CA   | 3:B:507:HOH:O    | 2.45                     | 0.64              |
| 1:C:21:GLU:OE2   | 3:C:422:HOH:O    | 2.14                     | 0.64              |
| 1:G:262:VAL:HG22 | 3:G:402:HOH:O    | 1.77                     | 0.64              |
| 2:F:346:ARG:HA   | 2:F:354:GLY:O    | 1.98                     | 0.64              |
| 1:G:46:LYS:C     | 3:G:406:HOH:O    | 2.23                     | 0.64              |
| 1:A:71:GLU:OE2   | 1:A:247:ARG:NH2  | 2.31                     | 0.64              |
| 2:H:382:GLN:NE2  | 3:H:523:HOH:O    | 2.29                     | 0.64              |
| 1:K:20:THR:C     | 3:K:403:HOH:O    | 2.33                     | 0.63              |
| 1:G:28:ASN:ND2   | 3:G:401:HOH:O    | 1.81                     | 0.63              |
| 2:H:382:GLN:CB   | 3:H:507:HOH:O    | 2.46                     | 0.63              |
| 1:G:128:ALA:CB   | 3:G:413:HOH:O    | 2.24                     | 0.63              |
| 2:D:415:TYR:OH   | 3:D:506:HOH:O    | 2.13                     | 0.62              |
| 1:K:15:LYS:NZ    | 3:K:419:HOH:O    | 2.32                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:20:THR:HG22  | 1:K:21:GLU:HG3   | 1.81                     | 0.62              |
| 2:B:480:HIS:CB   | 3:B:506:HOH:O    | 2.44                     | 0.62              |
| 1:E:267:ASN:N    | 3:E:402:HOH:O    | 1.98                     | 0.62              |
| 1:A:207:SER:CB   | 1:E:203:SER:OG   | 2.47                     | 0.62              |
| 2:F:446:GLN:C    | 3:F:506:HOH:O    | 2.42                     | 0.62              |
| 1:I:179:THR:HG23 | 3:I:415:HOH:O    | 1.98                     | 0.62              |
| 2:H:466:ASP:OD2  | 3:H:515:HOH:O    | 2.16                     | 0.62              |
| 1:A:81:ARG:HB2   | 3:A:407:HOH:O    | 1.98                     | 0.62              |
| 1:A:263:GLN:CD   | 3:A:418:HOH:O    | 2.43                     | 0.62              |
| 2:D:481:SER:N    | 3:D:509:HOH:O    | 2.31                     | 0.62              |
| 1:E:151:ALA:N    | 3:E:404:HOH:O    | 2.22                     | 0.62              |
| 1:I:20:THR:HG22  | 1:I:21:GLU:HG3   | 1.82                     | 0.62              |
| 1:E:151:ALA:CA   | 3:E:404:HOH:O    | 2.47                     | 0.62              |
| 2:B:346:ARG:HA   | 2:B:354:GLY:O    | 2.00                     | 0.62              |
| 1:C:4:CYS:HA     | 3:D:504:HOH:O    | 2.00                     | 0.62              |
| 2:D:394:VAL:HB   | 3:D:511:HOH:O    | 2.00                     | 0.62              |
| 1:G:75:ASP:HB2   | 3:G:406:HOH:O    | 1.98                     | 0.62              |
| 1:A:222:ASP:OD1  | 1:E:201:GLN:NE2  | 2.32                     | 0.61              |
| 2:B:341:GLY:HA3  | 3:B:507:HOH:O    | 2.01                     | 0.61              |
| 1:K:191:LYS:NZ   | 3:K:420:HOH:O    | 2.32                     | 0.61              |
| 1:G:128:ALA:CA   | 3:G:413:HOH:O    | 2.48                     | 0.61              |
| 2:H:468:ASP:HB3  | 3:H:515:HOH:O    | 2.00                     | 0.61              |
| 1:G:46:LYS:HB3   | 3:G:406:HOH:O    | 1.98                     | 0.61              |
| 1:A:166:PRO:O    | 3:A:420:HOH:O    | 2.16                     | 0.60              |
| 2:J:395:GLU:HB3  | 2:J:398:ILE:HG22 | 1.83                     | 0.60              |
| 2:L:339:ILE:N    | 3:L:517:HOH:O    | 2.28                     | 0.60              |
| 1:C:250:PHE:C    | 3:C:409:HOH:O    | 2.35                     | 0.60              |
| 2:H:382:GLN:CG   | 3:H:507:HOH:O    | 2.49                     | 0.60              |
| 1:K:71:GLU:OE2   | 1:K:247:ARG:NH2  | 2.34                     | 0.60              |
| 1:C:56:LEU:HB2   | 3:C:406:HOH:O    | 1.96                     | 0.60              |
| 1:I:313:ASN:HA   | 3:I:407:HOH:O    | 2.01                     | 0.60              |
| 1:I:122:THR:HA   | 3:I:413:HOH:O    | 1.96                     | 0.60              |
| 2:J:435:GLU:OE2  | 3:J:512:HOH:O    | 2.16                     | 0.60              |
| 2:D:380:THR:CG2  | 3:D:505:HOH:O    | 2.28                     | 0.60              |
| 1:A:201:GLN:HB2  | 1:C:211:ARG:HE   | 1.65                     | 0.60              |
| 1:A:298:ARG:NH2  | 2:D:411:GLU:OE1  | 2.35                     | 0.60              |
| 1:C:170:VAL:HG22 | 1:C:225:TRP:HB3  | 1.83                     | 0.60              |
| 1:I:172:GLY:HA2  | 1:I:222:ASP:O    | 2.02                     | 0.60              |
| 1:G:171:TRP:HZ3  | 1:G:226:LEU:HD22 | 1.68                     | 0.59              |
| 1:K:3:ILE:HG22   | 2:L:461:ILE:HD11 | 1.84                     | 0.59              |
| 2:L:480:HIS:HB2  | 3:L:506:HOH:O    | 2.02                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:12:ASN:HA    | 3:G:408:HOH:O    | 2.02                     | 0.59              |
| 2:L:479:ASP:CG   | 3:L:512:HOH:O    | 2.44                     | 0.59              |
| 2:H:395:GLU:HB3  | 2:H:398:ILE:HG22 | 1.84                     | 0.59              |
| 1:A:215:ASN:HA   | 2:H:353:GLU:HB2  | 1.82                     | 0.59              |
| 1:C:250:PHE:HB2  | 3:C:409:HOH:O    | 2.03                     | 0.59              |
| 1:I:170:VAL:HG22 | 1:I:225:TRP:HB3  | 1.85                     | 0.59              |
| 1:K:68:GLN:CD    | 3:K:401:HOH:O    | 2.13                     | 0.59              |
| 1:K:152:PHE:CB   | 3:K:420:HOH:O    | 2.49                     | 0.59              |
| 1:E:71:GLU:OE2   | 1:E:247:ARG:NH2  | 2.35                     | 0.59              |
| 2:B:480:HIS:C    | 3:B:506:HOH:O    | 2.42                     | 0.58              |
| 1:K:28:ASN:HB2   | 3:K:409:HOH:O    | 2.02                     | 0.58              |
| 1:K:172:GLY:HA2  | 1:K:222:ASP:O    | 2.03                     | 0.58              |
| 2:L:395:GLU:HB3  | 2:L:398:ILE:HG22 | 1.84                     | 0.58              |
| 1:E:15:LYS:NZ    | 3:E:417:HOH:O    | 2.31                     | 0.58              |
| 2:D:380:THR:HG22 | 2:D:382:GLN:H    | 1.69                     | 0.58              |
| 2:H:387:ILE:HG22 | 3:H:538:HOH:O    | 2.03                     | 0.58              |
| 1:A:130:ARG:NH1  | 2:H:458:CYS:SG   | 2.77                     | 0.58              |
| 1:G:120:ILE:N    | 3:G:411:HOH:O    | 2.36                     | 0.58              |
| 1:C:287:ASN:ND2  | 1:C:300:VAL:O    | 2.35                     | 0.57              |
| 2:F:381:ASN:C    | 3:F:503:HOH:O    | 2.33                     | 0.57              |
| 1:I:71:GLU:OE2   | 1:I:247:ARG:NH2  | 2.37                     | 0.57              |
| 2:J:380:THR:HG22 | 2:J:382:GLN:H    | 1.69                     | 0.57              |
| 1:A:100:GLN:NE2  | 3:A:408:HOH:O    | 1.90                     | 0.57              |
| 1:E:3:ILE:HG22   | 2:F:461:ILE:HD11 | 1.86                     | 0.57              |
| 1:I:110:LYS:NZ   | 1:I:139:GLU:OE2  | 2.35                     | 0.57              |
| 1:G:128:ALA:C    | 3:G:413:HOH:O    | 2.47                     | 0.57              |
| 1:G:194:THR:HB   | 1:G:237:SER:HB2  | 1.86                     | 0.57              |
| 2:H:380:THR:HG22 | 2:H:382:GLN:H    | 1.70                     | 0.57              |
| 2:L:469:CYS:HB2  | 3:L:536:HOH:O    | 2.02                     | 0.57              |
| 1:I:7:HIS:HD2    | 3:I:434:HOH:O    | 1.87                     | 0.57              |
| 1:A:305:LEU:HB3  | 2:B:421:VAL:HG21 | 1.87                     | 0.57              |
| 1:G:20:THR:HG22  | 1:G:21:GLU:HG3   | 1.87                     | 0.57              |
| 2:H:382:GLN:HG3  | 3:H:507:HOH:O    | 2.05                     | 0.57              |
| 1:K:170:VAL:HG22 | 1:K:225:TRP:HB3  | 1.86                     | 0.57              |
| 2:H:331:ILE:O    | 3:H:516:HOH:O    | 2.18                     | 0.56              |
| 2:J:464:LYS:C    | 3:J:509:HOH:O    | 2.43                     | 0.56              |
| 2:B:395:GLU:HB3  | 2:B:398:ILE:HG22 | 1.86                     | 0.56              |
| 1:C:110:LYS:NZ   | 1:C:139:GLU:OE2  | 2.38                     | 0.56              |
| 1:G:21:GLU:OE1   | 3:G:412:HOH:O    | 2.18                     | 0.56              |
| 1:G:110:LYS:NZ   | 1:G:139:GLU:OE2  | 2.38                     | 0.56              |
| 1:G:298:ARG:NH2  | 2:J:411:GLU:OE1  | 2.39                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:480:HIS:CG   | 3:B:506:HOH:O    | 2.58                     | 0.56              |
| 1:G:203:SER:O    | 1:G:203:SER:OG   | 2.22                     | 0.56              |
| 1:K:202:GLN:CA   | 1:K:203:SER:CB   | 2.83                     | 0.56              |
| 2:D:395:GLU:HB3  | 2:D:398:ILE:HG22 | 1.86                     | 0.56              |
| 2:F:395:GLU:HB3  | 2:F:398:ILE:HG22 | 1.86                     | 0.56              |
| 1:A:49:VAL:HG23  | 1:A:74:ALA:HB2   | 1.88                     | 0.56              |
| 1:E:110:LYS:NZ   | 1:E:139:GLU:OE2  | 2.38                     | 0.56              |
| 1:C:71:GLU:OE2   | 1:C:247:ARG:NH2  | 2.38                     | 0.56              |
| 1:E:170:VAL:HG22 | 1:E:225:TRP:HB3  | 1.88                     | 0.56              |
| 1:A:95:GLU:C     | 3:A:410:HOH:O    | 2.46                     | 0.56              |
| 2:B:346:ARG:CZ   | 3:B:502:HOH:O    | 2.39                     | 0.55              |
| 1:G:193:VAL:HG13 | 1:G:238:PHE:HB3  | 1.88                     | 0.55              |
| 1:K:36:THR:O     | 3:K:411:HOH:O    | 2.18                     | 0.55              |
| 1:C:178:SER:CB   | 3:C:404:HOH:O    | 2.43                     | 0.55              |
| 1:K:202:GLN:NE2  | 3:K:422:HOH:O    | 2.40                     | 0.55              |
| 1:A:68:GLN:CG    | 3:A:403:HOH:O    | 2.39                     | 0.55              |
| 1:G:3:ILE:HG22   | 2:H:461:ILE:HD11 | 1.88                     | 0.55              |
| 1:G:202:GLN:HA   | 1:G:203:SER:CB   | 2.37                     | 0.55              |
| 2:L:389:ASN:N    | 3:L:515:HOH:O    | 2.32                     | 0.55              |
| 1:G:169:ILE:O    | 1:G:225:TRP:HA   | 2.07                     | 0.55              |
| 1:A:287:ASN:ND2  | 1:A:300:VAL:O    | 2.35                     | 0.54              |
