



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:57 am BST

PDB ID : 3K2Q  
Title : Crystal structure of Pyrophosphate-dependent phosphofructokinase from *Marinobacter aquaeolei*, NORTHEAST STRUCTURAL GENOMICS CONSORTIUM TARGET MqR88  
Authors : Seetharaman, J.; Lew, S.; Wang, D.; Neely, H.; Janjua, K.; Cunningham, K.; Owens, L.; Xiao, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2009-09-30  
Resolution : 2.50 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.

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

|                                |   |                                                                    |
|--------------------------------|---|--------------------------------------------------------------------|
| MolProbity                     | : | 4.02b-467                                                          |
| Xtriage (Phenix)               | : | 1.13                                                               |
| EDS                            | : | 2.11                                                               |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac                         | : | 5.8.0158                                                           |
| CCP4                           | : | 7.0.044 (Gargrove)                                                 |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                                |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                            |
| Validation Pipeline (wwPDB-VP) | : | 2.11                                                               |

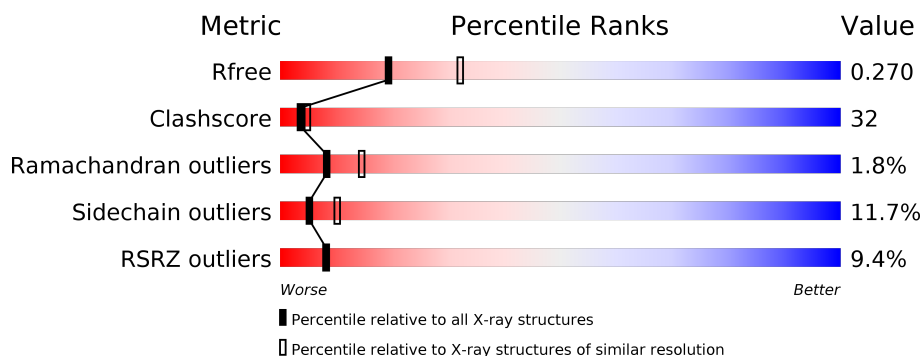
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 130704                      | 4661 (2.50-2.50)                                      |
| Clashscore            | 141614                      | 5346 (2.50-2.50)                                      |
| Ramachandran outliers | 138981                      | 5231 (2.50-2.50)                                      |
| Sidechain outliers    | 138945                      | 5233 (2.50-2.50)                                      |
| RSRZ outliers         | 127900                      | 4559 (2.50-2.50)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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     | 420    | <div> <div>5%</div> <div> <div>50%</div> <div>37%</div> <div>5% • 7%</div> </div> </div>  |
| 1   | B     | 420    | <div> <div>9%</div> <div> <div>45%</div> <div>42%</div> <div>5% • 7%</div> </div> </div>  |
| 1   | C     | 420    | <div> <div>13%</div> <div> <div>46%</div> <div>40%</div> <div>6% • 7%</div> </div> </div> |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9397 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 Pyrophosphate-dependent phosphofructokinase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 392      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3010  | 1909 | 519 | 566 | 16 |         |         |       |
| 1   | B     | 392      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3010  | 1909 | 519 | 566 | 16 |         |         |       |
| 1   | C     | 392      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3010  | 1909 | 519 | 566 | 16 |         |         |       |

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | B     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | A     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | C     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3   | A     | 136      | Total | O   | 0       | 0       |
|     |       |          | 136   | 136 |         |         |
| 3   | B     | 109      | Total | O   | 0       | 0       |
|     |       |          | 109   | 109 |         |         |
| 3   | C     | 119      | Total | O   | 0       | 0       |
|     |       |          | 119   | 119 |         |         |

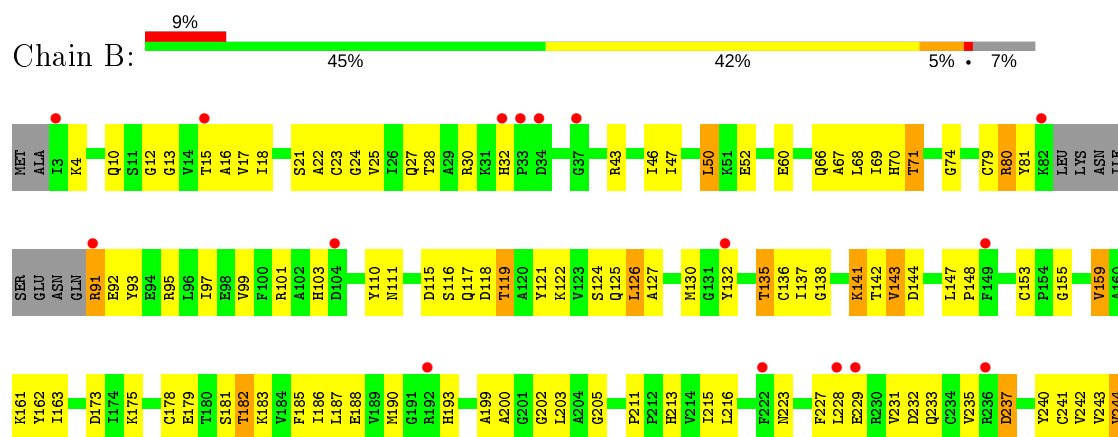
### 3 Residue-property plots [i](#)

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

- Molecule 1: Pyrophosphate-dependent phosphofructokinase



- Molecule 1: Pyrophosphate-dependent phosphofructokinase





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 151.53Å 100.75Å 101.58Å<br>90.00° 110.34° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 44.70 – 2.50<br>44.70 – 2.48                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 89.9 (44.70-2.50)<br>95.1 (44.70-2.48)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.09                                                        | Depositor        |
| $R_{sym}$                                                               | 0.06                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.77 (at 2.48Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.2                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.234 , 0.260<br>0.249 , 0.270                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3762 reflections (3.86%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 25.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.774                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 46.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.88                                                        | EDS              |
| Total number of atoms                                                   | 9397                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 33.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.87         | 23/3073 (0.7%) | 0.67        | 1/4157 (0.0%)  |
| 1   | B     | 0.71         | 15/3073 (0.5%) | 0.61        | 0/4157         |
| 1   | C     | 0.49         | 2/3073 (0.1%)  | 0.62        | 0/4157         |
| All | All   | 0.71         | 40/9219 (0.4%) | 0.63        | 1/12471 (0.0%) |