| 2:D:382:GLN:N    | 3:D:505:HOH:O    | 2.41                     | 0.54              |
| 1:A:312:LYS:HB2  | 2:B:429:ILE:HG23 | 1.89                     | 0.54              |
| 2:F:380:THR:HG22 | 2:F:382:GLN:H    | 1.72                     | 0.54              |
| 1:G:13:GLY:N     | 3:G:408:HOH:O    | 1.97                     | 0.54              |
| 1:G:170:VAL:HG22 | 1:G:225:TRP:HB3  | 1.89                     | 0.54              |
| 1:C:126:THR:HG23 | 1:C:129:CYS:H    | 1.72                     | 0.54              |
| 1:I:7:HIS:CD2    | 3:I:434:HOH:O    | 2.60                     | 0.54              |
| 1:A:170:VAL:HG22 | 1:A:225:TRP:HB3  | 1.90                     | 0.54              |
| 2:H:351:GLN:HB3  | 3:H:508:HOH:O    | 1.94                     | 0.54              |
| 1:K:110:LYS:NZ   | 1:K:139:GLU:OE2  | 2.40                     | 0.54              |
| 1:C:176:SER:C    | 3:C:401:HOH:O    | 2.43                     | 0.54              |
| 1:G:175:HIS:HB3  | 1:G:211:ARG:HH12 | 1.73                     | 0.54              |
| 1:C:177:VAL:C    | 3:C:404:HOH:O    | 2.42                     | 0.54              |
| 1:A:169:ILE:HB   | 1:A:226:LEU:HD23 | 1.90                     | 0.53              |
| 1:C:169:ILE:HB   | 1:C:226:LEU:HD23 | 1.90                     | 0.53              |
| 1:G:169:ILE:HB   | 1:G:226:LEU:HD23 | 1.89                     | 0.53              |
| 1:I:169:ILE:O    | 1:I:225:TRP:HA   | 2.08                     | 0.53              |
| 2:L:380:THR:HG22 | 2:L:382:GLN:H    | 1.73                     | 0.53              |
| 2:L:414:SER:O    | 3:L:504:HOH:O    | 2.08                     | 0.53              |
| 1:E:169:ILE:HB   | 1:E:226:LEU:HD23 | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:448:ARG:HG3  | 2:L:480:HIS:HB2  | 1.90                     | 0.53              |
| 1:A:177:VAL:HG23 | 3:A:444:HOH:O    | 2.08                     | 0.53              |
| 1:C:250:PHE:CB   | 3:C:409:HOH:O    | 2.56                     | 0.53              |
| 1:I:7:HIS:NE2    | 3:I:403:HOH:O    | 2.12                     | 0.53              |
| 2:L:484:ARG:HH11 | 2:L:488:MET:HG3  | 1.73                     | 0.53              |
| 1:G:171:TRP:CZ3  | 1:G:226:LEU:HD22 | 2.44                     | 0.53              |
| 1:A:292:ALA:C    | 3:A:406:HOH:O    | 2.37                     | 0.53              |
| 2:B:484:ARG:HH11 | 2:B:488:MET:HG3  | 1.73                     | 0.53              |
| 1:G:2:LYS:NZ     | 3:H:514:HOH:O    | 2.41                     | 0.53              |
| 1:I:287:ASN:ND2  | 1:I:300:VAL:O    | 2.36                     | 0.53              |
| 1:A:194:THR:HA   | 1:A:203:SER:H    | 1.74                     | 0.52              |
| 1:C:59:THR:N     | 3:C:414:HOH:O    | 2.02                     | 0.52              |
| 1:A:190:ASN:CA   | 1:A:191:LYS:HB2  | 2.38                     | 0.52              |
| 2:B:388:ASP:OD2  | 2:B:406:ARG:NH2  | 2.41                     | 0.52              |
| 1:E:13:GLY:HA2   | 3:E:412:HOH:O    | 2.09                     | 0.52              |
| 1:G:153:PRO:HB2  | 3:G:403:HOH:O    | 2.07                     | 0.52              |
| 1:A:5:LEU:HD11   | 2:B:440:TYR:HA   | 1.91                     | 0.52              |
| 1:C:20:THR:HG22  | 1:C:21:GLU:HG3   | 1.91                     | 0.52              |
| 1:C:57:LEU:C     | 3:C:414:HOH:O    | 2.43                     | 0.52              |
| 1:G:156:THR:HA   | 1:G:236:PHE:O    | 2.09                     | 0.52              |
| 1:K:169:ILE:O    | 1:K:225:TRP:HA   | 2.09                     | 0.52              |
| 2:H:348:GLN:HB2  | 2:H:353:GLU:HG2  | 1.89                     | 0.52              |
| 1:K:169:ILE:HB   | 1:K:226:LEU:HD23 | 1.91                     | 0.52              |
| 2:B:396:LYS:HB3  | 1:E:97:ALA:HB1   | 1.91                     | 0.52              |
| 1:G:301:LYS:HD2  | 3:G:417:HOH:O    | 2.08                     | 0.52              |
| 1:C:56:LEU:O     | 3:C:414:HOH:O    | 2.19                     | 0.52              |
| 2:B:442:ARG:NH1  | 2:B:443:VAL:HG23 | 2.24                     | 0.52              |
| 2:H:395:GLU:HG3  | 3:H:511:HOH:O    | 2.02                     | 0.52              |
| 1:I:169:ILE:HB   | 1:I:226:LEU:HD23 | 1.90                     | 0.52              |
| 1:K:47:ARG:NH2   | 1:K:73:SER:OG    | 2.42                     | 0.52              |
| 1:A:40:ARG:NE    | 3:A:421:HOH:O    | 2.25                     | 0.51              |
| 2:B:380:THR:HG22 | 2:B:382:GLN:H    | 1.75                     | 0.51              |
| 1:I:101:ILE:HD11 | 2:L:396:LYS:HG2  | 1.91                     | 0.51              |
| 1:K:198:SER:CA   | 3:K:402:HOH:O    | 2.47                     | 0.51              |
| 1:I:180:ALA:HB2  | 3:I:415:HOH:O    | 2.10                     | 0.51              |
| 1:E:122:THR:HG22 | 3:E:440:HOH:O    | 2.10                     | 0.51              |
| 1:G:196:GLY:O    | 1:G:235:THR:HB   | 2.10                     | 0.51              |
| 3:H:522:HOH:O    | 2:L:480:HIS:CD2  | 2.62                     | 0.51              |
| 1:K:287:ASN:ND2  | 1:K:300:VAL:O    | 2.38                     | 0.51              |
| 2:H:382:GLN:HB3  | 3:H:507:HOH:O    | 2.09                     | 0.51              |
| 1:A:172:GLY:HA2  | 1:A:222:ASP:O    | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:101:ILE:HD11 | 2:F:396:LYS:HG2  | 1.91                     | 0.51              |
| 1:K:21:GLU:HB3   | 3:K:405:HOH:O    | 2.06                     | 0.51              |
| 1:A:207:SER:O    | 1:A:211:ARG:NH2  | 2.40                     | 0.51              |
| 2:D:484:ARG:HH11 | 2:D:488:MET:HG3  | 1.76                     | 0.51              |
| 1:G:305:LEU:HB3  | 2:H:421:VAL:HG21 | 1.93                     | 0.51              |
| 1:E:172:GLY:HA2  | 1:E:222:ASP:O    | 2.11                     | 0.51              |
| 1:A:5:LEU:HD12   | 2:B:439:LEU:HG   | 1.91                     | 0.51              |
| 1:A:202:GLN:HA   | 1:A:203:SER:CB   | 2.40                     | 0.51              |
| 1:K:305:LEU:HB3  | 2:L:421:VAL:HG21 | 1.93                     | 0.51              |
| 1:A:203:SER:HB2  | 1:C:207:SER:HB3  | 1.93                     | 0.50              |
| 1:A:72:PHE:N     | 3:A:431:HOH:O    | 2.44                     | 0.50              |
| 2:D:345:PHE:O    | 2:D:355:THR:HA   | 2.12                     | 0.50              |
| 1:I:200:TYR:CZ   | 1:I:202:GLN:HG3  | 2.46                     | 0.50              |
| 2:F:400:ASN:ND2  | 3:F:511:HOH:O    | 2.44                     | 0.50              |
| 1:E:169:ILE:O    | 1:E:225:TRP:HA   | 2.11                     | 0.50              |
| 1:G:2:LYS:HE3    | 3:H:514:HOH:O    | 2.12                     | 0.50              |
| 1:K:12:ASN:ND2   | 1:K:12:ASN:O     | 2.45                     | 0.50              |
| 1:E:287:ASN:ND2  | 1:E:300:VAL:O    | 2.35                     | 0.50              |
| 2:F:484:ARG:HH11 | 2:F:488:MET:HG3  | 1.77                     | 0.50              |
| 1:G:193:VAL:HB   | 1:G:204:PHE:HB2  | 1.94                     | 0.50              |
| 1:C:25:GLU:CD    | 3:C:417:HOH:O    | 2.52                     | 0.50              |
| 1:G:63:PRO:CG    | 3:G:433:HOH:O    | 2.60                     | 0.50              |
| 1:I:156:THR:CG2  | 3:I:409:HOH:O    | 2.52                     | 0.50              |
| 2:J:346:ARG:HA   | 2:J:354:GLY:O    | 2.11                     | 0.50              |
| 2:J:403:ASN:ND2  | 3:J:520:HOH:O    | 2.43                     | 0.50              |
| 1:A:263:GLN:CB   | 3:A:418:HOH:O    | 2.51                     | 0.50              |
| 1:A:265:ASP:OD2  | 3:A:421:HOH:O    | 2.20                     | 0.50              |
| 1:I:120:ILE:HG12 | 3:I:413:HOH:O    | 2.11                     | 0.50              |
| 2:L:346:ARG:NH1  | 2:L:353:GLU:OE2  | 2.45                     | 0.50              |
| 2:L:388:ASP:OD2  | 2:L:406:ARG:NH2  | 2.45                     | 0.50              |
| 2:F:385:GLU:OE1  | 3:F:507:HOH:O    | 2.20                     | 0.49              |
| 1:I:131:ARG:NH1  | 1:I:136:PHE:O    | 2.38                     | 0.49              |
| 1:A:147:THR:OG1  | 1:A:148:ASP:N    | 2.42                     | 0.49              |
| 1:A:169:ILE:O    | 1:A:225:TRP:HA   | 2.12                     | 0.49              |
| 1:K:175:HIS:HB3  | 1:K:211:ARG:HH12 | 1.76                     | 0.49              |
| 1:A:233:THR:HB   | 1:C:212:THR:HG21 | 1.94                     | 0.49              |
| 1:C:110:LYS:HA   | 1:C:248:ALA:O    | 2.13                     | 0.49              |
| 1:G:171:TRP:CE2  | 1:G:195:VAL:HG21 | 2.48                     | 0.49              |
| 1:I:23:GLY:HA3   | 3:I:401:HOH:O    | 2.12                     | 0.49              |
| 1:C:146:ASN:HB2  | 3:C:415:HOH:O    | 2.11                     | 0.49              |
| 2:L:346:ARG:HA   | 2:L:354:GLY:O    | 2.13                     | 0.49              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:146:ASN:HB2  | 3:A:413:HOH:O   | 2.12                     | 0.49              |
| 1:C:168:LEU:HB3  | 1:C:249:SER:HB2 | 1.94                     | 0.49              |
| 1:G:47:ARG:NH2   | 1:G:73:SER:OG   | 2.46                     | 0.49              |
| 1:G:154:GLN:N    | 3:G:403:HOH:O   | 2.44                     | 0.49              |
| 1:G:201:GLN:O    | 1:G:202:GLN:HG3 | 2.09                     | 0.49              |
| 1:A:40:ARG:NH2   | 3:A:421:HOH:O   | 2.42                     | 0.48              |
| 2:B:345:PHE:O    | 2:B:355:THR:HA  | 2.14                     | 0.48              |
| 1:E:183:THR:HG22 | 1:E:188:SER:HA  | 1.95                     | 0.48              |
| 1:E:47:ARG:NH2   | 1:E:73:SER:OG   | 2.46                     | 0.48              |
| 1:E:228:LEU:HA   | 3:E:414:HOH:O   | 2.12                     | 0.48              |
| 1:G:287:ASN:ND2  | 1:G:300:VAL:O   | 2.35                     | 0.48              |
| 1:K:168:LEU:HB3  | 1:K:249:SER:HB2 | 1.94                     | 0.48              |
| 2:L:345:PHE:O    | 2:L:355:THR:HA  | 2.12                     | 0.48              |
| 2:B:392:ASN:CG   | 3:B:505:HOH:O   | 2.50                     | 0.48              |
| 1:E:168:LEU:HB3  | 1:E:249:SER:HB2 | 1.95                     | 0.48              |
| 2:J:397:GLN:HB2  | 3:J:510:HOH:O   | 2.13                     | 0.48              |
| 1:C:100:GLN:CG   | 3:C:421:HOH:O   | 2.62                     | 0.48              |
| 1:I:122:THR:HB   | 3:I:413:HOH:O   | 2.13                     | 0.48              |
| 1:C:157:LYS:CD   | 3:C:427:HOH:O   | 2.57                     | 0.48              |
| 1:C:173:ILE:C    | 3:C:410:HOH:O   | 2.50                     | 0.48              |
| 1:I:177:VAL:HG13 | 1:I:218:SER:HB2 | 1.96                     | 0.48              |
| 1:I:183:THR:HG22 | 1:I:188:SER:HA  | 1.94                     | 0.48              |
| 1:K:49:VAL:HG23  | 1:K:74:ALA:HB2  | 1.96                     | 0.48              |
| 1:A:143:LEU:HB2  | 3:A:419:HOH:O   | 2.14                     | 0.47              |
| 1:C:25:GLU:CG    | 3:C:417:HOH:O   | 2.55                     | 0.47              |
| 1:C:272:CYS:CA   | 3:C:436:HOH:O   | 2.44                     | 0.47              |
| 2:B:448:ARG:HG3  | 2:B:480:HIS:HB2 | 1.96                     | 0.47              |
| 2:D:462:PHE:HB3  | 2:D:490:ASN:HB2 | 1.97                     | 0.47              |
| 1:E:198:SER:CB   | 3:E:401:HOH:O   | 2.48                     | 0.47              |
| 1:E:212:THR:O    | 1:E:220:ARG:NH2 | 2.29                     | 0.47              |
| 2:F:345:PHE:O    | 2:F:355:THR:HA  | 2.14                     | 0.47              |
| 1:E:186:TYR:O    | 1:E:191:LYS:NZ  | 2.37                     | 0.47              |
| 2:F:480:HIS:O    | 3:F:508:HOH:O   | 2.20                     | 0.47              |
| 1:G:2:LYS:CE     | 3:H:514:HOH:O   | 2.62                     | 0.47              |
| 2:H:395:GLU:CD   | 3:H:511:HOH:O   | 2.45                     | 0.47              |
| 2:L:484:ARG:HD2  | 3:L:505:HOH:O   | 2.14                     | 0.47              |
| 1:I:49:VAL:HG23  | 1:I:74:ALA:HB2  | 1.97                     | 0.47              |
| 1:C:130:ARG:NH2  | 3:C:431:HOH:O   | 2.38                     | 0.47              |
| 1:I:47:ARG:NH2   | 1:I:73:SER:OG   | 2.47                     | 0.47              |
| 1:I:65:GLN:HG3   | 3:I:414:HOH:O   | 2.14                     | 0.47              |
| 1:A:120:ILE:HB   | 1:A:144:LEU:O   | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:293:VAL:C    | 3:A:406:HOH:O    | 2.38                     | 0.47              |
| 1:C:21:GLU:CG    | 3:C:422:HOH:O    | 2.61                     | 0.47              |
| 1:C:156:THR:HA   | 1:C:236:PHE:O    | 2.14                     | 0.47              |
| 1:E:110:LYS:HA   | 1:E:248:ALA:O    | 2.15                     | 0.47              |
| 1:E:298:ARG:CD   | 3:E:420:HOH:O    | 2.51                     | 0.47              |
| 1:G:49:VAL:HG23  | 1:G:74:ALA:HB2   | 1.96                     | 0.47              |
| 1:G:131:ARG:NH1  | 1:G:136:PHE:O    | 2.38                     | 0.47              |
| 1:G:143:LEU:HD12 | 1:G:242:PHE:HD2  | 1.80                     | 0.47              |
| 1:K:186:TYR:HB2  | 1:K:191:LYS:HE3  | 1.97                     | 0.47              |
| 2:B:411:GLU:OE1  | 1:E:298:ARG:NH2  | 2.48                     | 0.47              |
| 1:A:28:ASN:ND2   | 3:A:434:HOH:O    | 2.48                     | 0.47              |
| 1:A:56:LEU:CB    | 3:A:422:HOH:O    | 2.62                     | 0.47              |
| 1:A:71:GLU:C     | 3:A:431:HOH:O    | 2.58                     | 0.47              |
| 1:G:312:LYS:HB2  | 2:H:429:ILE:HG23 | 1.96                     | 0.47              |
| 1:A:168:LEU:HB3  | 1:A:249:SER:HB2  | 1.96                     | 0.47              |
| 2:H:340:ASP:CB   | 3:H:512:HOH:O    | 2.63                     | 0.47              |
| 2:J:397:GLN:CB   | 3:J:510:HOH:O    | 2.63                     | 0.47              |
| 1:C:169:ILE:O    | 1:C:225:TRP:HA   | 2.14                     | 0.46              |
| 1:I:296:CYS:N    | 3:I:423:HOH:O    | 2.47                     | 0.46              |
| 1:A:201:GLN:CB   | 1:C:211:ARG:HE   | 2.27                     | 0.46              |
| 1:E:49:VAL:HG23  | 1:E:74:ALA:HB2   | 1.96                     | 0.46              |
| 1:E:143:LEU:HB2  | 3:E:405:HOH:O    | 2.15                     | 0.46              |
| 1:C:30:THR:CA    | 3:C:402:HOH:O    | 2.40                     | 0.46              |
| 2:D:480:HIS:C    | 3:D:509:HOH:O    | 2.58                     | 0.46              |
| 2:J:345:PHE:O    | 2:J:355:THR:HA   | 2.15                     | 0.46              |
| 2:J:445:ARG:HB3  | 2:L:455:GLY:HA2  | 1.96                     | 0.46              |
| 1:K:110:LYS:HA   | 1:K:248:ALA:O    | 2.16                     | 0.46              |
| 1:C:171:TRP:CE2  | 1:C:195:VAL:HG21 | 2.51                     | 0.46              |
| 2:H:388:ASP:OD2  | 2:H:406:ARG:NH2  | 2.47                     | 0.46              |
| 1:G:195:VAL:HG22 | 1:G:236:PHE:CD2  | 2.51                     | 0.46              |
| 1:A:68:GLN:NE2   | 3:A:412:HOH:O    | 2.47                     | 0.46              |
| 1:C:31:GLU:N     | 3:C:418:HOH:O    | 2.37                     | 0.46              |
| 1:C:120:ILE:HB   | 1:C:144:LEU:O    | 2.16                     | 0.46              |
| 1:G:110:LYS:HA   | 1:G:248:ALA:O    | 2.16                     | 0.46              |
| 1:G:63:PRO:CD    | 3:G:433:HOH:O    | 2.64                     | 0.46              |
| 1:G:88:TYR:HD1   | 1:G:126:THR:HG21 | 1.81                     | 0.46              |
| 1:I:298:ARG:NH2  | 2:L:411:GLU:OE1  | 2.49                     | 0.46              |
| 2:H:335:TRP:CH2  | 2:H:346:ARG:HB2  | 2.51                     | 0.46              |
| 1:A:191:LYS:O    | 1:A:206:PRO:CD   | 2.64                     | 0.45              |
| 1:C:5:LEU:N      | 3:D:504:HOH:O    | 2.40                     | 0.45              |
| 1:C:21:GLU:HB3   | 3:C:422:HOH:O    | 2.15                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:466:ASP:CG   | 3:H:515:HOH:O    | 2.58                     | 0.45              |
| 2:D:450:ASN:OD1  | 2:D:450:ASN:N    | 2.48                     | 0.45              |
| 1:G:172:GLY:HA2  | 1:G:222:ASP:O    | 2.17                     | 0.45              |
| 1:I:291:ARG:CZ   | 3:I:406:HOH:O    | 2.40                     | 0.45              |
| 1:A:190:ASN:HA   | 1:A:191:LYS:CB   | 2.37                     | 0.45              |
| 1:C:47:ARG:NH2   | 1:C:73:SER:OG    | 2.46                     | 0.45              |
| 1:E:20:THR:HG22  | 1:E:21:GLU:HG3   | 1.99                     | 0.45              |
| 2:F:462:PHE:HB3  | 2:F:490:ASN:HB2  | 1.99                     | 0.45              |
| 1:I:180:ALA:CB   | 3:I:415:HOH:O    | 2.64                     | 0.45              |
| 1:K:174:HIS:ND1  | 1:K:186:TYR:OH   | 2.46                     | 0.45              |
| 1:I:15:LYS:HD3   | 3:I:401:HOH:O    | 2.16                     | 0.45              |
| 1:I:186:TYR:HB2  | 1:I:191:LYS:HE3  | 1.98                     | 0.45              |
| 1:A:20:THR:HG22  | 1:A:21:GLU:HG3   | 1.98                     | 0.45              |
| 1:C:49:VAL:HG23  | 1:C:74:ALA:HB2   | 1.97                     | 0.45              |
| 2:D:376:LEU:HD11 | 2:D:424:GLU:HG3  | 1.99                     | 0.45              |
| 1:I:168:LEU:HB3  | 1:I:249:SER:HB2  | 1.97                     | 0.45              |
| 1:A:202:GLN:HA   | 1:A:203:SER:HB2  | 1.99                     | 0.45              |
| 2:B:399:GLY:C    | 3:B:508:HOH:O    | 2.47                     | 0.45              |
| 1:G:63:PRO:HD2   | 3:G:433:HOH:O    | 2.17                     | 0.45              |
| 1:A:191:LYS:N    | 1:A:239:ASN:HD21 | 2.12                     | 0.45              |
| 1:A:232:ASP:OD1  | 1:A:233:THR:N    | 2.47                     | 0.45              |
| 1:G:198:SER:HA   | 1:I:220:ARG:HH21 | 1.81                     | 0.45              |
| 1:A:8:HIS:N      | 2:B:342:TRP:O    | 2.45                     | 0.45              |
| 2:B:462:PHE:HB3  | 2:B:490:ASN:HB2  | 1.99                     | 0.45              |
| 2:B:480:HIS:ND1  | 3:B:506:HOH:O    | 2.36                     | 0.45              |
| 1:C:220:ARG:CZ   | 3:C:412:HOH:O    | 2.46                     | 0.45              |
| 1:I:110:LYS:HA   | 1:I:248:ALA:O    | 2.16                     | 0.45              |
| 1:K:183:THR:HG22 | 1:K:188:SER:HA   | 1.99                     | 0.45              |
| 2:B:400:ASN:ND2  | 1:E:100:GLN:OE1  | 2.41                     | 0.45              |
| 1:K:175:HIS:HB3  | 1:K:211:ARG:NH1  | 2.32                     | 0.45              |
| 1:C:201:GLN:NE2  | 1:E:222:ASP:OD1  | 2.49                     | 0.44              |
| 2:J:388:ASP:OD2  | 2:J:406:ARG:NH2  | 2.48                     | 0.44              |
| 1:A:47:ARG:NH2   | 1:A:73:SER:OG    | 2.49                     | 0.44              |
| 2:F:450:ASN:N    | 2:F:450:ASN:OD1  | 2.50                     | 0.44              |
| 2:H:411:GLU:OE1  | 1:K:298:ARG:NH2  | 2.50                     | 0.44              |
| 1:C:114:GLY:N    | 3:C:411:HOH:O    | 1.89                     | 0.44              |
| 1:C:117:TYR:HB3  | 1:C:120:ILE:HD11 | 1.98                     | 0.44              |
| 1:C:120:ILE:HG22 | 3:C:415:HOH:O    | 2.16                     | 0.44              |
| 1:G:202:GLN:CA   | 1:G:203:SER:CB   | 2.95                     | 0.44              |
| 1:I:143:LEU:HD12 | 1:I:242:PHE:HD2  | 1.82                     | 0.44              |
| 1:A:228:LEU:HD22 | 1:A:232:ASP:HB3  | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:137:TYR:HB2  | 1:A:140:MET:HB2  | 2.00                     | 0.44              |
| 2:B:450:ASN:OD1  | 2:B:450:ASN:N    | 2.50                     | 0.44              |
| 1:C:121:ARG:HD2  | 1:C:146:ASN:O    | 2.18                     | 0.44              |
| 2:H:479:ASP:OD1  | 2:H:481:SER:OG   | 2.33                     | 0.44              |
| 1:A:12:ASN:ND2   | 1:A:12:ASN:O     | 2.51                     | 0.44              |
| 1:A:98:LEU:CA    | 3:A:410:HOH:O    | 2.34                     | 0.44              |
| 2:F:382:GLN:N    | 3:F:503:HOH:O    | 2.48                     | 0.44              |
| 1:I:12:ASN:O     | 1:I:12:ASN:ND2   | 2.51                     | 0.44              |
| 2:D:447:LEU:HA   | 3:D:501:HOH:O    | 2.08                     | 0.44              |