All (40) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 273 | GLY  | C-O    | -16.46 | 0.97        | 1.23     |
| 1   | B     | 420 | LEU  | C-OXT  | 15.37  | 1.52        | 1.23     |
| 1   | B     | 277 | ALA  | CA-CB  | -14.53 | 1.22        | 1.52     |
| 1   | C     | 273 | GLY  | C-O    | -12.65 | 1.03        | 1.23     |
| 1   | A     | 278 | LEU  | C-O    | -12.05 | 1.00        | 1.23     |
| 1   | A     | 277 | ALA  | C-O    | -9.04  | 1.06        | 1.23     |
| 1   | A     | 361 | LYS  | CD-CE  | -8.96  | 1.28        | 1.51     |
| 1   | B     | 276 | PRO  | CG-CD  | -8.74  | 1.21        | 1.50     |
| 1   | A     | 274 | VAL  | C-O    | -8.43  | 1.07        | 1.23     |
| 1   | A     | 361 | LYS  | CE-NZ  | -8.40  | 1.28        | 1.49     |
| 1   | A     | 276 | PRO  | CB-CG  | -7.97  | 1.10        | 1.50     |
| 1   | A     | 276 | PRO  | CG-CD  | -7.94  | 1.24        | 1.50     |
| 1   | A     | 277 | ALA  | CA-CB  | -7.86  | 1.35        | 1.52     |
| 1   | B     | 276 | PRO  | CB-CG  | -7.84  | 1.10        | 1.50     |
| 1   | B     | 276 | PRO  | C-O    | -7.44  | 1.08        | 1.23     |
| 1   | B     | 275 | ALA  | C-O    | -7.23  | 1.09        | 1.23     |
| 1   | A     | 273 | GLY  | CA-C   | -7.12  | 1.40        | 1.51     |
| 1   | B     | 275 | ALA  | CA-CB  | -7.02  | 1.37        | 1.52     |
| 1   | B     | 277 | ALA  | C-O    | -6.99  | 1.10        | 1.23     |
| 1   | A     | 360 | GLU  | CD-OE2 | -6.71  | 1.18        | 1.25     |
| 1   | B     | 274 | VAL  | C-O    | -6.60  | 1.10        | 1.23     |
| 1   | A     | 278 | LEU  | CA-C   | -6.38  | 1.36        | 1.52     |
| 1   | A     | 361 | LYS  | CB-CG  | -6.38  | 1.35        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 361 | LYS  | C-O    | -6.37 | 1.11        | 1.23     |
| 1   | A     | 276 | PRO  | C-O    | -6.34 | 1.10        | 1.23     |
| 1   | B     | 277 | ALA  | CA-C   | -6.07 | 1.37        | 1.52     |
| 1   | A     | 275 | ALA  | C-O    | -5.98 | 1.11        | 1.23     |
| 1   | B     | 276 | PRO  | CA-CB  | -5.97 | 1.41        | 1.53     |
| 1   | A     | 360 | GLU  | CD-OE1 | -5.91 | 1.19        | 1.25     |
| 1   | A     | 361 | LYS  | N-CA   | -5.81 | 1.34        | 1.46     |
| 1   | B     | 276 | PRO  | N-CD   | -5.75 | 1.39        | 1.47     |
| 1   | A     | 360 | GLU  | C-O    | -5.74 | 1.12        | 1.23     |
| 1   | A     | 275 | ALA  | CA-CB  | -5.73 | 1.40        | 1.52     |
| 1   | A     | 360 | GLU  | CB-CG  | -5.61 | 1.41        | 1.52     |
| 1   | C     | 275 | ALA  | CA-CB  | -5.54 | 1.40        | 1.52     |
| 1   | A     | 276 | PRO  | N-CD   | -5.44 | 1.40        | 1.47     |
| 1   | B     | 277 | ALA  | C-N    | -5.35 | 1.21        | 1.34     |
| 1   | B     | 275 | ALA  | N-CA   | -5.17 | 1.36        | 1.46     |
| 1   | B     | 276 | PRO  | N-CA   | -5.14 | 1.38        | 1.47     |
| 1   | A     | 278 | LEU  | CG-CD1 | -5.04 | 1.33        | 1.51     |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1   | A     | 278 | LEU  | CB-CG-CD2 | 5.63 | 120.57      | 111.00   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 3010  | 0        | 2950     | 175     | 0            |
| 1   | B     | 3010  | 0        | 2950     | 194     | 0            |
| 1   | C     | 3010  | 0        | 2950     | 206     | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 136   | 0        | 0        | 15      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | B     | 109   | 0        | 0        | 13      | 0            |
| 3   | C     | 119   | 0        | 0        | 14      | 0            |
| All | All   | 9397  | 0        | 8850     | 565     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (565) 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:C:15:THR:HG22  | 1:C:17:VAL:H     | 1.19                     | 1.08              |
| 1:B:15:THR:HG22  | 1:B:17:VAL:H     | 1.20                     | 1.06              |
| 1:A:15:THR:HG22  | 1:A:17:VAL:H     | 1.19                     | 1.03              |
| 1:B:342:LYS:HB2  | 1:B:343:PRO:HD2  | 1.38                     | 1.02              |
| 1:C:28:THR:HG21  | 1:C:319:LYS:HG3  | 1.44                     | 1.00              |
| 1:C:419:GLU:HG2  | 1:C:420:LEU:N    | 1.71                     | 0.99              |
| 1:A:99:VAL:HG12  | 1:A:414:LEU:CD2  | 1.97                     | 0.94              |
| 1:A:136:CYS:H    | 1:A:330:GLN:HE22 | 1.18                     | 0.92              |
| 1:A:342:LYS:HB2  | 1:A:343:PRO:HD2  | 1.52                     | 0.91              |
| 1:A:113:GLY:HA3  | 3:A:438:HOH:O    | 1.69                     | 0.91              |
| 1:B:138:GLY:O    | 1:B:334:PRO:HD2  | 1.70                     | 0.90              |
| 1:A:330:GLN:HE21 | 1:A:331:ALA:H    | 1.16                     | 0.90              |
| 1:A:60:GLU:HG2   | 1:A:405:LEU:HD22 | 1.53                     | 0.90              |
| 1:C:99:VAL:HG12  | 1:C:414:LEU:CD2  | 2.01                     | 0.90              |
| 1:A:138:GLY:O    | 1:A:334:PRO:HD2  | 1.73                     | 0.89              |
| 1:C:138:GLY:O    | 1:C:334:PRO:HD2  | 1.71                     | 0.89              |
| 1:C:416:THR:HA   | 3:C:488:HOH:O    | 1.72                     | 0.87              |
| 1:A:371:ASN:HD22 | 1:A:371:ASN:N    | 1.72                     | 0.86              |
| 1:A:375:ILE:HD11 | 1:A:379:CYS:SG   | 2.16                     | 0.86              |
| 1:C:136:CYS:H    | 1:C:330:GLN:NE2  | 1.73                     | 0.86              |
| 1:B:340:GLN:HG2  | 1:B:342:LYS:HG2  | 1.59                     | 0.85              |
| 1:A:213:HIS:HD2  | 1:A:242:VAL:H    | 1.24                     | 0.85              |
| 1:C:342:LYS:HB2  | 1:C:343:PRO:HD2  | 1.60                     | 0.84              |
| 1:A:371:ASN:H    | 1:A:371:ASN:HD22 | 1.22                     | 0.82              |
| 1:A:302:ALA:HB1  | 1:A:305:ILE:HD11 | 1.60                     | 0.81              |
| 1:C:136:CYS:H    | 1:C:330:GLN:HE22 | 1.22                     | 0.81              |
| 1:C:340:GLN:HG2  | 1:C:342:LYS:HG2  | 1.61                     | 0.80              |
| 1:B:136:CYS:H    | 1:B:330:GLN:HE22 | 1.27                     | 0.80              |
| 1:A:416:THR:HG22 | 1:A:417:GLU:H    | 1.47                     | 0.80              |
| 1:C:302:ALA:HB1  | 1:C:305:ILE:HD11 | 1.64                     | 0.80              |
| 1:B:213:HIS:HD2  | 1:B:242:VAL:H    | 1.27                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:213:HIS:HD2  | 1:C:242:VAL:H    | 1.27                     | 0.80              |
| 1:B:416:THR:HG23 | 3:B:506:HOH:O    | 1.82                     | 0.78              |
| 1:A:95:ARG:NH2   | 1:A:417:GLU:HB3  | 1.99                     | 0.78              |
| 1:C:380:ARG:O    | 1:C:384:GLN:HG2  | 1.84                     | 0.78              |
| 1:B:95:ARG:CZ    | 1:B:417:GLU:HB3  | 2.13                     | 0.78              |
| 1:C:371:ASN:N    | 1:C:371:ASN:HD22 | 1.81                     | 0.77              |
| 1:B:173:ASP:OD2  | 1:C:300:ARG:HD2  | 1.84                     | 0.77              |
| 1:B:99:VAL:HG12  | 1:B:414:LEU:CD2  | 2.16                     | 0.75              |
| 1:A:115:ASP:O    | 1:A:119:THR:HG22 | 1.87                     | 0.75              |
| 1:B:115:ASP:O    | 1:B:119:THR:HG22 | 1.86                     | 0.75              |
| 1:C:95:ARG:NH2   | 1:C:417:GLU:HB3  | 2.02                     | 0.75              |
| 1:C:115:ASP:O    | 1:C:119:THR:HG22 | 1.87                     | 0.74              |
| 1:C:302:ALA:HB1  | 1:C:305:ILE:CD1  | 2.17                     | 0.74              |
| 1:A:13:GLY:H     | 1:A:80:ARG:HH21  | 1.33                     | 0.74              |
| 1:B:13:GLY:H     | 1:B:80:ARG:HH21  | 1.34                     | 0.74              |
| 1:B:371:ASN:H    | 1:B:371:ASN:ND2  | 1.84                     | 0.73              |
| 1:C:15:THR:HG22  | 1:C:17:VAL:N     | 2.00                     | 0.73              |
| 1:B:95:ARG:NE    | 1:B:417:GLU:HG2  | 2.03                     | 0.73              |
| 1:A:15:THR:HG22  | 1:A:17:VAL:N     | 2.01                     | 0.73              |
| 1:B:70:HIS:HB2   | 1:B:393:PRO:HB3  | 1.69                     | 0.73              |
| 1:C:125:GLN:HG3  | 3:C:525:HOH:O    | 1.89                     | 0.73              |
| 1:C:143:VAL:HG22 | 1:C:159:VAL:HG11 | 1.71                     | 0.72              |
| 1:B:309:THR:O    | 1:B:313:GLN:HG3  | 1.89                     | 0.72              |
| 1:A:118:ASP:OD1  | 1:A:122:LYS:HE2  | 1.90                     | 0.72              |
| 1:B:213:HIS:CD2  | 1:B:241:CYS:HA   | 2.24                     | 0.72              |
| 1:B:302:ALA:HB1  | 1:B:305:ILE:CD1  | 2.19                     | 0.72              |
| 1:B:202:GLY:HA3  | 1:B:375:ILE:HD12 | 1.72                     | 0.72              |
| 1:B:296:ASP:O    | 1:B:299:GLN:HG2  | 1.90                     | 0.71              |
| 1:B:371:ASN:HD22 | 1:B:371:ASN:N    | 1.89                     | 0.71              |
| 1:C:118:ASP:OD1  | 1:C:122:LYS:HE2  | 1.90                     | 0.71              |
| 1:C:358:ASN:O    | 1:C:359:GLN:CG   | 2.38                     | 0.71              |
| 1:C:235:VAL:HG21 | 1:C:288:HIS:NE2  | 2.06                     | 0.71              |
| 1:C:213:HIS:CD2  | 1:C:241:CYS:HA   | 2.26                     | 0.70              |
| 1:C:324:MET:CE   | 1:C:350:GLU:HG2  | 2.20                     | 0.70              |
| 1:C:99:VAL:HG12  | 1:C:414:LEU:HD22 | 1.73                     | 0.70              |
| 1:C:95:ARG:NE    | 1:C:417:GLU:HG2  | 2.06                     | 0.69              |
| 1:C:142:THR:HG22 | 1:C:144:ASP:H    | 1.56                     | 0.69              |
| 1:C:24:GLY:O     | 1:C:28:THR:HG23  | 1.92                     | 0.69              |
| 1:B:371:ASN:N    | 1:B:371:ASN:ND2  | 2.38                     | 0.69              |
| 1:A:235:VAL:HG21 | 1:A:288:HIS:NE2  | 2.08                     | 0.69              |
| 1:A:24:GLY:O     | 1:A:28:THR:HG23  | 1.92                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:28:THR:HG21  | 1:C:319:LYS:CG   | 2.21                     | 0.69              |
| 1:B:15:THR:HG22  | 1:B:17:VAL:N     | 2.02                     | 0.69              |
| 1:C:419:GLU:HG2  | 1:C:420:LEU:H    | 1.56                     | 0.69              |
| 1:A:296:ASP:O    | 1:A:299:GLN:HG2  | 1.93                     | 0.69              |
| 1:C:324:MET:HE3  | 1:C:350:GLU:HG2  | 1.75                     | 0.69              |
| 1:C:60:GLU:HG2   | 1:C:405:LEU:HD22 | 1.74                     | 0.69              |