| 2:H:466:ASP:OD1  | 2:H:466:ASP:N    | 2.49                     | 0.44              |
| 1:K:143:LEU:HD12 | 1:K:242:PHE:HD2  | 1.83                     | 0.44              |
| 1:K:131:ARG:NH1  | 1:K:136:PHE:O    | 2.40                     | 0.43              |
| 1:A:176:SER:CB   | 3:A:416:HOH:O    | 2.62                     | 0.43              |
| 1:E:88:TYR:HD1   | 1:E:126:THR:HG21 | 1.83                     | 0.43              |
| 1:E:232:ASP:OD2  | 3:E:414:HOH:O    | 2.21                     | 0.43              |
| 2:H:487:ALA:CB   | 3:H:502:HOH:O    | 2.65                     | 0.43              |
| 1:K:316:GLU:HG3  | 2:L:336:GLU:HG3  | 2.00                     | 0.43              |
| 1:I:151:ALA:N    | 3:I:411:HOH:O    | 2.47                     | 0.43              |
| 2:B:469:CYS:O    | 2:B:473:ILE:HG13 | 2.19                     | 0.43              |
| 2:F:450:ASN:ND2  | 3:F:508:HOH:O    | 2.21                     | 0.43              |
| 1:K:48:THR:HB    | 3:K:418:HOH:O    | 2.17                     | 0.43              |
| 1:A:195:VAL:HG22 | 1:A:236:PHE:HD2  | 1.84                     | 0.43              |
| 1:E:198:SER:HB3  | 3:E:401:HOH:O    | 2.17                     | 0.43              |
| 2:J:379:LYS:C    | 3:J:511:HOH:O    | 2.52                     | 0.43              |
| 1:G:202:GLN:NE2  | 3:G:420:HOH:O    | 2.51                     | 0.43              |
| 2:H:484:ARG:C    | 3:H:502:HOH:O    | 2.47                     | 0.43              |
| 1:K:106:GLY:HA2  | 1:K:255:SER:HB3  | 2.00                     | 0.43              |
| 1:A:51:LEU:HB2   | 3:A:427:HOH:O    | 2.19                     | 0.43              |
| 2:B:369:ILE:HD11 | 2:B:428:THR:HG23 | 2.01                     | 0.43              |
| 1:G:106:GLY:HA2  | 1:G:255:SER:HB3  | 2.01                     | 0.43              |
| 1:G:197:SER:HB3  | 1:G:234:VAL:HG23 | 2.01                     | 0.43              |
| 2:H:487:ALA:HB3  | 3:H:502:HOH:O    | 2.18                     | 0.43              |
| 1:C:106:GLY:HA2  | 1:C:255:SER:HB3  | 2.01                     | 0.43              |
| 1:C:143:LEU:HD12 | 1:C:242:PHE:HD2  | 1.83                     | 0.43              |
| 1:G:301:LYS:CD   | 3:G:417:HOH:O    | 2.66                     | 0.43              |
| 2:H:346:ARG:HA   | 2:H:354:GLY:O    | 2.18                     | 0.43              |
| 1:I:23:GLY:CA    | 3:I:401:HOH:O    | 2.66                     | 0.43              |
| 2:J:450:ASN:OD1  | 2:J:450:ASN:N    | 2.52                     | 0.43              |
| 1:E:143:LEU:HD12 | 1:E:242:PHE:HD2  | 1.84                     | 0.43              |
| 1:I:305:LEU:HB3  | 2:J:421:VAL:HG21 | 2.01                     | 0.43              |
| 1:A:106:GLY:HA2  | 1:A:255:SER:HB3  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:174:HIS:ND1  | 1:C:186:TYR:OH   | 2.41                     | 0.42              |
| 1:C:191:LYS:HE2  | 3:C:419:HOH:O    | 2.18                     | 0.42              |
| 1:E:130:ARG:NH2  | 3:E:422:HOH:O    | 2.44                     | 0.42              |
| 1:C:93:VAL:HB    | 3:C:445:HOH:O    | 2.18                     | 0.42              |
| 2:D:458:CYS:HA   | 3:D:504:HOH:O    | 2.18                     | 0.42              |
| 1:G:96:GLU:HG2   | 2:H:394:VAL:HG12 | 2.00                     | 0.42              |
| 1:I:106:GLY:HA2  | 1:I:255:SER:HB3  | 2.01                     | 0.42              |
| 1:C:139:GLU:OE1  | 1:C:247:ARG:HD3  | 2.20                     | 0.42              |
| 1:E:139:GLU:OE1  | 1:E:247:ARG:HD3  | 2.19                     | 0.42              |
| 1:I:212:THR:HG22 | 1:I:213:GLN:H    | 1.84                     | 0.42              |
| 2:L:450:ASN:OD1  | 2:L:450:ASN:N    | 2.52                     | 0.42              |
| 2:L:480:HIS:CB   | 3:L:506:HOH:O    | 2.65                     | 0.42              |
| 1:A:298:ARG:HG2  | 2:B:413:TRP:CE2  | 2.55                     | 0.42              |
| 2:H:453:GLU:HG2  | 2:H:459:PHE:HE2  | 1.84                     | 0.42              |
| 1:E:202:GLN:CA   | 1:E:203:SER:CB   | 2.95                     | 0.42              |
| 1:G:171:TRP:CE2  | 1:G:224:HIS:HB2  | 2.55                     | 0.42              |
| 1:I:197:SER:OG   | 1:I:200:TYR:HB3  | 2.20                     | 0.42              |
| 1:A:110:LYS:HA   | 1:A:248:ALA:O    | 2.19                     | 0.42              |
| 2:B:383:GLN:NE2  | 2:B:385:GLU:OE2  | 2.48                     | 0.42              |
| 2:F:376:LEU:HD11 | 2:F:424:GLU:HG3  | 2.02                     | 0.42              |
| 1:C:105:SER:HB2  | 1:C:251:LEU:HD22 | 2.01                     | 0.42              |
| 1:C:177:VAL:HG13 | 1:C:218:SER:HB2  | 2.02                     | 0.42              |
| 1:E:151:ALA:HA   | 3:E:404:HOH:O    | 2.14                     | 0.42              |
| 1:G:301:LYS:NZ   | 3:G:417:HOH:O    | 2.29                     | 0.42              |
| 2:H:384:PHE:CD1  | 3:H:507:HOH:O    | 2.72                     | 0.42              |
| 2:H:345:PHE:O    | 2:H:355:THR:HA   | 2.20                     | 0.42              |
| 1:K:202:GLN:CA   | 1:K:203:SER:HB3  | 2.44                     | 0.42              |
| 1:C:305:LEU:HB3  | 2:D:421:VAL:HG21 | 2.01                     | 0.42              |
| 2:F:447:LEU:CD2  | 3:F:506:HOH:O    | 2.29                     | 0.42              |
| 1:G:186:TYR:O    | 1:G:191:LYS:NZ   | 2.47                     | 0.42              |
| 2:B:408:SER:HB3  | 2:F:409:ILE:HG12 | 2.02                     | 0.41              |
| 1:I:63:PRO:HD2   | 1:I:66:CYS:HB2   | 2.02                     | 0.41              |
| 1:I:174:HIS:ND1  | 1:I:186:TYR:OH   | 2.45                     | 0.41              |
| 1:I:180:ALA:HA   | 3:I:415:HOH:O    | 2.14                     | 0.41              |
| 2:H:376:LEU:HD11 | 2:H:424:GLU:HG3  | 2.01                     | 0.41              |
| 3:I:410:HOH:O    | 2:J:335:TRP:HA   | 2.20                     | 0.41              |
| 1:K:154:GLN:CG   | 3:K:404:HOH:O    | 2.05                     | 0.41              |
| 1:E:12:ASN:O     | 1:E:12:ASN:ND2   | 2.53                     | 0.41              |
| 1:K:156:THR:HA   | 1:K:236:PHE:O    | 2.21                     | 0.41              |
| 2:H:382:GLN:CD   | 3:H:523:HOH:O    | 2.62                     | 0.41              |
| 1:I:8:HIS:CG     | 3:I:402:HOH:O    | 2.57                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:379:LYS:CA   | 3:J:511:HOH:O    | 2.69                     | 0.41              |
| 1:G:12:ASN:O     | 1:G:12:ASN:ND2   | 2.53                     | 0.41              |
| 1:G:169:ILE:HB   | 1:G:226:LEU:CD2  | 2.49                     | 0.41              |
| 2:H:445:ARG:HB3  | 2:J:455:GLY:HA2  | 2.02                     | 0.41              |
| 1:C:166:PRO:HA   | 1:C:228:LEU:O    | 2.21                     | 0.41              |
| 3:I:402:HOH:O    | 2:J:342:TRP:CD1  | 2.73                     | 0.41              |
| 2:J:442:ARG:HB3  | 2:J:442:ARG:HH11 | 1.85                     | 0.41              |
| 1:C:21:GLU:CB    | 3:C:422:HOH:O    | 2.69                     | 0.41              |
| 1:G:163:ARG:HD3  | 1:G:250:PHE:CZ   | 2.56                     | 0.41              |
| 1:K:163:ARG:HD3  | 1:K:250:PHE:CZ   | 2.55                     | 0.41              |
| 2:B:390:GLU:CD   | 3:B:509:HOH:O    | 2.59                     | 0.41              |
| 1:E:106:GLY:HA2  | 1:E:255:SER:HB3  | 2.03                     | 0.41              |
| 1:E:116:THR:O    | 1:E:157:LYS:NZ   | 2.49                     | 0.41              |
| 1:G:141:LYS:HE2  | 1:G:246:ASP:OD2  | 2.21                     | 0.41              |
| 1:G:211:ARG:HG3  | 1:K:196:GLY:HA3  | 2.03                     | 0.41              |
| 2:J:462:PHE:HB3  | 2:J:490:ASN:HB2  | 2.01                     | 0.41              |
| 1:K:166:PRO:HA   | 1:K:228:LEU:O    | 2.20                     | 0.41              |
| 1:A:19:LEU:HG    | 2:F:424:GLU:OE2  | 2.21                     | 0.41              |
| 2:B:376:LEU:HD23 | 2:B:376:LEU:HA   | 1.91                     | 0.41              |
| 1:C:63:PRO:HD2   | 1:C:66:CYS:HB2   | 2.02                     | 0.41              |
| 2:D:388:ASP:OD2  | 2:D:406:ARG:NH2  | 2.51                     | 0.41              |
| 1:G:115:PHE:HE2  | 3:G:419:HOH:O    | 1.99                     | 0.41              |
| 1:G:170:VAL:O    | 1:G:245:PRO:HB3  | 2.21                     | 0.41              |
| 2:H:328:ALA:HA   | 3:H:516:HOH:O    | 2.21                     | 0.41              |
| 2:L:347:HIS:CD2  | 2:L:474:ARG:HH12 | 2.38                     | 0.41              |
| 2:L:466:ASP:OD1  | 2:L:466:ASP:N    | 2.49                     | 0.41              |
| 1:A:228:LEU:HD23 | 1:A:228:LEU:HA   | 1.94                     | 0.41              |
| 1:G:168:LEU:HB3  | 1:G:249:SER:HB2  | 2.04                     | 0.41              |
| 2:L:484:ARG:CG   | 3:L:510:HOH:O    | 2.53                     | 0.40              |
| 1:A:195:VAL:HG22 | 1:A:236:PHE:CD2  | 2.57                     | 0.40              |
| 1:C:12:ASN:O     | 1:C:12:ASN:ND2   | 2.54                     | 0.40              |
| 2:F:388:ASP:OD2  | 2:F:406:ARG:NH2  | 2.51                     | 0.40              |
| 2:F:392:ASN:ND2  | 3:F:513:HOH:O    | 2.54                     | 0.40              |
| 1:G:166:PRO:HA   | 1:G:228:LEU:O    | 2.21                     | 0.40              |
| 2:J:378:GLU:N    | 3:J:506:HOH:O    | 2.44                     | 0.40              |
| 1:C:163:ARG:HD3  | 1:C:250:PHE:CZ   | 2.57                     | 0.40              |
| 1:E:144:LEU:HD22 | 1:E:185:LEU:HD22 | 2.04                     | 0.40              |
| 1:E:305:LEU:HB3  | 2:F:421:VAL:HG21 | 2.03                     | 0.40              |
| 1:I:139:GLU:OE1  | 1:I:247:ARG:HD3  | 2.21                     | 0.40              |
| 2:L:481:SER:HA   | 2:L:484:ARG:HG3  | 2.03                     | 0.40              |
| 2:L:347:HIS:O    | 2:L:353:GLU:HG3  | 2.20                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:G:12:ASN:CA   | 3:G:408:HOH:O   | 2.62                     | 0.40              |
| 1:G:139:GLU:OE1 | 1:G:247:ARG:HD3 | 2.22                     | 0.40              |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|------------------------|--------------------------|-------------------|
| 3:C:456:HOH:O | 3:K:429:HOH:O[2_775]   | 1.87                     | 0.33              |
| 1:E:215:ASN:O | 2:J:346:ARG:NH1[3_675] | 2.08                     | 0.12              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 312/321 (97%)   | 290 (93%)  | 21 (7%)  | 1 (0%)   | 36          | 60  |
| 1   | C     | 312/321 (97%)   | 290 (93%)  | 22 (7%)  | 0        | 100         | 100 |
| 1   | E     | 312/321 (97%)   | 292 (94%)  | 18 (6%)  | 2 (1%)   | 21          | 44  |
| 1   | G     | 314/321 (98%)   | 290 (92%)  | 21 (7%)  | 3 (1%)   | 12          | 32  |
| 1   | I     | 314/321 (98%)   | 294 (94%)  | 20 (6%)  | 0        | 100         | 100 |
| 1   | K     | 314/321 (98%)   | 294 (94%)  | 18 (6%)  | 2 (1%)   | 21          | 44  |
| 2   | B     | 161/177 (91%)   | 151 (94%)  | 10 (6%)  | 0        | 100         | 100 |
| 2   | D     | 161/177 (91%)   | 150 (93%)  | 11 (7%)  | 0        | 100         | 100 |
| 2   | F     | 161/177 (91%)   | 151 (94%)  | 10 (6%)  | 0        | 100         | 100 |
| 2   | H     | 161/177 (91%)   | 155 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 2   | J     | 161/177 (91%)   | 153 (95%)  | 7 (4%)   | 1 (1%)   | 21          | 44  |
| 2   | L     | 161/177 (91%)   | 151 (94%)  | 9 (6%)   | 1 (1%)   | 21          | 44  |
| All | All   | 2844/2988 (95%) | 2661 (94%) | 173 (6%) | 10 (0%)  | 30          | 54  |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 202 | GLN  |
| 1   | G     | 202 | GLN  |
| 1   | K     | 203 | SER  |
| 1   | K     | 202 | GLN  |
| 1   | E     | 203 | SER  |
| 1   | G     | 203 | SER  |
| 1   | A     | 203 | SER  |
| 1   | G     | 189 | GLY  |
| 2   | J     | 394 | VAL  |
| 2   | L     | 394 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 263/269 (98%)   | 246 (94%)  | 17 (6%)  | 15          | 37 |
| 1   | C     | 263/269 (98%)   | 254 (97%)  | 9 (3%)   | 32          | 62 |
| 1   | E     | 263/269 (98%)   | 252 (96%)  | 11 (4%)  | 26          | 55 |
| 1   | G     | 265/269 (98%)   | 254 (96%)  | 11 (4%)  | 26          | 55 |
| 1   | I     | 265/269 (98%)   | 255 (96%)  | 10 (4%)  | 29          | 58 |
| 1   | K     | 265/269 (98%)   | 256 (97%)  | 9 (3%)   | 32          | 62 |
| 2   | B     | 141/152 (93%)   | 137 (97%)  | 4 (3%)   | 38          | 68 |
| 2   | D     | 141/152 (93%)   | 137 (97%)  | 4 (3%)   | 38          | 68 |
| 2   | F     | 141/152 (93%)   | 137 (97%)  | 4 (3%)   | 38          | 68 |
| 2   | H     | 141/152 (93%)   | 130 (92%)  | 11 (8%)  | 11          | 29 |
| 2   | J     | 141/152 (93%)   | 137 (97%)  | 4 (3%)   | 38          | 68 |
| 2   | L     | 141/152 (93%)   | 135 (96%)  | 6 (4%)   | 26          | 54 |
| All | All   | 2430/2526 (96%) | 2330 (96%) | 100 (4%) | 27          | 56 |

All (100) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | ILE  |
| 1   | A     | 7   | HIS  |
| 1   | A     | 19  | LEU  |
| 1   | A     | 120 | ILE  |
| 1   | A     | 121 | ARG  |
| 1   | A     | 147 | THR  |
| 1   | A     | 148 | ASP  |
| 1   | A     | 160 | LYS  |
| 1   | A     | 183 | THR  |
| 1   | A     | 190 | ASN  |
| 1   | A     | 191 | LYS  |
| 1   | A     | 194 | THR  |
| 1   | A     | 202 | GLN  |
| 1   | A     | 213 | GLN  |
| 1   | A     | 226 | LEU  |
| 1   | A     | 237 | SER  |
| 1   | A     | 312 | LYS  |
| 2   | B     | 442 | ARG  |
| 2   | B     | 448 | ARG  |
| 2   | B     | 450 | ASN  |
| 2   | B     | 454 | ASP  |
| 1   | C     | 7   | HIS  |
| 1   | C     | 19  | LEU  |
| 1   | C     | 91  | LYS  |
| 1   | C     | 120 | ILE  |
| 1   | C     | 121 | ARG  |
| 1   | C     | 192 | LEU  |
| 1   | C     | 194 | THR  |
| 1   | C     | 282 | ASN  |
| 1   | C     | 312 | LYS  |
| 2   | D     | 373 | LEU  |
| 2   | D     | 442 | ARG  |
| 2   | D     | 450 | ASN  |
| 2   | D     | 454 | ASP  |
| 1   | E     | 7   | HIS  |
| 1   | E     | 19  | LEU  |
| 1   | E     | 120 | ILE  |
| 1   | E     | 127 | SER  |
| 1   | E     | 148 | ASP  |
| 1   | E     | 199 | ASN  |
| 1   | E     | 203 | SER  |
| 1   | E     | 213 | GLN  |
| 1   | E     | 226 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 282 | ASN  |
| 1   | E     | 312 | LYS  |
| 2   | F     | 373 | LEU  |
| 2   | F     | 442 | ARG  |
| 2   | F     | 450 | ASN  |
| 2   | F     | 454 | ASP  |
| 1   | G     | 5   | LEU  |
| 1   | G     | 19  | LEU  |
| 1   | G     | 38  | ILE  |
| 1   | G     | 120 | ILE  |
| 1   | G     | 148 | ASP  |
| 1   | G     | 194 | THR  |
| 1   | G     | 199 | ASN  |
| 1   | G     | 201 | GLN  |
| 1   | G     | 202 | GLN  |
| 1   | G     | 282 | ASN  |
| 1   | G     | 312 | LYS  |
| 2   | H     | 332 | GLU  |
| 2   | H     | 346 | ARG  |
| 2   | H     | 348 | GLN  |
| 2   | H     | 373 | LEU  |
| 2   | H     | 442 | ARG  |
| 2   | H     | 448 | ARG  |
| 2   | H     | 449 | GLU  |
| 2   | H     | 454 | ASP  |
| 2   | H     | 464 | LYS  |
| 2   | H     | 481 | SER  |
| 2   | H     | 482 | LYS  |
| 1   | I     | 1   | ASP  |
| 1   | I     | 7   | HIS  |
| 1   | I     | 19  | LEU  |
| 1   | I     | 120 | ILE  |
| 1   | I     | 146 | ASN  |
| 1   | I     | 148 | ASP  |
| 1   | I     | 207 | SER  |
| 1   | I     | 212 | THR  |
| 1   | I     | 282 | ASN  |
| 1   | I     | 316 | GLU  |
| 2   | J     | 373 | LEU  |
| 2   | J     | 442 | ARG  |
| 2   | J     | 450 | ASN  |
| 2   | J     | 454 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 1   | ASP  |
| 1   | K     | 7   | HIS  |
| 1   | K     | 19  | LEU  |
| 1   | K     | 120 | ILE  |
| 1   | K     | 148 | ASP  |
| 1   | K     | 194 | THR  |
| 1   | K     | 226 | LEU  |
| 1   | K     | 282 | ASN  |
| 1   | K     | 312 | LYS  |
| 2   | L     | 373 | LEU  |
| 2   | L     | 442 | ARG  |
| 2   | L     | 447 | LEU  |
| 2   | L     | 449 | GLU  |
| 2   | L     | 450 | ASN  |
| 2   | L     | 454 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | ASN  |
| 1   | C     | 12  | ASN  |
| 1   | E     | 12  | ASN  |
| 2   | F     | 397 | GLN  |
| 1   | G     | 12  | ASN  |
| 1   | G     | 146 | ASN  |
| 2   | H     | 351 | GLN  |
| 2   | H     | 381 | ASN  |
| 1   | I     | 12  | ASN  |
| 1   | I     | 146 | ASN  |
| 2   | J     | 381 | ASN  |
| 1   | K     | 202 | GLN  |
| 1   | K     | 213 | GLN  |
| 2   | L     | 351 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2                     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|-----------------------------|-----------------------|-------|
| 1   | A     | 314/321 (97%)   | 1.54   | 96 (30%) <b>1</b> <b>1</b>  | 27, 43, 82, 123       | 0     |
| 1   | C     | 314/321 (97%)   | 0.98   | 59 (18%) <b>3</b> <b>3</b>  | 24, 40, 75, 117       | 0     |
| 1   | E     | 314/321 (97%)   | 1.00   | 52 (16%) <b>4</b> <b>4</b>  | 25, 40, 76, 105       | 0     |
| 1   | G     | 316/321 (98%)   | 2.28   | 167 (52%) <b>0</b> <b>0</b> | 29, 74, 112, 143      | 0     |
| 1   | I     | 316/321 (98%)   | 1.88   | 124 (39%) <b>1</b> <b>0</b> | 20, 75, 115, 148      | 0     |
| 1   | K     | 316/321 (98%)   | 1.45   | 84 (26%) <b>1</b> <b>1</b>  | 27, 64, 98, 122       | 0     |
| 2   | B     | 163/177 (92%)   | 1.77   | 62 (38%) <b>1</b> <b>0</b>  | 20, 69, 105, 137      | 0     |
| 2   | D     | 163/177 (92%)   | 1.99   | 68 (41%) <b>0</b> <b>0</b>  | 30, 75, 115, 140      | 0     |
| 2   | F     | 163/177 (92%)   | 1.80   | 67 (41%) <b>0</b> <b>0</b>  | 26, 76, 115, 138      | 0     |
| 2   | H     | 163/177 (92%)   | 1.04   | 26 (15%) <b>5</b> <b>4</b>  | 21, 41, 72, 121       | 0     |
| 2   | J     | 163/177 (92%)   | 1.49   | 44 (26%) <b>1</b> <b>1</b>  | 23, 42, 79, 111       | 0     |
| 2   | L     | 163/177 (92%)   | 1.51   | 42 (25%) <b>1</b> <b>1</b>  | 22, 45, 82, 132       | 0     |
| All | All   | 2868/2988 (95%) | 1.55   | 891 (31%) <b>1</b> <b>1</b> | 20, 54, 105, 148      | 0     |

All (891) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | J     | 464 | LYS  | 10.3 |
| 1   | A     | 4   | CYS  | 9.3  |
| 1   | A     | 7   | HIS  | 8.9  |
| 2   | B     | 328 | ALA  | 8.8  |
| 1   | G     | 147 | THR  | 8.6  |
| 1   | A     | 3   | ILE  | 8.5  |
| 1   | I     | 222 | ASP  | 8.3  |
| 2   | D     | 328 | ALA  | 7.7  |
| 2   | L     | 379 | LYS  | 7.6  |
| 1   | G     | 130 | ARG  | 7.5  |
| 1   | I     | 194 | THR  | 7.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | D     | 464 | LYS  | 7.4  |
| 2   | F     | 464 | LYS  | 7.3  |
| 2   | F     | 480 | HIS  | 6.9  |
| 2   | D     | 480 | HIS  | 6.9  |
| 2   | L     | 348 | GLN  | 6.9  |
| 2   | B     | 480 | HIS  | 6.8  |
| 1   | K     | 216 | GLY  | 6.7  |
| 1   | G     | 151 | ALA  | 6.7  |
| 2   | L     | 328 | ALA  | 6.7  |
| 2   | D     | 378 | GLU  | 6.6  |
| 2   | D     | 351 | GLN  | 6.6  |
| 1   | A     | 179 | THR  | 6.6  |
| 1   | A     | 6   | GLY  | 6.5  |
| 1   | I     | 91  | LYS  | 6.5  |
| 2   | D     | 379 | LYS  | 6.5  |
| 2   | J     | 348 | GLN  | 6.5  |
| 2   | H     | 379 | LYS  | 6.4  |
| 1   | I     | 195 | VAL  | 6.3  |
| 1   | A     | 261 | GLY  | 6.3  |
| 2   | L     | 480 | HIS  | 6.2  |
| 2   | H     | 380 | THR  | 6.2  |
| 1   | G     | 236 | PHE  | 6.2  |
| 1   | G     | 240 | GLY  | 6.2  |
| 1   | G     | 235 | THR  | 6.1  |
| 1   | A     | 150 | ALA  | 6.1  |
| 2   | F     | 328 | ALA  | 6.1  |
| 1   | A     | 5   | LEU  | 6.1  |
| 1   | C     | 3   | ILE  | 6.0  |
| 1   | G     | 156 | THR  | 6.0  |
| 1   | G     | 230 | PRO  | 6.0  |
| 1   | G     | 158 | SER  | 5.9  |
| 1   | E     | 3   | ILE  | 5.9  |
| 2   | J     | 462 | PHE  | 5.9  |
| 1   | G     | 232 | ASP  | 5.8  |
| 1   | I     | 153 | PRO  | 5.8  |
| 1   | G     | 90  | GLY  | 5.7  |
| 1   | E     | 148 | ASP  | 5.7  |
| 1   | A     | 24  | VAL  | 5.7  |
| 2   | F     | 380 | THR  | 5.7  |
| 2   | B     | 350 | ALA  | 5.5  |
| 1   | G     | 144 | LEU  | 5.5  |
| 1   | G     | 150 | ALA  | 5.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | J     | 396 | LYS  | 5.5  |
| 2   | D     | 350 | ALA  | 5.4  |
| 1   | I     | 239 | ASN  | 5.4  |
| 1   | A     | 20  | THR  | 5.4  |
| 1   | I     | 210 | ALA  | 5.4  |
| 1   | G     | 234 | VAL  | 5.3  |
| 1   | G     | 160 | LYS  | 5.3  |
| 2   | F     | 379 | LYS  | 5.3  |
| 2   | L     | 395 | GLU  | 5.3  |