| 1:A:13:GLY:H     | 1:A:80:ARG:NH2   | 1.91                     | 0.69              |
| 1:B:136:CYS:H    | 1:B:330:GLN:NE2  | 1.91                     | 0.69              |
| 1:C:13:GLY:H     | 1:C:80:ARG:HH21  | 1.39                     | 0.69              |
| 1:B:235:VAL:HG21 | 1:B:288:HIS:NE2  | 2.07                     | 0.68              |
| 1:B:358:ASN:O    | 1:B:359:GLN:HG2  | 1.93                     | 0.68              |
| 1:A:142:THR:HG22 | 1:A:144:ASP:H    | 1.56                     | 0.68              |
| 1:B:118:ASP:OD1  | 1:B:122:LYS:HE2  | 1.93                     | 0.68              |
| 1:C:27:GLN:HE22  | 1:C:66:GLN:NE2   | 1.91                     | 0.68              |
| 1:A:371:ASN:ND2  | 1:A:371:ASN:H    | 1.91                     | 0.68              |
| 1:B:27:GLN:HE22  | 1:B:66:GLN:NE2   | 1.91                     | 0.68              |
| 1:A:67:ALA:O     | 1:A:71:THR:HG22  | 1.94                     | 0.68              |
| 1:A:213:HIS:CD2  | 1:A:241:CYS:HA   | 2.28                     | 0.68              |
| 1:B:60:GLU:HG2   | 1:B:405:LEU:HD22 | 1.75                     | 0.68              |
| 1:A:309:THR:O    | 1:A:313:GLN:HG3  | 1.93                     | 0.67              |
| 1:B:143:VAL:HG22 | 1:B:159:VAL:HG11 | 1.77                     | 0.67              |
| 1:B:305:ILE:HD12 | 1:B:305:ILE:H    | 1.58                     | 0.67              |
| 1:B:13:GLY:H     | 1:B:80:ARG:NH2   | 1.92                     | 0.67              |
| 1:B:142:THR:HG22 | 1:B:144:ASP:H    | 1.58                     | 0.67              |
| 1:A:27:GLN:HE22  | 1:A:66:GLN:NE2   | 1.92                     | 0.67              |
| 1:A:309:THR:HG23 | 1:A:388:ALA:O    | 1.94                     | 0.67              |
| 1:B:135:THR:HA   | 1:B:330:GLN:OE1  | 1.95                     | 0.67              |
| 1:A:330:GLN:HE21 | 1:A:331:ALA:N    | 1.91                     | 0.67              |
| 1:C:274:VAL:O    | 1:C:274:VAL:HG12 | 1.95                     | 0.67              |
| 1:C:148:PRO:HG3  | 1:C:359:GLN:O    | 1.95                     | 0.67              |
| 1:A:95:ARG:CZ    | 1:A:417:GLU:HB3  | 2.25                     | 0.66              |
| 1:C:194:ALA:HB1  | 3:C:432:HOH:O    | 1.95                     | 0.66              |
| 1:B:203:LEU:HD12 | 1:B:384:GLN:OE1  | 1.96                     | 0.66              |
| 1:A:302:ALA:HB1  | 1:A:305:ILE:CD1  | 2.24                     | 0.66              |
| 1:A:136:CYS:H    | 1:A:330:GLN:NE2  | 1.93                     | 0.66              |
| 1:A:118:ASP:HB2  | 1:A:357:ALA:HB2  | 1.77                     | 0.66              |
| 1:B:67:ALA:O     | 1:B:71:THR:HG22  | 1.95                     | 0.65              |
| 1:C:118:ASP:HB2  | 1:C:357:ALA:HB2  | 1.79                     | 0.65              |
| 1:C:371:ASN:ND2  | 1:C:371:ASN:N    | 2.44                     | 0.65              |
| 1:A:283:LYS:HD2  | 1:A:290:TYR:HE1  | 1.62                     | 0.65              |
| 1:B:24:GLY:O     | 1:B:28:THR:HG23  | 1.97                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:13:GLY:H     | 1:C:80:ARG:NH2   | 1.95                     | 0.65              |
| 1:C:367:TYR:O    | 1:C:376:THR:HG23 | 1.96                     | 0.65              |
| 1:A:99:VAL:HG12  | 1:A:414:LEU:HD22 | 1.77                     | 0.64              |
| 1:B:95:ARG:NH2   | 1:B:417:GLU:HB3  | 2.12                     | 0.64              |
| 1:C:67:ALA:O     | 1:C:71:THR:HG22  | 1.97                     | 0.64              |
| 1:B:302:ALA:HB1  | 1:B:305:ILE:HD11 | 1.78                     | 0.64              |
| 1:B:307:SER:HB3  | 1:B:310:ASP:HB2  | 1.80                     | 0.64              |
| 1:C:70:HIS:HB2   | 1:C:393:PRO:HB3  | 1.80                     | 0.64              |
| 1:C:418:PHE:HA   | 3:C:511:HOH:O    | 1.97                     | 0.64              |
| 1:C:283:LYS:HD2  | 1:C:290:TYR:HE1  | 1.63                     | 0.64              |
| 1:C:232:ASP:HB2  | 1:C:286:LEU:HD13 | 1.80                     | 0.64              |
| 1:A:95:ARG:NH1   | 1:A:414:LEU:HD23 | 2.13                     | 0.63              |
| 1:B:417:GLU:O    | 1:B:417:GLU:HG3  | 1.97                     | 0.63              |
| 1:C:342:LYS:CB   | 1:C:343:PRO:HD2  | 2.28                     | 0.63              |
| 1:B:380:ARG:HH11 | 1:B:380:ARG:HG3  | 1.64                     | 0.63              |
| 1:A:136:CYS:N    | 1:A:330:GLN:HE22 | 1.94                     | 0.63              |
| 1:B:415:ARG:HB2  | 3:B:468:HOH:O    | 1.99                     | 0.62              |
| 1:B:342:LYS:CB   | 1:B:343:PRO:HD2  | 2.22                     | 0.62              |
| 1:A:10:GLN:HE22  | 1:A:74:GLY:CA    | 2.12                     | 0.62              |
| 1:B:199:ALA:O    | 1:B:375:ILE:HD11 | 1.99                     | 0.62              |
| 1:B:283:LYS:HD2  | 1:B:290:TYR:HE1  | 1.63                     | 0.62              |
| 1:B:10:GLN:HE22  | 1:B:74:GLY:CA    | 2.12                     | 0.62              |
| 1:B:27:GLN:HE22  | 1:B:66:GLN:HE21  | 1.48                     | 0.62              |
| 1:A:416:THR:HG22 | 1:A:417:GLU:N    | 2.13                     | 0.62              |
| 1:A:342:LYS:O    | 1:A:343:PRO:C    | 2.38                     | 0.62              |
| 1:C:10:GLN:HE22  | 1:C:74:GLY:CA    | 2.12                     | 0.61              |
| 1:C:136:CYS:N    | 1:C:330:GLN:HE22 | 1.94                     | 0.61              |
| 1:B:232:ASP:HB2  | 1:B:286:LEU:HD13 | 1.82                     | 0.61              |
| 1:C:211:PRO:HB3  | 1:C:242:VAL:HG21 | 1.82                     | 0.61              |
| 1:A:91:ARG:N     | 3:A:423:HOH:O    | 2.33                     | 0.61              |
| 1:B:342:LYS:O    | 1:B:344:TYR:N    | 2.33                     | 0.61              |
| 1:A:50:LEU:O     | 1:A:417:GLU:HG2  | 2.00                     | 0.61              |
| 1:A:91:ARG:HG3   | 1:A:92:GLU:H     | 1.65                     | 0.61              |
| 1:B:99:VAL:HG12  | 1:B:414:LEU:HD22 | 1.83                     | 0.61              |
| 1:C:417:GLU:O    | 1:C:417:GLU:HG3  | 2.00                     | 0.61              |
| 1:C:331:ALA:HA   | 1:C:353:LEU:HD12 | 1.83                     | 0.61              |
| 1:A:322:VAL:O    | 1:A:326:LEU:HD22 | 2.01                     | 0.60              |
| 1:B:396:ASP:O    | 1:B:397:ASP:HB2  | 2.01                     | 0.60              |
| 1:B:91:ARG:HG3   | 1:B:92:GLU:H     | 1.66                     | 0.60              |
| 1:C:91:ARG:HG3   | 1:C:92:GLU:H     | 1.66                     | 0.60              |
| 1:C:358:ASN:O    | 1:C:359:GLN:HG3  | 2.02                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:47:ILE:HD11  | 1:A:81:TYR:CG    | 2.37                     | 0.60              |
| 1:A:27:GLN:HE22  | 1:A:66:GLN:HE21  | 1.50                     | 0.60              |
| 1:A:232:ASP:HB2  | 1:A:286:LEU:HD13 | 1.84                     | 0.59              |
| 1:A:138:GLY:O    | 1:A:334:PRO:CD   | 2.48                     | 0.59              |
| 1:C:342:LYS:O    | 1:C:343:PRO:C    | 2.39                     | 0.59              |
| 1:A:357:ALA:HB3  | 3:A:510:HOH:O    | 2.01                     | 0.59              |
| 1:C:161:LYS:NZ   | 1:C:390:GLU:HG3  | 2.17                     | 0.59              |
| 1:C:27:GLN:HE22  | 1:C:66:GLN:HE21  | 1.48                     | 0.59              |
| 1:C:47:ILE:HD11  | 1:C:81:TYR:CG    | 2.38                     | 0.59              |
| 1:A:403:ALA:O    | 1:A:404:LYS:HB2  | 2.02                     | 0.58              |
| 1:C:182:THR:HG21 | 1:C:291:HIS:CD2  | 2.38                     | 0.58              |
| 1:C:382:TYR:O    | 1:C:385:PRO:HD2  | 2.03                     | 0.58              |
| 1:A:375:ILE:CD1  | 1:A:379:CYS:SG   | 2.91                     | 0.58              |
| 1:B:47:ILE:HD11  | 1:B:81:TYR:CG    | 2.39                     | 0.58              |
| 1:C:279:ALA:HB1  | 1:C:290:TYR:CD2  | 2.39                     | 0.58              |
| 1:A:15:THR:CG2   | 1:A:16:ALA:N     | 2.67                     | 0.58              |
| 1:B:279:ALA:HB1  | 1:B:290:TYR:CD2  | 2.38                     | 0.58              |
| 1:B:342:LYS:HB2  | 1:B:343:PRO:CD   | 2.23                     | 0.58              |
| 1:C:216:LEU:HD12 | 1:C:278:LEU:HD11 | 1.84                     | 0.58              |
| 1:B:300:ARG:HD3  | 1:C:173:ASP:OD2  | 2.04                     | 0.57              |
| 1:C:364:PRO:HB2  | 1:C:366:HIS:CD2  | 2.39                     | 0.57              |
| 1:C:296:ASP:O    | 1:C:299:GLN:HG2  | 2.04                     | 0.57              |
| 1:B:116:SER:O    | 1:B:119:THR:HG23 | 2.04                     | 0.57              |
| 1:A:18:ILE:HD12  | 1:A:141:LYS:HG3  | 1.86                     | 0.57              |
| 1:A:60:GLU:CG    | 1:A:405:LEU:HD22 | 2.32                     | 0.57              |
| 1:A:329:LYS:NZ   | 1:B:340:GLN:HG3  | 2.20                     | 0.57              |
| 1:A:295:ALA:O    | 1:A:298:LEU:HB2  | 2.04                     | 0.57              |
| 1:A:21:SER:O     | 1:A:25:VAL:HG12  | 2.04                     | 0.57              |
| 1:C:50:LEU:O     | 1:C:417:GLU:HG2  | 2.05                     | 0.57              |
| 1:C:156:PHE:CE2  | 1:C:196:TRP:HB3  | 2.40                     | 0.56              |
| 1:A:335:THR:O    | 1:A:348:ILE:HA   | 2.05                     | 0.56              |
| 1:C:145:ASN:HA   | 1:C:153:CYS:SG   | 2.45                     | 0.56              |
| 1:C:3:ILE:O      | 1:C:3:ILE:HG23   | 2.06                     | 0.56              |
| 1:A:375:ILE:HG13 | 1:A:379:CYS:HB3  | 1.86                     | 0.56              |
| 1:B:342:LYS:O    | 1:B:343:PRO:C    | 2.44                     | 0.56              |
| 1:C:15:THR:CG2   | 1:C:16:ALA:N     | 2.69                     | 0.56              |
| 1:A:24:GLY:HA2   | 1:A:315:TYR:CE1  | 2.41                     | 0.56              |
| 1:A:70:HIS:HB2   | 1:A:393:PRO:HB3  | 1.88                     | 0.56              |
| 1:B:18:ILE:HD12  | 1:B:141:LYS:HG3  | 1.88                     | 0.56              |
| 1:B:200:ALA:HA   | 1:B:203:LEU:HD23 | 1.88                     | 0.56              |
| 1:B:211:PRO:HB3  | 1:B:242:VAL:HG21 | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:147:LEU:HB2  | 1:A:153:CYS:SG   | 2.45                     | 0.55              |
| 1:A:305:ILE:HD12 | 1:A:305:ILE:H    | 1.71                     | 0.55              |
| 1:B:337:VAL:HG22 | 1:B:347:SER:O    | 2.07                     | 0.55              |
| 1:C:18:ILE:HD12  | 1:C:141:LYS:HG3  | 1.87                     | 0.55              |
| 1:B:141:LYS:C    | 1:B:141:LYS:HD2  | 2.27                     | 0.55              |