| 1   | G     | 268 | CYS  | 5.2  |
| 2   | D     | 353 | GLU  | 5.2  |
| 2   | B     | 351 | GLN  | 5.2  |
| 2   | D     | 462 | PHE  | 5.2  |
| 1   | G     | 117 | TYR  | 5.1  |
| 1   | G     | 228 | LEU  | 5.1  |
| 2   | L     | 385 | GLU  | 5.1  |
| 2   | J     | 487 | ALA  | 5.1  |
| 1   | G     | 233 | THR  | 5.1  |
| 1   | G     | 164 | LYS  | 5.1  |
| 1   | A     | 21  | GLU  | 5.1  |
| 1   | G     | 261 | GLY  | 5.1  |
| 1   | I     | 176 | SER  | 5.1  |
| 2   | L     | 386 | LEU  | 5.0  |
| 1   | A     | 8   | HIS  | 5.0  |
| 2   | F     | 392 | ASN  | 5.0  |
| 1   | G     | 134 | SER  | 5.0  |
| 1   | I     | 151 | ALA  | 5.0  |
| 1   | A     | 12  | ASN  | 4.9  |
| 1   | K     | 237 | SER  | 4.9  |
| 1   | A     | 268 | CYS  | 4.9  |
| 2   | D     | 380 | THR  | 4.9  |
| 1   | G     | 256 | MET  | 4.9  |
| 1   | G     | 237 | SER  | 4.8  |
| 2   | H     | 328 | ALA  | 4.8  |
| 2   | D     | 463 | HIS  | 4.8  |
| 1   | G     | 296 | CYS  | 4.8  |
| 1   | I     | 145 | SER  | 4.8  |
| 1   | I     | 12  | ASN  | 4.8  |
| 1   | E     | 121 | ARG  | 4.8  |
| 1   | A     | 10  | VAL  | 4.8  |
| 1   | G     | 203 | SER  | 4.8  |
| 1   | I     | 217 | LEU  | 4.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 177 | VAL  | 4.7  |
| 1   | A     | 314 | VAL  | 4.7  |
| 1   | A     | 23  | GLY  | 4.7  |
| 1   | A     | 87  | CYS  | 4.7  |
| 1   | E     | 219 | GLY  | 4.7  |
| 2   | J     | 380 | THR  | 4.7  |
| 1   | G     | 122 | THR  | 4.7  |
| 1   | G     | 152 | PHE  | 4.7  |
| 2   | B     | 462 | PHE  | 4.7  |
| 1   | G     | 44  | LYS  | 4.7  |
| 1   | I     | 214 | VAL  | 4.7  |
| 1   | G     | 114 | GLY  | 4.6  |
| 2   | B     | 378 | GLU  | 4.6  |
| 1   | G     | 118 | SER  | 4.6  |
| 1   | G     | 229 | ASN  | 4.6  |
| 1   | G     | 116 | THR  | 4.6  |
| 1   | C     | 315 | PRO  | 4.6  |
| 1   | G     | 104 | GLU  | 4.6  |
| 2   | D     | 396 | LYS  | 4.6  |
| 1   | G     | 20  | THR  | 4.6  |
| 1   | G     | 115 | PHE  | 4.6  |
| 2   | B     | 441 | GLU  | 4.5  |
| 1   | E     | 29  | ALA  | 4.5  |
| 1   | G     | 231 | ASN  | 4.5  |
| 2   | H     | 388 | ASP  | 4.5  |
| 1   | G     | 43  | SER  | 4.5  |
| 1   | G     | 132 | SER  | 4.5  |
| 1   | I     | 237 | SER  | 4.5  |
| 2   | B     | 352 | GLY  | 4.5  |
| 1   | C     | 311 | MET  | 4.5  |
| 2   | F     | 395 | GLU  | 4.5  |
| 1   | G     | 108 | ILE  | 4.4  |
| 2   | F     | 489 | GLN  | 4.4  |
| 2   | L     | 381 | ASN  | 4.4  |
| 1   | G     | 23  | GLY  | 4.4  |
| 2   | D     | 352 | GLY  | 4.4  |
| 2   | B     | 379 | LYS  | 4.4  |
| 1   | I     | 120 | ILE  | 4.4  |
| 2   | B     | 464 | LYS  | 4.3  |
| 2   | D     | 483 | TYR  | 4.3  |
| 1   | I     | 191 | LYS  | 4.3  |
| 1   | K     | 199 | ASN  | 4.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | J     | 328 | ALA  | 4.3  |
| 1   | K     | 219 | GLY  | 4.3  |
| 1   | I     | 193 | VAL  | 4.3  |
| 1   | I     | 275 | SER  | 4.2  |
| 1   | I     | 192 | LEU  | 4.2  |
| 2   | B     | 353 | GLU  | 4.2  |
| 2   | F     | 462 | PHE  | 4.2  |
| 1   | A     | 219 | GLY  | 4.2  |
| 1   | C     | 257 | GLY  | 4.2  |
| 1   | I     | 152 | PHE  | 4.2  |
| 1   | I     | 238 | PHE  | 4.2  |
| 1   | K     | 120 | ILE  | 4.2  |
| 1   | A     | 316 | GLU  | 4.2  |
| 2   | D     | 344 | GLY  | 4.2  |
| 1   | I     | 164 | LYS  | 4.2  |
| 1   | K     | 151 | ALA  | 4.1  |
| 2   | B     | 356 | ALA  | 4.1  |
| 1   | E     | 198 | SER  | 4.1  |
| 1   | I     | 215 | ASN  | 4.1  |
| 2   | D     | 465 | CYS  | 4.1  |
| 1   | A     | 14  | THR  | 4.1  |
| 2   | L     | 380 | THR  | 4.1  |
| 1   | I     | 117 | TYR  | 4.1  |
| 1   | K     | 197 | SER  | 4.1  |
| 1   | I     | 183 | THR  | 4.1  |
| 2   | B     | 485 | GLU  | 4.0  |
| 1   | G     | 148 | ASP  | 4.0  |
| 1   | K     | 127 | SER  | 4.0  |
| 1   | I     | 254 | LYS  | 4.0  |
| 2   | B     | 329 | GLY  | 4.0  |
| 1   | G     | 161 | ASN  | 4.0  |
| 2   | F     | 453 | GLU  | 4.0  |
| 2   | L     | 339 | ILE  | 4.0  |
| 1   | A     | 19  | LEU  | 4.0  |
| 1   | K     | 190 | ASN  | 4.0  |
| 2   | H     | 396 | LYS  | 4.0  |
| 2   | D     | 441 | GLU  | 4.0  |
| 2   | H     | 377 | ILE  | 4.0  |
| 1   | I     | 116 | THR  | 3.9  |
| 1   | G     | 280 | ILE  | 3.9  |
| 1   | K     | 19  | LEU  | 3.9  |
| 2   | B     | 482 | LYS  | 3.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 159 | TYR  | 3.9  |
| 2   | D     | 482 | LYS  | 3.9  |
| 1   | K     | 122 | THR  | 3.9  |
| 2   | B     | 380 | THR  | 3.9  |
| 1   | G     | 167 | ALA  | 3.9  |
| 2   | F     | 354 | GLY  | 3.9  |
| 1   | K     | 236 | PHE  | 3.9  |
| 1   | A     | 315 | PRO  | 3.9  |
| 1   | I     | 181 | GLU  | 3.8  |
| 2   | F     | 485 | GLU  | 3.8  |
| 1   | I     | 165 | SER  | 3.8  |
| 1   | K     | 144 | LEU  | 3.8  |
| 1   | A     | 282 | ASN  | 3.8  |
| 1   | I     | 190 | ASN  | 3.8  |
| 1   | E     | 150 | ALA  | 3.8  |
| 2   | B     | 349 | ASN  | 3.8  |
| 2   | J     | 379 | LYS  | 3.8  |
| 2   | H     | 378 | GLU  | 3.8  |
| 1   | A     | 256 | MET  | 3.8  |
| 1   | C     | 9   | ALA  | 3.8  |
| 1   | K     | 241 | ALA  | 3.8  |
| 2   | B     | 484 | ARG  | 3.8  |
| 2   | D     | 485 | GLU  | 3.8  |
| 1   | A     | 53  | GLN  | 3.7  |
| 1   | A     | 181 | GLU  | 3.7  |
| 1   | G     | 21  | GLU  | 3.7  |
| 1   | I     | 155 | MET  | 3.7  |
| 2   | L     | 376 | LEU  | 3.7  |
| 1   | K     | 132 | SER  | 3.7  |
| 2   | J     | 378 | GLU  | 3.7  |
| 1   | G     | 143 | LEU  | 3.7  |
| 2   | F     | 461 | ILE  | 3.7  |
| 1   | I     | 158 | SER  | 3.7  |
| 2   | F     | 350 | ALA  | 3.7  |
| 1   | A     | 254 | LYS  | 3.7  |
| 2   | D     | 346 | ARG  | 3.7  |
| 1   | C     | 177 | VAL  | 3.7  |
| 1   | K     | 155 | MET  | 3.7  |
| 2   | D     | 343 | TYR  | 3.7  |
| 1   | A     | 310 | GLY  | 3.7  |
| 1   | K     | 125 | ALA  | 3.7  |
| 1   | G     | 145 | SER  | 3.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 132 | SER  | 3.7  |
| 2   | B     | 344 | GLY  | 3.7  |
| 1   | G     | 264 | VAL  | 3.7  |
| 2   | D     | 348 | GLN  | 3.7  |
| 2   | H     | 441 | GLU  | 3.7  |
| 1   | E     | 216 | GLY  | 3.7  |
| 2   | B     | 395 | GLU  | 3.7  |
| 2   | F     | 378 | GLU  | 3.7  |
| 1   | I     | 156 | THR  | 3.6  |
| 1   | C     | 239 | ASN  | 3.6  |
| 1   | G     | 81  | ARG  | 3.6  |
| 2   | B     | 445 | ARG  | 3.6  |
| 1   | A     | 308 | ALA  | 3.6  |
| 2   | L     | 481 | SER  | 3.6  |
| 1   | I     | 242 | PHE  | 3.6  |
| 1   | K     | 147 | THR  | 3.6  |
| 1   | C     | 310 | GLY  | 3.6  |
| 2   | J     | 465 | CYS  | 3.6  |
| 1   | G     | 73  | SER  | 3.6  |
| 1   | G     | 127 | SER  | 3.6  |
| 2   | L     | 353 | GLU  | 3.6  |
| 1   | K     | 20  | THR  | 3.6  |
| 1   | I     | 112 | ALA  | 3.6  |
| 1   | I     | 196 | GLY  | 3.6  |
| 1   | I     | 118 | SER  | 3.6  |
| 1   | I     | 154 | GLN  | 3.6  |
| 1   | I     | 229 | ASN  | 3.6  |
| 1   | K     | 148 | ASP  | 3.6  |
| 2   | F     | 381 | ASN  | 3.6  |
| 2   | B     | 347 | HIS  | 3.5  |
| 1   | G     | 12  | ASN  | 3.5  |
| 1   | I     | 189 | GLY  | 3.5  |
| 1   | I     | 122 | THR  | 3.5  |
| 1   | K     | 116 | THR  | 3.5  |
| 1   | A     | 28  | ASN  | 3.5  |
| 1   | A     | 37  | ASN  | 3.5  |
| 1   | A     | 9   | ALA  | 3.5  |
| 1   | I     | 209 | GLY  | 3.5  |
| 2   | J     | 377 | ILE  | 3.5  |
| 1   | E     | 282 | ASN  | 3.5  |
| 2   | J     | 433 | ASP  | 3.5  |
| 1   | A     | 89  | PRO  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 69  | PHE  | 3.5  |
| 1   | I     | 144 | LEU  | 3.5  |
| 1   | A     | 178 | SER  | 3.5  |
| 2   | L     | 377 | ILE  | 3.5  |
| 1   | E     | 87  | CYS  | 3.5  |
| 1   | A     | 44  | LYS  | 3.5  |
| 1   | C     | 12  | ASN  | 3.5  |
| 1   | G     | 128 | ALA  | 3.5  |
| 1   | I     | 240 | GLY  | 3.5  |
| 2   | L     | 329 | GLY  | 3.5  |
| 2   | B     | 463 | HIS  | 3.5  |
| 2   | J     | 461 | ILE  | 3.4  |
| 2   | L     | 378 | GLU  | 3.4  |
| 1   | K     | 130 | ARG  | 3.4  |
| 1   | G     | 119 | GLY  | 3.4  |
| 1   | G     | 123 | ASN  | 3.4  |
| 2   | B     | 453 | GLU  | 3.4  |
| 2   | H     | 353 | GLU  | 3.4  |
| 1   | I     | 121 | ARG  | 3.4  |
| 1   | I     | 228 | LEU  | 3.4  |
| 1   | I     | 148 | ASP  | 3.4  |
| 1   | K     | 121 | ARG  | 3.4  |
| 1   | K     | 44  | LYS  | 3.4  |
| 1   | A     | 132 | SER  | 3.4  |
| 2   | F     | 332 | GLU  | 3.4  |
| 2   | F     | 487 | ALA  | 3.4  |
| 1   | I     | 149 | ASN  | 3.4  |
| 2   | L     | 388 | ASP  | 3.4  |
| 1   | G     | 69  | PHE  | 3.4  |
| 1   | I     | 223 | PHE  | 3.4  |
| 1   | K     | 165 | SER  | 3.3  |
| 1   | A     | 13  | GLY  | 3.3  |
| 1   | I     | 53  | GLN  | 3.3  |
| 2   | J     | 340 | ASP  | 3.3  |
| 2   | J     | 349 | ASN  | 3.3  |
| 1   | I     | 260 | SER  | 3.3  |
| 1   | A     | 25  | GLU  | 3.3  |
| 2   | H     | 332 | GLU  | 3.3  |
| 1   | G     | 267 | ASN  | 3.3  |
| 1   | G     | 76  | LEU  | 3.3  |
| 1   | G     | 133 | GLY  | 3.3  |
| 1   | I     | 216 | GLY  | 3.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 78  | ILE  | 3.3  |
| 1   | A     | 296 | CYS  | 3.3  |
| 1   | C     | 47  | ARG  | 3.3  |
| 1   | E     | 5   | LEU  | 3.3  |
| 1   | E     | 147 | THR  | 3.3  |
| 2   | L     | 390 | GLU  | 3.3  |
| 1   | A     | 311 | MET  | 3.3  |
| 1   | I     | 119 | GLY  | 3.3  |
| 1   | K     | 90  | GLY  | 3.3  |
| 1   | K     | 240 | GLY  | 3.3  |
| 2   | F     | 352 | GLY  | 3.3  |
| 1   | G     | 92  | PHE  | 3.3  |
| 1   | C     | 17  | ASN  | 3.3  |
| 1   | I     | 60  | ILE  | 3.3  |
| 1   | I     | 282 | ASN  | 3.3  |
| 2   | J     | 392 | ASN  | 3.3  |
| 2   | L     | 392 | ASN  | 3.3  |
| 1   | C     | 268 | CYS  | 3.2  |
| 1   | E     | 268 | CYS  | 3.2  |
| 2   | D     | 386 | LEU  | 3.2  |
| 1   | K     | 91  | LYS  | 3.2  |
| 1   | K     | 179 | THR  | 3.2  |
| 2   | J     | 463 | HIS  | 3.2  |
| 1   | E     | 202 | GLN  | 3.2  |
| 2   | D     | 329 | GLY  | 3.2  |
| 1   | I     | 128 | ALA  | 3.2  |
| 1   | G     | 262 | VAL  | 3.2  |
| 2   | J     | 388 | ASP  | 3.2  |
| 2   | D     | 390 | GLU  | 3.2  |
| 2   | F     | 386 | LEU  | 3.2  |
| 1   | I     | 147 | THR  | 3.2  |
| 1   | C     | 275 | SER  | 3.2  |
| 1   | K     | 178 | SER  | 3.2  |
| 2   | J     | 398 | ILE  | 3.2  |
| 2   | L     | 340 | ASP  | 3.2  |
| 2   | B     | 488 | MET  | 3.2  |
| 1   | C     | 316 | GLU  | 3.2  |
| 1   | E     | 20  | THR  | 3.2  |
| 1   | C     | 11  | SER  | 3.2  |
| 1   | G     | 275 | SER  | 3.2  |
| 1   | K     | 118 | SER  | 3.2  |
| 2   | F     | 459 | PHE  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 149 | ASN  | 3.2  |
| 2   | B     | 490 | ASN  | 3.2  |
| 2   | D     | 392 | ASN  | 3.2  |
| 1   | K     | 143 | LEU  | 3.2  |
| 2   | D     | 453 | GLU  | 3.2  |
| 1   | C     | 6   | GLY  | 3.2  |
| 2   | F     | 329 | GLY  | 3.2  |
| 2   | F     | 455 | GLY  | 3.2  |
| 1   | A     | 84  | SER  | 3.2  |
| 1   | C     | 118 | SER  | 3.2  |
| 2   | D     | 478 | TYR  | 3.2  |
| 1   | A     | 81  | ARG  | 3.1  |
| 1   | A     | 312 | LYS  | 3.1  |
| 1   | G     | 19  | LEU  | 3.1  |
| 1   | E     | 21  | GLU  | 3.1  |
| 1   | G     | 100 | GLN  | 3.1  |
| 1   | I     | 68  | GLN  | 3.1  |
| 1   | G     | 41  | ILE  | 3.1  |
| 1   | G     | 260 | SER  | 3.1  |
| 1   | C     | 27  | VAL  | 3.1  |
| 1   | I     | 220 | ARG  | 3.1  |
| 2   | F     | 482 | LYS  | 3.1  |
| 1   | G     | 113 | MET  | 3.1  |
| 1   | I     | 231 | ASN  | 3.1  |
| 2   | D     | 340 | ASP  | 3.1  |
| 1   | A     | 27  | VAL  | 3.1  |
| 1   | A     | 223 | PHE  | 3.1  |
| 1   | G     | 93  | VAL  | 3.1  |
| 1   | I     | 188 | SER  | 3.1  |
| 2   | D     | 459 | PHE  | 3.1  |
| 1   | E     | 22  | ARG  | 3.1  |
| 2   | B     | 433 | ASP  | 3.1  |
| 1   | G     | 181 | GLU  | 3.1  |
| 1   | K     | 154 | GLN  | 3.1  |
| 1   | I     | 187 | GLY  | 3.1  |
| 2   | L     | 461 | ILE  | 3.1  |
| 1   | C     | 44  | LYS  | 3.1  |
| 1   | A     | 203 | SER  | 3.1  |
| 2   | H     | 340 | ASP  | 3.1  |
| 1   | C     | 4   | CYS  | 3.1  |
| 1   | G     | 24  | VAL  | 3.1  |
| 2   | B     | 481 | SER  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 200 | TYR  | 3.0  |
| 2   | F     | 385 | GLU  | 3.0  |
| 1   | A     | 276 | GLY  | 3.0  |
| 1   | C     | 20  | THR  | 3.0  |
| 1   | I     | 233 | THR  | 3.0  |
| 2   | B     | 471 | ALA  | 3.0  |
| 1   | G     | 84  | SER  | 3.0  |
| 1   | I     | 127 | SER  | 3.0  |
| 1   | I     | 143 | LEU  | 3.0  |
| 1   | K     | 200 | TYR  | 3.0  |
| 2   | L     | 351 | GLN  | 3.0  |
| 2   | L     | 396 | LYS  | 3.0  |
| 1   | A     | 22  | ARG  | 3.0  |
| 2   | D     | 461 | ILE  | 3.0  |
| 2   | F     | 377 | ILE  | 3.0  |
| 1   | G     | 293 | VAL  | 3.0  |
| 1   | I     | 170 | VAL  | 3.0  |
| 2   | D     | 443 | VAL  | 3.0  |
| 1   | G     | 166 | PRO  | 3.0  |
| 2   | F     | 475 | ASN  | 3.0  |
| 1   | G     | 46  | LYS  | 3.0  |
| 1   | G     | 157 | LYS  | 3.0  |
| 1   | C     | 22  | ARG  | 3.0  |
| 1   | K     | 183 | THR  | 3.0  |
| 1   | A     | 128 | ALA  | 3.0  |
| 2   | B     | 447 | LEU  | 3.0  |
| 2   | H     | 390 | GLU  | 3.0  |
| 1   | E     | 12  | ASN  | 3.0  |
| 2   | D     | 381 | ASN  | 3.0  |
| 2   | D     | 437 | ASP  | 3.0  |
| 1   | E     | 6   | GLY  | 3.0  |
| 1   | I     | 212 | THR  | 3.0  |
| 1   | A     | 180 | ALA  | 3.0  |
| 1   | I     | 125 | ALA  | 3.0  |
| 1   | I     | 150 | ALA  | 3.0  |
| 2   | B     | 376 | LEU  | 2.9  |
| 2   | H     | 453 | GLU  | 2.9  |
| 1   | G     | 64  | PRO  | 2.9  |
| 1   | G     | 89  | PRO  | 2.9  |
| 1   | K     | 198 | SER  | 2.9  |
| 1   | K     | 282 | ASN  | 2.9  |
| 1   | G     | 97  | ALA  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 332 | GLU  | 2.9  |
| 1   | A     | 17  | ASN  | 2.9  |
| 1   | E     | 28  | ASN  | 2.9  |
| 2   | D     | 475 | ASN  | 2.9  |
| 1   | A     | 221 | ILE  | 2.9  |
| 1   | G     | 120 | ILE  | 2.9  |
| 1   | K     | 189 | GLY  | 2.9  |
| 1   | C     | 26  | VAL  | 2.9  |
| 1   | G     | 254 | LYS  | 2.9  |
| 1   | K     | 164 | LYS  | 2.9  |
| 2   | F     | 463 | HIS  | 2.9  |
| 2   | L     | 441 | GLU  | 2.9  |
| 1   | K     | 275 | SER  | 2.9  |
| 2   | J     | 397 | GLN  | 2.9  |
| 1   | G     | 291 | ARG  | 2.9  |
| 1   | I     | 130 | ARG  | 2.9  |
| 1   | I     | 199 | ASN  | 2.9  |
| 2   | F     | 490 | ASN  | 2.9  |
| 2   | B     | 354 | GLY  | 2.9  |
| 1   | G     | 248 | ALA  | 2.9  |
| 1   | C     | 164 | LYS  | 2.9  |
| 1   | E     | 254 | LYS  | 2.9  |
| 1   | G     | 153 | PRO  | 2.9  |
| 1   | G     | 4   | CYS  | 2.9  |
| 2   | D     | 466 | ASP  | 2.9  |
| 2   | D     | 360 | LYS  | 2.9  |
| 2   | H     | 464 | LYS  | 2.9  |
| 2   | L     | 350 | ALA  | 2.9  |
| 1   | K     | 181 | GLU  | 2.8  |
| 2   | J     | 453 | GLU  | 2.8  |
| 2   | J     | 351 | GLN  | 2.8  |
| 1   | C     | 282 | ASN  | 2.8  |
| 1   | G     | 196 | GLY  | 2.8  |
| 1   | I     | 1   | ASP  | 2.8  |
| 2   | B     | 468 | ASP  | 2.8  |
| 2   | F     | 437 | ASP  | 2.8  |
| 1   | I     | 186 | TYR  | 2.8  |
| 2   | B     | 483 | TYR  | 2.8  |
| 1   | A     | 30  | THR  | 2.8  |
| 2   | J     | 441 | GLU  | 2.8  |
| 2   | D     | 474 | ARG  | 2.8  |
| 1   | K     | 231 | ASN  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 222 | ASP  | 2.8  |
| 2   | F     | 340 | ASP  | 2.8  |
| 2   | F     | 447 | LEU  | 2.8  |
| 2   | F     | 394 | VAL  | 2.8  |
| 1   | G     | 82  | GLU  | 2.8  |
| 1   | G     | 96  | GLU  | 2.8  |
| 2   | F     | 346 | ARG  | 2.8  |
| 1   | G     | 102 | LEU  | 2.8  |
| 2   | D     | 468 | ASP  | 2.8  |
| 1   | K     | 205 | VAL  | 2.8  |
| 1   | G     | 87  | CYS  | 2.8  |
| 1   | A     | 68  | GLN  | 2.8  |
| 1   | G     | 259 | GLN  | 2.8  |
| 2   | H     | 387 | ILE  | 2.8  |
| 2   | D     | 388 | ASP  | 2.8  |
| 2   | J     | 454 | ASP  | 2.8  |
| 1   | G     | 155 | MET  | 2.8  |
| 2   | L     | 355 | THR  | 2.8  |
| 1   | G     | 136 | PHE  | 2.8  |
| 1   | I     | 211 | ARG  | 2.8  |
| 1   | G     | 154 | GLN  | 2.7  |
| 1   | I     | 221 | ILE  | 2.7  |
| 1   | A     | 11  | SER  | 2.7  |
| 1   | A     | 226 | LEU  | 2.7  |
| 1   | A     | 237 | SER  | 2.7  |
| 1   | G     | 5   | LEU  | 2.7  |
| 1   | I     | 142 | TRP  | 2.7  |
| 2   | F     | 344 | GLY  | 2.7  |
| 2   | H     | 381 | ASN  | 2.7  |
| 2   | J     | 381 | ASN  | 2.7  |
| 1   | E     | 316 | GLU  | 2.7  |
| 1   | G     | 49  | VAL  | 2.7  |
| 2   | H     | 395 | GLU  | 2.7  |
| 2   | F     | 345 | PHE  | 2.7  |
| 1   | I     | 208 | PRO  | 2.7  |
| 2   | B     | 465 | CYS  | 2.7  |
| 2   | L     | 360 | LYS  | 2.7  |
| 1   | K     | 207 | SER  | 2.7  |
| 2   | D     | 488 | MET  | 2.7  |
| 2   | L     | 349 | ASN  | 2.7  |
| 1   | A     | 130 | ARG  | 2.7  |
| 1   | C     | 181 | GLU  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | D     | 395 | GLU  | 2.7  |
| 2   | L     | 485 | GLU  | 2.7  |
| 1   | A     | 147 | THR  | 2.7  |
| 1   | G     | 222 | ASP  | 2.7  |
| 1   | I     | 184 | LYS  | 2.7  |
| 1   | G     | 217 | LEU  | 2.7  |
| 2   | B     | 338 | LEU  | 2.7  |
| 1   | G     | 146 | ASN  | 2.7  |
| 1   | G     | 149 | ASN  | 2.7  |
| 1   | I     | 178 | SER  | 2.7  |
| 1   | K     | 21  | GLU  | 2.7  |
| 1   | K     | 161 | ASN  | 2.7  |
| 2   | D     | 385 | GLU  | 2.7  |
| 2   | H     | 475 | ASN  | 2.7  |
| 1   | A     | 29  | ALA  | 2.7  |
| 1   | A     | 309 | THR  | 2.7  |
| 1   | A     | 202 | GLN  | 2.7  |
| 2   | F     | 348 | GLN  | 2.7  |
| 1   | G     | 189 | GLY  | 2.7  |
| 2   | F     | 484 | ARG  | 2.7  |
| 1   | A     | 313 | ASN  | 2.7  |
| 1   | G     | 269 | GLU  | 2.7  |
| 1   | I     | 171 | TRP  | 2.7  |
| 1   | G     | 162 | THR  | 2.7  |
| 2   | B     | 479 | ASP  | 2.7  |
| 1   | G     | 263 | GLN  | 2.6  |
| 2   | B     | 348 | GLN  | 2.6  |
| 1   | E     | 217 | LEU  | 2.6  |
| 1   | G     | 272 | CYS  | 2.6  |
| 1   | I     | 87  | CYS  | 2.6  |
| 1   | G     | 171 | TRP  | 2.6  |
| 2   | J     | 434 | SER  | 2.6  |
| 1   | G     | 48  | THR  | 2.6  |
| 1   | I     | 20  | THR  | 2.6  |
| 1   | I     | 179 | THR  | 2.6  |
| 2   | B     | 388 | ASP  | 2.6  |
| 2   | D     | 358 | ASP  | 2.6  |
| 1   | A     | 280 | ILE  | 2.6  |
| 2   | F     | 483 | TYR  | 2.6  |
| 1   | G     | 140 | MET  | 2.6  |
| 1   | K     | 217 | LEU  | 2.6  |
| 1   | I     | 268 | CYS  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | F     | 347 | HIS  | 2.6  |
| 1   | A     | 104 | GLU  | 2.6  |
| 1   | A     | 270 | GLY  | 2.6  |
| 1   | C     | 104 | GLU  | 2.6  |
| 2   | F     | 452 | GLU  | 2.6  |
| 2   | J     | 353 | GLU  | 2.6  |
| 1   | C     | 314 | VAL  | 2.6  |
| 1   | I     | 267 | ASN  | 2.6  |
| 2   | L     | 374 | ASN  | 2.6  |
| 1   | E     | 89  | PRO  | 2.6  |
| 2   | F     | 330 | PHE  | 2.6  |
| 2   | B     | 440 | TYR  | 2.6  |
| 2   | D     | 359 | TYR  | 2.6  |
| 1   | E     | 47  | ARG  | 2.6  |
| 2   | J     | 395 | GLU  | 2.6  |
| 2   | L     | 332 | GLU  | 2.6  |
| 1   | A     | 133 | GLY  | 2.6  |
| 2   | J     | 337 | GLY  | 2.6  |
| 1   | C     | 267 | ASN  | 2.6  |
| 1   | E     | 128 | ALA  | 2.6  |
| 1   | I     | 146 | ASN  | 2.6  |
| 1   | I     | 241 | ALA  | 2.6  |
| 2   | B     | 381 | ASN  | 2.6  |
| 1   | E     | 233 | THR  | 2.6  |
| 2   | F     | 382 | GLN  | 2.6  |
| 2   | F     | 446 | GLN  | 2.6  |
| 1   | G     | 109 | ASP  | 2.6  |
| 1   | G     | 98  | LEU  | 2.6  |
| 1   | K     | 186 | TYR  | 2.6  |
| 1   | C     | 8   | HIS  | 2.6  |
| 1   | I     | 21  | GLU  | 2.6  |
| 2   | B     | 455 | GLY  | 2.6  |
| 2   | D     | 354 | GLY  | 2.6  |
| 2   | L     | 459 | PHE  | 2.6  |
| 1   | A     | 222 | ASP  | 2.5  |
| 1   | K     | 1   | ASP  | 2.5  |
| 1   | C     | 5   | LEU  | 2.5  |
| 1   | G     | 47  | ARG  | 2.5  |
| 1   | I     | 44  | LYS  | 2.5  |
| 1   | E     | 8   | HIS  | 2.5  |
| 1   | G     | 68  | GLN  | 2.5  |
| 1   | G     | 80  | ARG  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 47  | ARG  | 2.5  |
| 2   | B     | 343 | TYR  | 2.5  |
| 1   | A     | 216 | GLY  | 2.5  |
| 1   | K     | 128 | ALA  | 2.5  |
| 2   | B     | 489 | GLN  | 2.5  |
| 1   | G     | 239 | ASN  | 2.5  |
| 1   | I     | 126 | THR  | 2.5  |
| 2   | D     | 374 | ASN  | 2.5  |
| 1   | C     | 165 | SER  | 2.5  |
| 1   | G     | 249 | SER  | 2.5  |
| 1   | E     | 44  | LYS  | 2.5  |
| 1   | A     | 217 | LEU  | 2.5  |
| 1   | K     | 185 | LEU  | 2.5  |
| 2   | J     | 430 | ASP  | 2.5  |
| 2   | D     | 455 | GLY  | 2.5  |
| 1   | I     | 234 | VAL  | 2.5  |