| 1:B:380:ARG:NH1  | 1:B:380:ARG:HG3  | 2.20                     | 0.55              |
| 1:C:200:ALA:HA   | 1:C:203:LEU:HD23 | 1.88                     | 0.55              |
| 1:B:216:LEU:HD12 | 1:B:278:LEU:HD11 | 1.89                     | 0.55              |
| 1:A:186:ILE:HG12 | 1:A:243:VAL:HG22 | 1.89                     | 0.55              |
| 1:A:200:ALA:HA   | 1:A:203:LEU:HD23 | 1.89                     | 0.55              |
| 1:C:320:ALA:HB1  | 1:C:348:ILE:HG21 | 1.89                     | 0.55              |
| 1:A:279:ALA:HB1  | 1:A:290:TYR:CD2  | 2.42                     | 0.54              |
| 1:A:59:LEU:HB3   | 3:A:483:HOH:O    | 2.08                     | 0.54              |
| 1:B:10:GLN:NE2   | 3:B:430:HOH:O    | 2.40                     | 0.54              |
| 1:A:182:THR:HG21 | 1:A:291:HIS:CD2  | 2.42                     | 0.54              |
| 1:B:186:ILE:HG12 | 1:B:243:VAL:HG22 | 1.90                     | 0.54              |
| 1:B:320:ALA:HB1  | 1:B:348:ILE:HG21 | 1.90                     | 0.54              |
| 1:B:338:ARG:NH1  | 1:B:344:TYR:CE1  | 2.75                     | 0.54              |
| 1:B:199:ALA:O    | 1:B:375:ILE:CD1  | 2.55                     | 0.54              |
| 1:B:147:LEU:HB2  | 1:B:153:CYS:SG   | 2.48                     | 0.54              |
| 1:B:340:GLN:HG2  | 1:B:342:LYS:CG   | 2.36                     | 0.54              |
| 1:C:355:GLU:HB3  | 3:C:515:HOH:O    | 2.08                     | 0.54              |
| 1:A:10:GLN:NE2   | 3:A:422:HOH:O    | 2.40                     | 0.54              |
| 1:C:142:THR:HA   | 3:C:502:HOH:O    | 2.08                     | 0.54              |
| 1:B:358:ASN:O    | 1:B:359:GLN:CG   | 2.56                     | 0.54              |
| 1:C:116:SER:O    | 1:C:119:THR:HG23 | 2.07                     | 0.54              |
| 1:C:127:ALA:HB1  | 1:C:132:TYR:O    | 2.05                     | 0.54              |
| 1:C:135:THR:HA   | 1:C:330:GLN:HE22 | 1.74                     | 0.53              |
| 1:C:419:GLU:CG   | 1:C:420:LEU:N    | 2.53                     | 0.53              |
| 1:A:116:SER:O    | 1:A:119:THR:HG23 | 2.09                     | 0.53              |
| 1:A:275:ALA:HB3  | 1:A:276:PRO:CD   | 2.39                     | 0.53              |
| 1:B:300:ARG:CD   | 1:C:173:ASP:OD2  | 2.57                     | 0.53              |
| 1:A:291:HIS:HB2  | 3:A:424:HOH:O    | 2.08                     | 0.53              |
| 1:A:371:ASN:ND2  | 1:A:371:ASN:N    | 2.45                     | 0.53              |
| 1:B:127:ALA:HB1  | 1:B:132:TYR:O    | 2.09                     | 0.53              |
| 1:C:338:ARG:NH1  | 1:C:344:TYR:CD1  | 2.77                     | 0.53              |
| 1:C:95:ARG:CZ    | 1:C:417:GLU:CB   | 2.86                     | 0.53              |
| 1:A:211:PRO:HB3  | 1:A:242:VAL:HG21 | 1.89                     | 0.53              |
| 1:B:307:SER:HB3  | 1:B:310:ASP:CB   | 2.39                     | 0.53              |
| 1:C:143:VAL:HG22 | 1:C:159:VAL:CG1  | 2.37                     | 0.53              |
| 1:C:178:CYS:O    | 1:C:183:LYS:HE2  | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:93:TYR:HB3   | 1:A:126:LEU:HD12 | 1.91                     | 0.53              |
| 1:A:141:LYS:HD2  | 1:A:141:LYS:C    | 2.30                     | 0.53              |
| 1:B:305:ILE:N    | 1:B:305:ILE:HD12 | 2.21                     | 0.52              |
| 1:C:135:THR:HA   | 1:C:330:GLN:NE2  | 2.24                     | 0.52              |
| 1:A:143:VAL:HG22 | 1:A:159:VAL:HG11 | 1.91                     | 0.52              |
| 1:A:348:ILE:HD12 | 1:A:348:ILE:N    | 2.23                     | 0.52              |
| 1:B:15:THR:CG2   | 1:B:16:ALA:N     | 2.72                     | 0.52              |
| 1:B:227:PHE:O    | 1:B:231:VAL:HG12 | 2.10                     | 0.52              |
| 1:C:95:ARG:HE    | 1:C:417:GLU:HG2  | 1.75                     | 0.52              |
| 1:A:127:ALA:HB1  | 1:A:132:TYR:O    | 2.09                     | 0.52              |
| 1:B:186:ILE:O    | 1:B:292:TRP:HA   | 2.09                     | 0.52              |
| 1:C:274:VAL:CG1  | 1:C:274:VAL:O    | 2.56                     | 0.52              |
| 1:C:309:THR:O    | 1:C:313:GLN:HG3  | 2.09                     | 0.52              |
| 1:C:324:MET:HE2  | 1:C:350:GLU:HG2  | 1.90                     | 0.52              |
| 1:A:330:GLN:NE2  | 1:A:331:ALA:H    | 1.97                     | 0.52              |
| 1:A:227:PHE:O    | 1:A:231:VAL:HG12 | 2.10                     | 0.52              |
| 1:B:320:ALA:CB   | 1:B:348:ILE:HG21 | 2.40                     | 0.51              |
| 1:C:21:SER:O     | 1:C:25:VAL:HG12  | 2.10                     | 0.51              |
| 1:C:93:TYR:HB3   | 1:C:126:LEU:HD12 | 1.92                     | 0.51              |
| 1:A:178:CYS:O    | 1:A:183:LYS:HE2  | 2.10                     | 0.51              |
| 1:A:99:VAL:HG12  | 1:A:414:LEU:HD21 | 1.85                     | 0.51              |
| 1:C:141:LYS:C    | 1:C:141:LYS:HD2  | 2.31                     | 0.51              |
| 1:B:70:HIS:HB2   | 1:B:393:PRO:CB   | 2.37                     | 0.51              |
| 1:C:231:VAL:HG13 | 1:C:232:ASP:H    | 1.76                     | 0.51              |
| 1:A:40:TYR:CE1   | 1:A:410:VAL:HG21 | 2.46                     | 0.51              |
| 1:B:23:CYS:SG    | 1:B:69:ILE:CG2   | 2.99                     | 0.51              |
| 1:A:4:LYS:NZ     | 3:A:455:HOH:O    | 2.44                     | 0.51              |
| 1:C:182:THR:HG21 | 1:C:291:HIS:HD2  | 1.76                     | 0.51              |
| 1:A:199:ALA:HB1  | 1:A:375:ILE:HD11 | 1.93                     | 0.51              |
| 1:C:320:ALA:CB   | 1:C:348:ILE:HG21 | 2.41                     | 0.51              |
| 1:C:330:GLN:HE21 | 1:C:331:ALA:H    | 1.59                     | 0.51              |
| 1:A:10:GLN:HE22  | 1:A:74:GLY:HA2   | 1.75                     | 0.51              |
| 1:A:316:ALA:HB1  | 1:A:348:ILE:HD11 | 1.93                     | 0.51              |
| 1:A:95:ARG:CZ    | 1:A:417:GLU:CB   | 2.88                     | 0.51              |
| 1:B:95:ARG:HE    | 1:B:417:GLU:HG2  | 1.74                     | 0.51              |
| 3:B:507:HOH:O    | 1:C:305:ILE:HG23 | 2.11                     | 0.51              |
| 1:C:313:GLN:HB3  | 1:C:336:ILE:HD12 | 1.92                     | 0.51              |
| 1:C:161:LYS:HE3  | 1:C:389:GLY:O    | 2.11                     | 0.51              |
| 1:A:291:HIS:N    | 3:A:424:HOH:O    | 2.44                     | 0.50              |
| 1:A:340:GLN:O    | 1:A:344:TYR:HA   | 2.10                     | 0.50              |
| 1:B:178:CYS:O    | 1:B:183:LYS:HE2  | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:185:PHE:HA   | 1:B:291:HIS:O    | 2.10                     | 0.50              |
| 1:C:337:VAL:O    | 1:C:346:TRP:HA   | 2.11                     | 0.50              |
| 1:B:71:THR:HG21  | 1:B:403:ALA:HB2  | 1.92                     | 0.50              |
| 1:B:117:GLN:HE21 | 1:B:333:MET:HB2  | 1.77                     | 0.50              |
| 1:B:30:ARG:HB3   | 3:B:449:HOH:O    | 2.10                     | 0.50              |
| 1:C:52:GLU:OE1   | 1:C:413:LYS:N    | 2.40                     | 0.50              |
| 1:C:349:GLY:O    | 1:C:350:GLU:HG3  | 2.12                     | 0.50              |
| 1:A:327:ALA:HB1  | 1:B:339:ASP:O    | 2.11                     | 0.50              |
| 1:B:21:SER:O     | 1:B:25:VAL:HG12  | 2.11                     | 0.50              |
| 1:C:186:ILE:HG12 | 1:C:243:VAL:HG22 | 1.92                     | 0.50              |
| 1:C:255:ARG:HB3  | 1:C:256:PHE:HD1  | 1.75                     | 0.50              |
| 1:B:279:ALA:O    | 1:B:282:VAL:HG22 | 2.11                     | 0.50              |
| 1:C:419:GLU:CG   | 1:C:420:LEU:H    | 2.20                     | 0.50              |
| 1:C:91:ARG:CG    | 1:C:92:GLU:H     | 2.25                     | 0.50              |
| 1:B:93:TYR:HB3   | 1:B:126:LEU:HD12 | 1.93                     | 0.50              |
| 1:C:273:GLY:O    | 1:C:276:PRO:HD2  | 2.11                     | 0.50              |
| 1:A:182:THR:HG21 | 1:A:291:HIS:HD2  | 1.75                     | 0.50              |
| 1:B:143:VAL:HG22 | 1:B:159:VAL:CG1  | 2.41                     | 0.50              |
| 1:B:200:ALA:O    | 1:B:203:LEU:HD23 | 2.12                     | 0.50              |
| 1:B:231:VAL:HG13 | 1:B:232:ASP:H    | 1.77                     | 0.50              |
| 1:C:95:ARG:CZ    | 1:C:417:GLU:HB3  | 2.42                     | 0.50              |
| 1:A:91:ARG:CG    | 1:A:92:GLU:H     | 2.24                     | 0.49              |
| 1:A:255:ARG:HB3  | 1:A:256:PHE:HD1  | 1.77                     | 0.49              |
| 1:A:417:GLU:O    | 1:A:417:GLU:HG3  | 2.10                     | 0.49              |
| 1:C:121:TYR:O    | 1:C:124:SER:HB3  | 2.12                     | 0.49              |
| 1:C:147:LEU:HB2  | 1:C:153:CYS:SG   | 2.53                     | 0.49              |
| 1:B:125:GLN:NE2  | 3:B:529:HOH:O    | 2.44                     | 0.49              |
| 1:B:213:HIS:CD2  | 1:B:242:VAL:H    | 2.18                     | 0.49              |
| 1:B:10:GLN:HE22  | 1:B:74:GLY:HA2   | 1.77                     | 0.49              |
| 1:B:10:GLN:HE22  | 1:B:74:GLY:HA3   | 1.77                     | 0.49              |
| 1:B:91:ARG:CG    | 1:B:92:GLU:H     | 2.25                     | 0.49              |
| 1:C:342:LYS:O    | 1:C:344:TYR:N    | 2.45                     | 0.49              |
| 1:C:360:GLU:HB3  | 3:C:506:HOH:O    | 2.11                     | 0.49              |
| 1:A:23:CYS:SG    | 1:A:69:ILE:CG2   | 3.00                     | 0.49              |
| 1:B:316:ALA:HB1  | 1:B:348:ILE:HD11 | 1.94                     | 0.49              |
| 1:C:10:GLN:HE22  | 1:C:74:GLY:HA2   | 1.77                     | 0.49              |
| 1:B:216:LEU:HA   | 3:B:517:HOH:O    | 2.12                     | 0.49              |
| 1:B:357:ALA:O    | 1:B:358:ASN:HB2  | 2.12                     | 0.49              |
| 1:C:233:GLN:O    | 1:C:237:ASP:HB2  | 2.12                     | 0.49              |
| 1:B:317:VAL:O    | 1:B:334:PRO:HG3  | 2.13                     | 0.49              |
| 1:C:162:TYR:HD2  | 1:C:163:ILE:HD12 | 1.77                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:279:ALA:O    | 1:C:282:VAL:HG22 | 2.11                     | 0.49              |
| 1:C:23:CYS:SG    | 1:C:69:ILE:CG2   | 3.01                     | 0.49              |
| 1:A:15:THR:HG22  | 1:A:16:ALA:N     | 2.28                     | 0.49              |