| 1   | A     | 92  | PHE  | 2.5  |
| 1   | E     | 9   | ALA  | 2.5  |
| 1   | G     | 191 | LYS  | 2.5  |
| 2   | B     | 373 | LEU  | 2.5  |
| 2   | B     | 442 | ARG  | 2.5  |
| 2   | D     | 377 | ILE  | 2.5  |
| 2   | B     | 466 | ASP  | 2.5  |
| 2   | F     | 468 | ASP  | 2.5  |
| 2   | J     | 385 | GLU  | 2.5  |
| 2   | L     | 453 | GLU  | 2.5  |
| 1   | A     | 26  | VAL  | 2.5  |
| 1   | K     | 150 | ALA  | 2.5  |
| 1   | C     | 312 | LYS  | 2.4  |
| 1   | A     | 267 | ASN  | 2.4  |
| 1   | C     | 94  | ASN  | 2.4  |
| 1   | I     | 163 | ARG  | 2.4  |
| 2   | B     | 346 | ARG  | 2.4  |
| 1   | E     | 19  | LEU  | 2.4  |
| 1   | E     | 143 | LEU  | 2.4  |
| 1   | G     | 251 | LEU  | 2.4  |
| 2   | D     | 373 | LEU  | 2.4  |
| 1   | G     | 129 | CYS  | 2.4  |
| 2   | H     | 433 | ASP  | 2.4  |
| 1   | A     | 39  | PRO  | 2.4  |
| 1   | C     | 23  | GLY  | 2.4  |
| 2   | J     | 482 | LYS  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 167 | ALA  | 2.4  |
| 1   | G     | 266 | ALA  | 2.4  |
| 1   | C     | 309 | THR  | 2.4  |
| 1   | E     | 179 | THR  | 2.4  |
| 1   | G     | 279 | ILE  | 2.4  |
| 2   | D     | 490 | ASN  | 2.4  |
| 1   | G     | 165 | SER  | 2.4  |
| 1   | A     | 148 | ASP  | 2.4  |
| 2   | F     | 335 | TRP  | 2.4  |
| 1   | I     | 113 | MET  | 2.4  |
| 1   | G     | 27  | VAL  | 2.4  |
| 1   | G     | 273 | TYR  | 2.4  |
| 1   | I     | 159 | TYR  | 2.4  |
| 1   | G     | 22  | ARG  | 2.4  |
| 1   | I     | 180 | ALA  | 2.4  |
| 2   | B     | 474 | ARG  | 2.4  |
| 2   | D     | 445 | ARG  | 2.4  |
| 2   | F     | 356 | ALA  | 2.4  |
| 1   | I     | 185 | LEU  | 2.4  |
| 2   | B     | 387 | ILE  | 2.4  |
| 2   | J     | 355 | THR  | 2.4  |
| 1   | G     | 199 | ASN  | 2.4  |
| 1   | G     | 198 | SER  | 2.4  |
| 1   | I     | 198 | SER  | 2.4  |
| 1   | I     | 75  | ASP  | 2.4  |
| 2   | F     | 488 | MET  | 2.4  |
| 1   | I     | 157 | LYS  | 2.4  |
| 1   | K     | 208 | PRO  | 2.4  |
| 1   | C     | 234 | VAL  | 2.4  |
| 1   | C     | 117 | TYR  | 2.4  |
| 1   | G     | 112 | ALA  | 2.4  |
| 1   | G     | 204 | PHE  | 2.4  |
| 2   | L     | 384 | PHE  | 2.4  |
| 2   | J     | 447 | LEU  | 2.4  |
| 2   | B     | 475 | ASN  | 2.4  |
| 2   | H     | 392 | ASN  | 2.4  |
| 1   | A     | 275 | SER  | 2.4  |
| 1   | I     | 269 | GLU  | 2.4  |
| 2   | D     | 454 | ASP  | 2.4  |
| 1   | G     | 142 | TRP  | 2.4  |
| 2   | J     | 455 | GLY  | 2.4  |
| 1   | A     | 91  | LYS  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | F     | 467 | ASP  | 2.3  |
| 1   | I     | 202 | GLN  | 2.3  |
| 1   | K     | 133 | GLY  | 2.3  |
| 2   | H     | 354 | GLY  | 2.3  |
| 1   | K     | 22  | ARG  | 2.3  |
| 2   | F     | 474 | ARG  | 2.3  |
| 2   | J     | 448 | ARG  | 2.3  |
| 1   | K     | 193 | VAL  | 2.3  |
| 1   | G     | 74  | ALA  | 2.3  |
| 1   | I     | 244 | ALA  | 2.3  |
| 2   | F     | 357 | ALA  | 2.3  |
| 1   | G     | 186 | TYR  | 2.3  |
| 2   | J     | 490 | ASN  | 2.3  |
| 2   | L     | 475 | ASN  | 2.3  |
| 2   | B     | 449 | GLU  | 2.3  |
| 1   | K     | 119 | GLY  | 2.3  |
| 2   | D     | 484 | ARG  | 2.3  |
| 1   | I     | 250 | PHE  | 2.3  |
| 2   | J     | 459 | PHE  | 2.3  |
| 1   | A     | 266 | ALA  | 2.3  |
| 1   | A     | 164 | LYS  | 2.3  |
| 1   | C     | 15  | LYS  | 2.3  |
| 1   | I     | 111 | GLU  | 2.3  |
| 1   | K     | 157 | LYS  | 2.3  |
| 2   | F     | 396 | LYS  | 2.3  |
| 2   | D     | 349 | ASN  | 2.3  |
| 1   | C     | 237 | SER  | 2.3  |
| 1   | G     | 85  | ASP  | 2.3  |
| 2   | D     | 481 | SER  | 2.3  |
| 1   | G     | 298 | ARG  | 2.3  |
| 1   | G     | 187 | GLY  | 2.3  |
| 1   | I     | 124 | GLY  | 2.3  |
| 1   | I     | 182 | GLN  | 2.3  |
| 1   | C     | 150 | ALA  | 2.3  |
| 1   | E     | 183 | THR  | 2.3  |
| 1   | G     | 227 | MET  | 2.3  |
| 1   | C     | 269 | GLU  | 2.3  |
| 1   | I     | 232 | ASP  | 2.3  |
| 2   | H     | 474 | ARG  | 2.3  |
| 1   | A     | 228 | LEU  | 2.3  |
| 1   | I     | 93  | VAL  | 2.3  |
| 2   | B     | 431 | LEU  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 301 | LYS  | 2.2  |
| 2   | D     | 470 | MET  | 2.2  |
| 2   | F     | 360 | LYS  | 2.2  |
| 1   | A     | 269 | GLU  | 2.2  |
| 1   | C     | 25  | GLU  | 2.2  |
| 1   | K     | 82  | GLU  | 2.2  |
| 2   | D     | 440 | TYR  | 2.2  |
| 2   | F     | 478 | TYR  | 2.2  |
| 1   | C     | 149 | ASN  | 2.2  |
| 1   | C     | 303 | ARG  | 2.2  |
| 1   | C     | 39  | PRO  | 2.2  |
| 1   | G     | 246 | ASP  | 2.2  |
| 1   | K     | 203 | SER  | 2.2  |
| 2   | B     | 340 | ASP  | 2.2  |
| 2   | B     | 430 | ASP  | 2.2  |
| 1   | G     | 195 | VAL  | 2.2  |
| 1   | K     | 254 | LYS  | 2.2  |
| 1   | E     | 256 | MET  | 2.2  |
| 2   | D     | 347 | HIS  | 2.2  |
| 1   | C     | 21  | GLU  | 2.2  |
| 1   | C     | 179 | THR  | 2.2  |
| 2   | D     | 452 | GLU  | 2.2  |
| 1   | E     | 88  | TYR  | 2.2  |
| 1   | K     | 12  | ASN  | 2.2  |
| 1   | E     | 310 | GLY  | 2.2  |
| 1   | G     | 11  | SER  | 2.2  |
| 1   | G     | 50  | ASP  | 2.2  |
| 1   | G     | 188 | SER  | 2.2  |
| 1   | I     | 109 | ASP  | 2.2  |
| 2   | B     | 337 | GLY  | 2.2  |
| 2   | F     | 481 | SER  | 2.2  |
| 1   | G     | 10  | VAL  | 2.2  |
| 1   | K     | 140 | MET  | 2.2  |
| 2   | B     | 339 | ILE  | 2.2  |
| 2   | D     | 339 | ILE  | 2.2  |
| 2   | J     | 391 | PHE  | 2.2  |
| 1   | K     | 210 | ALA  | 2.2  |
| 2   | D     | 356 | ALA  | 2.2  |
| 2   | J     | 350 | ALA  | 2.2  |
| 1   | E     | 4   | CYS  | 2.2  |
| 2   | F     | 465 | CYS  | 2.2  |
| 2   | J     | 370 | THR  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | L     | 458 | CYS  | 2.2  |
| 2   | F     | 448 | ARG  | 2.2  |
| 1   | G     | 94  | ASN  | 2.2  |
| 1   | G     | 190 | ASN  | 2.2  |
| 1   | K     | 88  | TYR  | 2.2  |
| 1   | G     | 91  | LYS  | 2.2  |
| 2   | F     | 341 | GLY  | 2.2  |
| 1   | G     | 135 | SER  | 2.2  |
| 1   | K     | 145 | SER  | 2.2  |
| 1   | E     | 214 | VAL  | 2.2  |
| 1   | C     | 7   | HIS  | 2.2  |
| 1   | G     | 77  | ILE  | 2.2  |
| 2   | H     | 459 | PHE  | 2.2  |
| 1   | A     | 151 | ALA  | 2.2  |
| 1   | K     | 156 | THR  | 2.2  |
| 2   | L     | 370 | THR  | 2.2  |
| 1   | I     | 131 | ARG  | 2.2  |
| 1   | I     | 296 | CYS  | 2.2  |
| 1   | A     | 94  | ASN  | 2.2  |
| 2   | D     | 368 | GLN  | 2.2  |
| 1   | A     | 16  | VAL  | 2.2  |
| 1   | E     | 73  | SER  | 2.2  |
| 1   | K     | 176 | SER  | 2.2  |
| 1   | K     | 234 | VAL  | 2.2  |
| 2   | F     | 339 | ILE  | 2.2  |
| 2   | B     | 459 | PHE  | 2.2  |
| 1   | E     | 30  | THR  | 2.1  |
| 1   | G     | 131 | ARG  | 2.1  |
| 1   | G     | 163 | ARG  | 2.1  |
| 2   | F     | 456 | THR  | 2.1  |
| 1   | G     | 42  | CYS  | 2.1  |
| 1   | A     | 190 | ASN  | 2.1  |
| 1   | E     | 199 | ASN  | 2.1  |
| 2   | F     | 359 | TYR  | 2.1  |
| 2   | L     | 478 | TYR  | 2.1  |
| 1   | C     | 19  | LEU  | 2.1  |
| 1   | I     | 90  | GLY  | 2.1  |
| 1   | C     | 222 | ASP  | 2.1  |
| 1   | C     | 73  | SER  | 2.1  |
| 1   | G     | 314 | VAL  | 2.1  |
| 2   | B     | 377 | ILE  | 2.1  |
| 1   | I     | 236 | PHE  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 180 | ALA  | 2.1  |
| 1   | A     | 225 | TRP  | 2.1  |
| 1   | G     | 111 | GLU  | 2.1  |
| 2   | D     | 335 | TRP  | 2.1  |
| 1   | G     | 121 | ARG  | 2.1  |
| 1   | I     | 22  | ARG  | 2.1  |
| 1   | K     | 153 | PRO  | 2.1  |
| 1   | C     | 37  | ASN  | 2.1  |
| 1   | E     | 144 | LEU  | 2.1  |
| 1   | K     | 256 | MET  | 2.1  |
| 2   | J     | 376 | LEU  | 2.1  |
| 1   | C     | 119 | GLY  | 2.1  |
| 1   | G     | 276 | GLY  | 2.1  |
| 1   | I     | 133 | GLY  | 2.1  |
| 1   | G     | 101 | ILE  | 2.1  |
| 1   | G     | 214 | VAL  | 2.1  |
| 2   | B     | 331 | ILE  | 2.1  |
| 2   | D     | 394 | VAL  | 2.1  |
| 1   | E     | 158 | SER  | 2.1  |
| 1   | K     | 285 | PHE  | 2.1  |
| 1   | G     | 210 | ALA  | 2.1  |
| 2   | H     | 471 | ALA  | 2.1  |
| 1   | G     | 211 | ARG  | 2.1  |
| 1   | G     | 194 | THR  | 2.1  |
| 1   | E     | 164 | LYS  | 2.1  |
| 1   | I     | 206 | PRO  | 2.1  |
| 2   | B     | 386 | LEU  | 2.1  |
| 2   | J     | 475 | ASN  | 2.1  |
| 1   | A     | 224 | HIS  | 2.1  |
| 2   | J     | 437 | ASP  | 2.1  |
| 1   | A     | 47  | ARG  | 2.1  |
| 1   | A     | 74  | ALA  | 2.1  |
| 1   | A     | 96  | GLU  | 2.1  |
| 1   | G     | 141 | LYS  | 2.1  |
| 2   | L     | 482 | LYS  | 2.1  |
| 1   | K     | 194 | THR  | 2.1  |
| 2   | F     | 477 | THR  | 2.1  |
| 1   | E     | 267 | ASN  | 2.1  |
| 1   | A     | 253 | GLY  | 2.1  |
| 1   | A     | 272 | CYS  | 2.1  |
| 1   | C     | 114 | GLY  | 2.1  |
| 1   | I     | 219 | GLY  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | L     | 354 | GLY  | 2.1  |
| 1   | G     | 173 | ILE  | 2.1  |
| 2   | F     | 473 | ILE  | 2.1  |
| 1   | K     | 204 | PHE  | 2.1  |
| 1   | A     | 95  | GLU  | 2.0  |
| 1   | C     | 298 | ARG  | 2.0  |
| 1   | E     | 298 | ARG  | 2.0  |
| 1   | K     | 247 | ARG  | 2.0  |
| 2   | F     | 479 | ASP  | 2.0  |
| 2   | F     | 390 | GLU  | 2.0  |
| 1   | A     | 255 | SER  | 2.0  |
| 1   | G     | 105 | SER  | 2.0  |
| 1   | I     | 73  | SER  | 2.0  |
| 1   | K     | 141 | LYS  | 2.0  |
| 2   | F     | 370 | THR  | 2.0  |
| 1   | E     | 140 | MET  | 2.0  |
| 1   | K     | 227 | MET  | 2.0  |
| 1   | C     | 217 | LEU  | 2.0  |
| 1   | I     | 213 | GLN  | 2.0  |
| 2   | H     | 373 | LEU  | 2.0  |
| 1   | G     | 282 | ASN  | 2.0  |
| 1   | K     | 229 | ASN  | 2.0  |
| 1   | K     | 239 | ASN  | 2.0  |
| 1   | E     | 133 | GLY  | 2.0  |
| 1   | G     | 169 | ILE  | 2.0  |
| 2   | D     | 473 | ILE  | 2.0  |
| 1   | E     | 27  | VAL  | 2.0  |
| 1   | K     | 87  | CYS  | 2.0  |
| 2   | D     | 469 | CYS  | 2.0  |
| 1   | G     | 247 | ARG  | 2.0  |
| 2   | F     | 441 | GLU  | 2.0  |
| 1   | K     | 248 | ALA  | 2.0  |
| 2   | L     | 487 | ALA  | 2.0  |
| 1   | C     | 132 | SER  | 2.0  |
| 1   | K     | 235 | THR  | 2.0  |
| 2   | D     | 355 | THR  | 2.0  |
| 1   | E     | 53  | GLN  | 2.0  |
| 2   | L     | 431 | LEU  | 2.0  |
| 1   | G     | 216 | GLY  | 2.0  |
| 2   | H     | 352 | GLY  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.