| 1:C:330:GLN:HG3  | 1:C:331:ALA:N    | 2.26                     | 0.49              |
| 1:A:231:VAL:HG13 | 1:A:232:ASP:H    | 1.78                     | 0.49              |
| 1:A:365:ILE:C    | 1:A:367:TYR:H    | 2.16                     | 0.49              |
| 1:C:126:LEU:HD22 | 1:C:130:MET:HG3  | 1.94                     | 0.49              |
| 1:C:384:GLN:HG3  | 1:C:385:PRO:HD3  | 1.94                     | 0.49              |
| 1:A:158:SER:HB3  | 3:A:453:HOH:O    | 2.13                     | 0.48              |
| 1:A:380:ARG:HD3  | 3:A:470:HOH:O    | 2.11                     | 0.48              |
| 1:C:159:VAL:CG2  | 1:C:160:ALA:N    | 2.76                     | 0.48              |
| 1:A:162:TYR:HD2  | 1:A:163:ILE:HD12 | 1.77                     | 0.48              |
| 1:A:275:ALA:HB3  | 1:A:276:PRO:HD3  | 1.94                     | 0.48              |
| 1:A:411:GLU:O    | 1:A:412:LYS:O    | 2.30                     | 0.48              |
| 1:C:10:GLN:HE22  | 1:C:74:GLY:HA3   | 1.79                     | 0.48              |
| 1:C:307:SER:HB3  | 1:C:310:ASP:HB2  | 1.95                     | 0.48              |
| 1:C:363:MET:HB2  | 3:C:432:HOH:O    | 2.12                     | 0.48              |
| 1:C:394:PRO:HG3  | 1:C:401:ARG:NH1  | 2.28                     | 0.48              |
| 1:C:40:TYR:CE1   | 1:C:410:VAL:HG21 | 2.48                     | 0.48              |
| 1:A:91:ARG:HG2   | 3:A:423:HOH:O    | 2.12                     | 0.48              |
| 1:B:119:THR:HG21 | 3:B:422:HOH:O    | 2.12                     | 0.48              |
| 1:B:255:ARG:HB3  | 1:B:256:PHE:HD1  | 1.78                     | 0.48              |
| 1:C:28:THR:CG2   | 1:C:319:LYS:HG3  | 2.27                     | 0.48              |
| 1:B:162:TYR:HD2  | 1:B:163:ILE:HD12 | 1.78                     | 0.48              |
| 1:B:242:VAL:O    | 1:B:242:VAL:HG23 | 2.13                     | 0.48              |
| 1:C:149:PHE:O    | 1:C:335:THR:HG21 | 2.14                     | 0.48              |
| 1:B:375:ILE:HG23 | 1:B:379:CYS:HB3  | 1.96                     | 0.48              |
| 1:C:126:LEU:CD2  | 1:C:130:MET:HG3  | 2.44                     | 0.48              |
| 1:C:70:HIS:HA    | 1:C:303:ARG:CZ   | 2.43                     | 0.48              |
| 1:C:371:ASN:ND2  | 1:C:371:ASN:H    | 2.09                     | 0.48              |
| 1:A:340:GLN:HG2  | 1:A:342:LYS:HG3  | 1.95                     | 0.48              |
| 1:C:81:TYR:CZ    | 1:C:419:GLU:HG3  | 2.48                     | 0.48              |
| 1:B:4:LYS:HB2    | 1:B:4:LYS:NZ     | 2.29                     | 0.48              |
| 1:C:133:PRO:HA   | 3:C:441:HOH:O    | 2.12                     | 0.48              |
| 1:A:126:LEU:CD2  | 1:A:130:MET:HG3  | 2.43                     | 0.48              |
| 1:A:215:ILE:HG12 | 1:A:244:VAL:CG1  | 2.44                     | 0.48              |
| 1:A:279:ALA:O    | 1:A:282:VAL:HG22 | 2.13                     | 0.48              |
| 1:B:308:ALA:HB2  | 1:B:390:GLU:O    | 2.14                     | 0.48              |
| 1:A:233:GLN:O    | 1:A:237:ASP:HB2  | 2.14                     | 0.48              |
| 1:A:71:THR:HG21  | 1:A:403:ALA:HB2  | 1.96                     | 0.48              |
| 1:A:360:GLU:OE1  | 1:A:362:LYS:HD2  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:121:TYR:O    | 1:B:124:SER:HB3  | 2.13                     | 0.47              |
| 1:B:233:GLN:O    | 1:B:237:ASP:HB2  | 2.14                     | 0.47              |
| 1:C:39:VAL:HG23  | 3:C:462:HOH:O    | 2.13                     | 0.47              |
| 1:A:161:LYS:NZ   | 1:A:390:GLU:HG3  | 2.30                     | 0.47              |
| 1:A:135:THR:HA   | 1:A:330:GLN:HE22 | 1.79                     | 0.47              |
| 1:A:342:LYS:O    | 1:A:344:TYR:N    | 2.47                     | 0.47              |
| 1:C:215:ILE:HG12 | 1:C:244:VAL:CG1  | 2.44                     | 0.47              |
| 1:C:24:GLY:HA2   | 1:C:315:TYR:CE1  | 2.49                     | 0.47              |
| 1:C:242:VAL:O    | 1:C:242:VAL:HG23 | 2.13                     | 0.47              |
| 1:B:415:ARG:O    | 1:B:416:THR:O    | 2.32                     | 0.47              |
| 1:C:339:ASP:N    | 1:C:345:ARG:O    | 2.48                     | 0.47              |
| 1:B:12:GLY:HA2   | 1:B:80:ARG:HE    | 1.79                     | 0.47              |
| 1:A:21:SER:HA    | 1:A:314:ALA:O    | 2.15                     | 0.47              |
| 1:A:47:ILE:HG12  | 1:A:79:CYS:SG    | 2.55                     | 0.47              |
| 1:B:297:TYR:OH   | 1:C:182:THR:HG21 | 2.15                     | 0.47              |
| 1:B:322:VAL:O    | 1:B:325:ALA:HB3  | 2.15                     | 0.47              |
| 1:C:227:PHE:O    | 1:C:231:VAL:HG12 | 2.14                     | 0.47              |
| 1:A:126:LEU:HD22 | 1:A:130:MET:HG3  | 1.97                     | 0.47              |
| 1:B:28:THR:HG21  | 1:B:319:LYS:HG3  | 1.97                     | 0.47              |
| 1:C:15:THR:CG2   | 1:C:17:VAL:H     | 2.08                     | 0.47              |
| 1:A:213:HIS:CD2  | 1:A:242:VAL:H    | 2.16                     | 0.46              |
| 1:A:290:TYR:C    | 3:A:424:HOH:O    | 2.54                     | 0.46              |
| 1:A:347:SER:HB2  | 3:A:448:HOH:O    | 2.16                     | 0.46              |
| 1:B:355:GLU:C    | 1:B:357:ALA:N    | 2.68                     | 0.46              |
| 1:A:133:PRO:HA   | 3:A:467:HOH:O    | 2.15                     | 0.46              |
| 1:A:199:ALA:HB1  | 1:A:375:ILE:CD1  | 2.46                     | 0.46              |
| 1:A:364:PRO:O    | 1:A:367:TYR:HB2  | 2.15                     | 0.46              |
| 1:C:200:ALA:O    | 1:C:203:LEU:HD23 | 2.15                     | 0.46              |
| 1:B:297:TYR:CE1  | 1:B:300:ARG:NH1  | 2.84                     | 0.46              |
| 1:C:97:ILE:HD13  | 1:C:127:ALA:HA   | 1.97                     | 0.46              |
| 1:B:126:LEU:HD22 | 1:B:130:MET:HG3  | 1.98                     | 0.46              |
| 1:C:285:ALA:O    | 1:C:286:LEU:HD23 | 2.16                     | 0.46              |
| 1:B:126:LEU:CD2  | 1:B:130:MET:HG3  | 2.45                     | 0.46              |
| 1:B:215:ILE:HG12 | 1:B:244:VAL:CG1  | 2.45                     | 0.46              |
| 1:C:182:THR:N    | 1:C:289:LYS:HD3  | 2.30                     | 0.46              |
| 1:C:32:HIS:CG    | 1:C:326:LEU:HD21 | 2.51                     | 0.46              |
| 1:B:60:GLU:CG    | 1:B:405:LEU:HD22 | 2.44                     | 0.46              |
| 1:B:95:ARG:CZ    | 1:B:417:GLU:CB   | 2.91                     | 0.46              |
| 1:A:302:ALA:O    | 1:A:305:ILE:HD12 | 2.16                     | 0.46              |
| 1:A:357:ALA:O    | 1:A:358:ASN:HB2  | 2.15                     | 0.46              |
| 1:B:297:TYR:O    | 1:B:300:ARG:HG3  | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:91:ARG:HB3   | 1:C:91:ARG:HE    | 1.10                     | 0.46              |
| 1:A:121:TYR:O    | 1:A:124:SER:HB3  | 2.16                     | 0.46              |
| 1:A:242:VAL:O    | 1:A:242:VAL:HG23 | 2.15                     | 0.46              |
| 1:B:228:LEU:HD11 | 1:B:281:MET:HB3  | 1.97                     | 0.46              |
| 1:C:337:VAL:CG2  | 1:C:347:SER:OG   | 2.64                     | 0.46              |
| 1:C:12:GLY:HA2   | 1:C:80:ARG:HE    | 1.80                     | 0.46              |
| 1:A:375:ILE:CG1  | 1:A:379:CYS:SG   | 3.04                     | 0.46              |
| 1:A:12:GLY:HA2   | 1:A:80:ARG:HE    | 1.81                     | 0.46              |
| 1:A:307:SER:O    | 1:A:311:VAL:HG13 | 2.16                     | 0.45              |
| 1:A:383:LEU:C    | 1:A:385:PRO:HD2  | 2.37                     | 0.45              |
| 1:C:302:ALA:O    | 1:C:305:ILE:HD12 | 2.16                     | 0.45              |
| 1:A:228:LEU:HD11 | 1:A:281:MET:HB3  | 1.99                     | 0.45              |
| 1:B:367:TYR:O    | 1:B:376:THR:HG23 | 2.16                     | 0.45              |
| 1:C:213:HIS:CD2  | 1:C:242:VAL:H    | 2.18                     | 0.45              |
| 1:B:70:HIS:CD2   | 1:B:401:ARG:O    | 2.70                     | 0.45              |
| 1:C:292:TRP:C    | 1:C:292:TRP:CD1  | 2.89                     | 0.45              |
| 1:C:367:TYR:C    | 1:C:376:THR:HG23 | 2.37                     | 0.45              |
| 1:C:231:VAL:HG13 | 1:C:232:ASP:N    | 2.32                     | 0.45              |
| 1:A:161:LYS:HE3  | 1:A:389:GLY:O    | 2.16                     | 0.45              |
| 1:C:15:THR:HG22  | 1:C:16:ALA:N     | 2.31                     | 0.45              |
| 1:A:22:ALA:HA    | 1:A:25:VAL:CG1   | 2.47                     | 0.45              |
| 1:C:380:ARG:HG3  | 1:C:380:ARG:HH11 | 1.82                     | 0.45              |
| 1:B:223:ASN:CB   | 3:B:490:HOH:O    | 2.64                     | 0.45              |
| 1:B:99:VAL:HG12  | 1:B:414:LEU:HD23 | 1.95                     | 0.45              |
| 1:A:341:ALA:C    | 1:A:342:LYS:O    | 2.54                     | 0.44              |
| 1:B:338:ARG:NH1  | 1:B:344:TYR:CD1  | 2.83                     | 0.44              |
| 1:C:313:GLN:HB3  | 1:C:336:ILE:CD1  | 2.48                     | 0.44              |
| 1:C:161:LYS:HZ2  | 1:C:390:GLU:HG3  | 1.82                     | 0.44              |
| 1:B:143:VAL:CG2  | 1:B:159:VAL:HG11 | 2.45                     | 0.44              |
| 1:B:314:ALA:O    | 1:B:317:VAL:HG22 | 2.17                     | 0.44              |
| 1:B:28:THR:O     | 1:B:32:HIS:HD2   | 2.00                     | 0.44              |
| 1:C:255:ARG:HB3  | 1:C:256:PHE:CD1  | 2.52                     | 0.44              |
| 1:C:148:PRO:CG   | 1:C:359:GLN:O    | 2.65                     | 0.44              |
| 1:C:375:ILE:HD11 | 1:C:379:CYS:SG   | 2.58                     | 0.44              |
| 1:C:47:ILE:HG12  | 1:C:79:CYS:SG    | 2.57                     | 0.44              |
| 1:A:52:GLU:OE2   | 1:A:414:LEU:HB2  | 2.18                     | 0.44              |
| 1:B:213:HIS:HD2  | 1:B:242:VAL:N    | 2.05                     | 0.44              |
| 1:B:50:LEU:O     | 1:B:417:GLU:HG2  | 2.17                     | 0.44              |
| 1:B:81:TYR:OH    | 1:B:419:GLU:HB2  | 2.18                     | 0.44              |
| 1:C:118:ASP:HB2  | 1:C:357:ALA:CB   | 2.46                     | 0.44              |
| 1:A:329:LYS:HZ3  | 1:B:340:GLN:HG3  | 1.81                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:352:ASN:O    | 1:C:356:VAL:HG23 | 2.18                     | 0.44              |
| 1:B:331:ALA:O    | 1:B:353:LEU:HG   | 2.18                     | 0.44              |
| 1:C:28:THR:O     | 1:C:32:HIS:HD2   | 2.01                     | 0.44              |
| 1:B:231:VAL:HG13 | 1:B:232:ASP:N    | 2.33                     | 0.44              |
| 1:B:326:LEU:CD1  | 1:B:326:LEU:N    | 2.80                     | 0.44              |
| 1:B:47:ILE:HG12  | 1:B:79:CYS:SG    | 2.57                     | 0.44              |
| 1:C:143:VAL:CG2  | 1:C:159:VAL:HG11 | 2.46                     | 0.44              |
| 1:C:70:HIS:HA    | 1:C:303:ARG:NH2  | 2.33                     | 0.44              |
| 1:C:364:PRO:O    | 1:C:367:TYR:HB2  | 2.18                     | 0.44              |
| 1:C:91:ARG:N     | 3:C:436:HOH:O    | 2.51                     | 0.44              |
| 1:A:97:ILE:HD13  | 1:A:127:ALA:HA   | 2.00                     | 0.43              |
| 1:B:97:ILE:HD13  | 1:B:127:ALA:HA   | 1.99                     | 0.43              |
| 1:C:186:ILE:HG23 | 1:C:243:VAL:CG2  | 2.48                     | 0.43              |
| 1:B:161:LYS:HE3  | 1:B:389:GLY:O    | 2.18                     | 0.43              |
| 1:B:296:ASP:CG   | 1:B:297:TYR:H    | 2.21                     | 0.43              |
| 1:A:210:GLU:HA   | 1:A:211:PRO:HD3  | 1.81                     | 0.43              |
| 1:A:182:THR:HA   | 1:A:289:LYS:HB3  | 2.00                     | 0.43              |
| 1:B:52:GLU:OE2   | 1:B:414:LEU:HB2  | 2.19                     | 0.43              |
| 1:C:403:ALA:O    | 1:C:404:LYS:HB2  | 2.18                     | 0.43              |
| 1:A:188:GLU:HA   | 1:A:245:ALA:O    | 2.18                     | 0.43              |
| 1:A:369:THR:HG23 | 1:A:374:GLY:C    | 2.38                     | 0.43              |
| 1:B:182:THR:HA   | 1:B:289:LYS:HB3  | 2.00                     | 0.43              |
| 1:C:188:GLU:HA   | 1:C:245:ALA:O    | 2.18                     | 0.43              |
| 1:C:358:ASN:O    | 1:C:359:GLN:CB   | 2.67                     | 0.43              |
| 1:A:10:GLN:HE22  | 1:A:74:GLY:HA3   | 1.81                     | 0.43              |
| 1:A:285:ALA:O    | 1:A:286:LEU:HD23 | 2.19                     | 0.43              |
| 1:A:28:THR:O     | 1:A:32:HIS:HD2   | 2.01                     | 0.43              |
| 1:A:91:ARG:HB3   | 1:A:91:ARG:HE    | 1.10                     | 0.43              |
| 1:C:304:HIS:CE1  | 1:C:305:ILE:HG13 | 2.53                     | 0.43              |
| 1:C:228:LEU:HD11 | 1:C:281:MET:HB3  | 1.99                     | 0.43              |
| 1:A:162:TYR:CD2  | 1:A:299:GLN:HA   | 2.53                     | 0.43              |
| 1:B:101:ARG:NH1  | 1:B:132:TYR:CE2  | 2.87                     | 0.43              |
| 1:B:255:ARG:HB3  | 1:B:256:PHE:CD1  | 2.53                     | 0.43              |
| 1:A:296:ASP:CG   | 1:A:297:TYR:H    | 2.22                     | 0.43              |
| 1:A:348:ILE:CD1  | 1:A:348:ILE:N    | 2.82                     | 0.43              |
| 1:B:16:ALA:O     | 1:B:303:ARG:HD3  | 2.18                     | 0.43              |
| 1:B:377:GLN:NE2  | 1:B:381:ASP:OD2  | 2.46                     | 0.43              |
| 1:B:103:HIS:CE1  | 1:B:413:LYS:HD2  | 2.54                     | 0.43              |
| 1:A:200:ALA:O    | 1:A:203:LEU:HD23 | 2.18                     | 0.43              |
| 1:B:332:LEU:HA   | 1:B:351:ALA:O    | 2.18                     | 0.43              |
| 1:C:211:PRO:HB3  | 1:C:242:VAL:CG2  | 2.47                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:338:ARG:NH1  | 1:B:344:TYR:HE1  | 2.15                     | 0.42              |
| 1:A:70:HIS:HA    | 1:A:303:ARG:NE   | 2.33                     | 0.42              |
| 1:B:148:PRO:HG3  | 1:B:359:GLN:O    | 2.19                     | 0.42              |
| 1:C:416:THR:HG22 | 3:C:488:HOH:O    | 2.18                     | 0.42              |
| 1:C:182:THR:HA   | 1:C:289:LYS:HB3  | 2.01                     | 0.42              |
| 1:C:22:ALA:HA    | 1:C:25:VAL:CG1   | 2.49                     | 0.42              |
| 1:C:303:ARG:HH11 | 1:C:303:ARG:HG3  | 1.83                     | 0.42              |
| 1:A:95:ARG:NE    | 1:A:417:GLU:HG2  | 2.34                     | 0.42              |
| 1:B:311:VAL:O    | 1:B:311:VAL:HG23 | 2.19                     | 0.42              |
| 1:A:182:THR:N    | 1:A:289:LYS:HD3  | 2.34                     | 0.42              |
| 1:B:205:GLY:HA3  | 1:B:211:PRO:O    | 2.20                     | 0.42              |
| 1:B:285:ALA:O    | 1:B:286:LEU:HD23 | 2.20                     | 0.42              |
| 1:B:182:THR:HG21 | 1:B:291:HIS:CD2  | 2.54                     | 0.42              |
| 1:B:302:ALA:O    | 1:B:305:ILE:HD12 | 2.20                     | 0.42              |
| 1:C:275:ALA:N    | 1:C:276:PRO:CD   | 2.82                     | 0.42              |
| 1:A:255:ARG:HB3  | 1:A:256:PHE:CD1  | 2.54                     | 0.42              |
| 1:C:348:ILE:N    | 1:C:348:ILE:HD12 | 2.34                     | 0.42              |
| 1:A:138:GLY:O    | 1:A:333:MET:HA   | 2.20                     | 0.42              |
| 1:A:213:HIS:HD2  | 1:A:242:VAL:N    | 2.03                     | 0.42              |
| 1:B:183:LYS:HE2  | 1:B:183:LYS:HB3  | 1.82                     | 0.42              |
| 1:B:330:GLN:HG3  | 1:B:331:ALA:N    | 2.34                     | 0.42              |
| 1:C:365:ILE:C    | 1:C:367:TYR:H    | 2.23                     | 0.42              |
| 1:C:411:GLU:HA   | 3:C:456:HOH:O    | 2.20                     | 0.42              |
| 1:A:143:VAL:HG22 | 1:A:159:VAL:CG1  | 2.49                     | 0.42              |
| 1:A:205:GLY:HA3  | 1:A:211:PRO:O    | 2.20                     | 0.42              |
| 1:A:186:ILE:HG23 | 1:A:243:VAL:CG2  | 2.50                     | 0.42              |
| 1:A:95:ARG:CZ    | 1:A:414:LEU:HD23 | 2.49                     | 0.42              |
| 1:B:22:ALA:HA    | 1:B:25:VAL:CG1   | 2.49                     | 0.42              |
| 1:C:232:ASP:HB2  | 1:C:286:LEU:CD1  | 2.50                     | 0.42              |
| 1:B:190:MET:HE3  | 3:B:504:HOH:O    | 2.19                     | 0.41              |
| 1:B:202:GLY:HA3  | 1:B:375:ILE:CD1  | 2.47                     | 0.41              |
| 1:B:91:ARG:HB3   | 1:B:91:ARG:HE    | 1.10                     | 0.41              |
| 1:C:117:GLN:HE22 | 1:C:138:GLY:HA3  | 1.84                     | 0.41              |
| 1:C:338:ARG:NH1  | 1:C:344:TYR:HD1  | 2.18                     | 0.41              |
| 1:C:50:LEU:O     | 1:C:417:GLU:CG   | 2.68                     | 0.41              |
| 1:A:126:LEU:HD22 | 1:A:130:MET:SD   | 2.60                     | 0.41              |
| 1:A:231:VAL:HG13 | 1:A:232:ASP:N    | 2.34                     | 0.41              |
| 1:B:362:LYS:HB3  | 1:B:362:LYS:HE2  | 1.91                     | 0.41              |
| 1:B:396:ASP:O    | 1:B:397:ASP:CB   | 2.67                     | 0.41              |
| 1:C:205:GLY:HA3  | 1:C:211:PRO:O    | 2.21                     | 0.41              |
| 1:C:213:HIS:HD2  | 1:C:242:VAL:N    | 2.06                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:203:LEU:O    | 1:C:399:LEU:HD11 | 2.20                     | 0.41              |
| 1:B:188:GLU:HA   | 1:B:245:ALA:O    | 2.19                     | 0.41              |
| 1:C:340:GLN:O    | 1:C:344:TYR:HA   | 2.20                     | 0.41              |
| 1:B:17:VAL:HG22  | 1:B:155:GLY:HA2  | 2.01                     | 0.41              |
| 1:B:182:THR:N    | 1:B:289:LYS:HD3  | 2.35                     | 0.41              |
| 1:C:342:LYS:HB2  | 1:C:343:PRO:CD   | 2.40                     | 0.41              |
| 1:A:417:GLU:OE2  | 1:A:418:PHE:O    | 2.39                     | 0.41              |
| 1:B:136:CYS:N    | 1:B:330:GLN:HE22 | 2.07                     | 0.41              |
| 1:A:135:THR:HA   | 1:A:330:GLN:NE2  | 2.35                     | 0.41              |
| 1:B:117:GLN:HE22 | 1:B:138:GLY:HA3  | 1.86                     | 0.41              |
| 1:B:278:LEU:O    | 1:B:281:MET:HB2  | 2.21                     | 0.41              |
| 1:B:312:GLU:OE2  | 1:B:346:TRP:HZ2  | 2.03                     | 0.41              |
| 1:C:275:ALA:H    | 1:C:276:PRO:CD   | 2.33                     | 0.41              |
| 1:C:416:THR:O    | 1:C:417:GLU:CB   | 2.68                     | 0.41              |
| 1:B:137:ILE:HG23 | 1:B:332:LEU:O    | 2.20                     | 0.41              |
| 1:B:68:LEU:HA    | 1:B:71:THR:CG2   | 2.50                     | 0.41              |
| 1:C:113:GLY:HA3  | 3:C:434:HOH:O    | 2.19                     | 0.41              |
| 1:C:99:VAL:HG12  | 1:C:414:LEU:HD23 | 1.94                     | 0.41              |
| 1:C:342:LYS:CB   | 1:C:343:PRO:CD   | 2.98                     | 0.41              |
| 1:B:293:ALA:HB2  | 1:C:296:ASP:HB3  | 2.02                     | 0.41              |
| 1:C:145:ASN:HB2  | 1:C:156:PHE:CD2  | 2.56                     | 0.41              |
| 1:C:203:LEU:HD22 | 1:C:203:LEU:N    | 2.36                     | 0.41              |
| 1:A:361:LYS:O    | 1:A:361:LYS:CG   | 2.67                     | 0.41              |
| 1:B:15:THR:HG22  | 1:B:16:ALA:N     | 2.35                     | 0.41              |
| 1:C:256:PHE:N    | 1:C:256:PHE:CD1  | 2.89                     | 0.41              |
| 1:B:304:HIS:HE1  | 1:C:304:HIS:HE1  | 1.68                     | 0.41              |
| 1:A:142:THR:HG22 | 1:A:144:ASP:N    | 2.32                     | 0.40              |
| 1:A:364:PRO:HG2  | 1:A:367:TYR:CD2  | 2.55                     | 0.40              |
| 1:A:4:LYS:HB2    | 3:A:547:HOH:O    | 2.21                     | 0.40              |
| 1:A:70:HIS:HB2   | 1:A:393:PRO:CB   | 2.50                     | 0.40              |
| 1:B:186:ILE:HG23 | 1:B:243:VAL:CG2  | 2.50                     | 0.40              |
| 1:B:256:PHE:HA   | 3:B:427:HOH:O    | 2.21                     | 0.40              |
| 1:B:52:GLU:O     | 1:B:52:GLU:HG2   | 2.21                     | 0.40              |
| 1:B:175:LYS:HG2  | 1:B:240:TYR:CE2  | 2.56                     | 0.40              |
| 1:B:193:HIS:HD2  | 3:B:455:HOH:O    | 2.03                     | 0.40              |
| 1:B:390:GLU:HG2  | 1:B:392:PHE:CZ   | 2.57                     | 0.40              |
| 1:B:70:HIS:HD2   | 1:B:401:ARG:O    | 2.03                     | 0.40              |
| 1:C:183:LYS:HE2  | 1:C:183:LYS:HB3  | 1.82                     | 0.40              |
| 1:B:331:ALA:C    | 1:B:353:LEU:HG   | 2.42                     | 0.40              |
| 1:A:232:ASP:O    | 1:A:235:VAL:HG22 | 2.21                     | 0.40              |
| 1:A:404:LYS:HA   | 1:A:404:LYS:HD3  | 1.88                     | 0.40              |

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| Atom-1          | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|---------------|--------------------------|-------------------|
| 1:B:413:LYS:HE2 | 3:B:470:HOH:O | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 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     | 384/420 (91%)   | 348 (91%)  | 30 (8%)  | 6 (2%)   | 9           | 17 |
| 1   | B     | 384/420 (91%)   | 348 (91%)  | 29 (8%)  | 7 (2%)   | 8           | 14 |
| 1   | C     | 384/420 (91%)   | 339 (88%)  | 37 (10%) | 8 (2%)   | 7           | 11 |
| All | All   | 1152/1260 (91%) | 1035 (90%) | 96 (8%)  | 21 (2%)  | 8           | 14 |

All (21) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 343 | PRO  |
| 1   | A     | 412 | LYS  |
| 1   | B     | 343 | PRO  |
| 1   | B     | 344 | TYR  |
| 1   | B     | 359 | GLN  |
| 1   | C     | 343 | PRO  |
| 1   | C     | 359 | GLN  |
| 1   | C     | 417 | GLU  |
| 1   | A     | 403 | ALA  |
| 1   | B     | 416 | THR  |
| 1   | C     | 416 | THR  |
| 1   | A     | 344 | TYR  |
| 1   | A     | 414 | LEU  |
| 1   | A     | 417 | GLU  |
| 1   | B     | 397 | ASP  |
| 1   | B     | 417 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 344 | TYR  |
| 1   | C     | 369 | THR  |
| 1   | C     | 414 | LEU  |
| 1   | B     | 365 | ILE  |
| 1   | C     | 365 | ILE  |

### 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     | 308/330 (93%) | 268 (87%) | 40 (13%)  | 4           | 7  |
| 1   | B     | 308/330 (93%) | 275 (89%) | 33 (11%)  | 6           | 13 |
| 1   | C     | 308/330 (93%) | 273 (89%) | 35 (11%)  | 5           | 11 |
| All | All   | 924/990 (93%) | 816 (88%) | 108 (12%) | 5           | 10 |

All (108) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | ILE  |
| 1   | A     | 43  | ARG  |
| 1   | A     | 46  | ILE  |
| 1   | A     | 50  | LEU  |
| 1   | A     | 60  | GLU  |
| 1   | A     | 71  | THR  |
| 1   | A     | 80  | ARG  |
| 1   | A     | 91  | ARG  |
| 1   | A     | 110 | TYR  |
| 1   | A     | 111 | ASN  |
| 1   | A     | 119 | THR  |
| 1   | A     | 126 | LEU  |
| 1   | A     | 135 | THR  |
| 1   | A     | 141 | LYS  |
| 1   | A     | 143 | VAL  |
| 1   | A     | 179 | GLU  |
| 1   | A     | 181 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 182 | THR  |
| 1   | A     | 187 | LEU  |
| 1   | A     | 229 | GLU  |
| 1   | A     | 237 | ASP  |
| 1   | A     | 244 | VAL  |
| 1   | A     | 255 | ARG  |
| 1   | A     | 276 | PRO  |
| 1   | A     | 291 | HIS  |
| 1   | A     | 292 | TRP  |
| 1   | A     | 300 | ARG  |
| 1   | A     | 305 | ILE  |
| 1   | A     | 311 | VAL  |
| 1   | A     | 323 | GLU  |
| 1   | A     | 326 | LEU  |
| 1   | A     | 343 | PRO  |
| 1   | A     | 355 | GLU  |
| 1   | A     | 360 | GLU  |
| 1   | A     | 361 | LYS  |
| 1   | A     | 371 | ASN  |
| 1   | A     | 409 | LEU  |
| 1   | A     | 413 | LYS  |
| 1   | A     | 414 | LEU  |
| 1   | A     | 417 | GLU  |
| 1   | B     | 43  | ARG  |
| 1   | B     | 46  | ILE  |
| 1   | B     | 50  | LEU  |
| 1   | B     | 71  | THR  |
| 1   | B     | 80  | ARG  |
| 1   | B     | 91  | ARG  |
| 1   | B     | 110 | TYR  |
| 1   | B     | 111 | ASN  |
| 1   | B     | 119 | THR  |
| 1   | B     | 126 | LEU  |
| 1   | B     | 135 | THR  |
| 1   | B     | 141 | LYS  |
| 1   | B     | 143 | VAL  |
| 1   | B     | 159 | VAL  |
| 1   | B     | 179 | GLU  |
| 1   | B     | 181 | SER  |
| 1   | B     | 182 | THR  |
| 1   | B     | 187 | LEU  |
| 1   | B     | 229 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 237 | ASP  |
| 1   | B     | 244 | VAL  |
| 1   | B     | 255 | ARG  |
| 1   | B     | 292 | TRP  |
| 1   | B     | 300 | ARG  |
| 1   | B     | 305 | ILE  |
| 1   | B     | 323 | GLU  |
| 1   | B     | 326 | LEU  |
| 1   | B     | 343 | PRO  |
| 1   | B     | 371 | ASN  |
| 1   | B     | 409 | LEU  |
| 1   | B     | 414 | LEU  |
| 1   | B     | 416 | THR  |
| 1   | B     | 417 | GLU  |
| 1   | C     | 43  | ARG  |
| 1   | C     | 46  | ILE  |
| 1   | C     | 50  | LEU  |
| 1   | C     | 71  | THR  |
| 1   | C     | 80  | ARG  |
| 1   | C     | 91  | ARG  |
| 1   | C     | 110 | TYR  |
| 1   | C     | 111 | ASN  |
| 1   | C     | 119 | THR  |
| 1   | C     | 126 | LEU  |
| 1   | C     | 135 | THR  |
| 1   | C     | 141 | LYS  |
| 1   | C     | 143 | VAL  |
| 1   | C     | 179 | GLU  |
| 1   | C     | 181 | SER  |
| 1   | C     | 182 | THR  |
| 1   | C     | 187 | LEU  |
| 1   | C     | 229 | GLU  |
| 1   | C     | 237 | ASP  |
| 1   | C     | 244 | VAL  |
| 1   | C     | 255 | ARG  |
| 1   | C     | 291 | HIS  |
| 1   | C     | 292 | TRP  |
| 1   | C     | 300 | ARG  |
| 1   | C     | 305 | ILE  |
| 1   | C     | 343 | PRO  |
| 1   | C     | 355 | GLU  |
| 1   | C     | 370 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 371 | ASN  |
| 1   | C     | 408 | GLN  |
| 1   | C     | 409 | LEU  |
| 1   | C     | 411 | GLU  |
| 1   | C     | 414 | LEU  |
| 1   | C     | 416 | THR  |
| 1   | C     | 419 | GLU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | GLN  |
| 1   | A     | 32  | HIS  |
| 1   | A     | 44  | ASN  |
| 1   | A     | 66  | GLN  |
| 1   | A     | 70  | HIS  |
| 1   | A     | 111 | ASN  |
| 1   | A     | 117 | GLN  |
| 1   | A     | 206 | GLN  |
| 1   | A     | 213 | HIS  |
| 1   | A     | 284 | GLN  |
| 1   | A     | 291 | HIS  |
| 1   | A     | 330 | GLN  |
| 1   | A     | 352 | ASN  |
| 1   | A     | 371 | ASN  |
| 1   | B     | 10  | GLN  |
| 1   | B     | 32  | HIS  |
| 1   | B     | 44  | ASN  |
| 1   | B     | 66  | GLN  |
| 1   | B     | 70  | HIS  |
| 1   | B     | 103 | HIS  |
| 1   | B     | 111 | ASN  |
| 1   | B     | 117 | GLN  |
| 1   | B     | 206 | GLN  |
| 1   | B     | 213 | HIS  |
| 1   | B     | 284 | GLN  |
| 1   | B     | 330 | GLN  |
| 1   | B     | 352 | ASN  |
| 1   | B     | 371 | ASN  |
| 1   | C     | 10  | GLN  |
| 1   | C     | 32  | HIS  |
| 1   | C     | 44  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 66  | GLN  |
| 1   | C     | 70  | HIS  |
| 1   | C     | 111 | ASN  |
| 1   | C     | 117 | GLN  |
| 1   | C     | 213 | HIS  |
| 1   | C     | 284 | GLN  |
| 1   | C     | 304 | HIS  |
| 1   | C     | 330 | GLN  |
| 1   | C     | 366 | HIS  |
| 1   | C     | 371 | ASN  |
| 1   | C     | 384 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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     | 392/420 (93%)   | 0.31   | 19 (4%) 30 32 | 7, 27, 47, 62         | 2 (0%) |
| 1   | B     | 392/420 (93%)   | 0.73   | 36 (9%) 9 9   | 12, 33, 54, 66        | 2 (0%) |
| 1   | C     | 392/420 (93%)   | 0.95   | 56 (14%) 2 2  | 12, 34, 60, 67        | 2 (0%) |
| All | All   | 1176/1260 (93%) | 0.66   | 111 (9%) 8 8  | 7, 32, 55, 67         | 6 (0%) |

All (111) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 372 | GLY  | 9.8  |
| 1   | B     | 416 | THR  | 7.6  |
| 1   | B     | 91  | ARG  | 5.8  |
| 1   | C     | 369 | THR  | 5.7  |
| 1   | C     | 418 | PHE  | 5.6  |
| 1   | C     | 416 | THR  | 5.6  |
| 1   | B     | 418 | PHE  | 5.5  |
| 1   | A     | 418 | PHE  | 5.4  |
| 1   | C     | 251 | TYR  | 5.3  |
| 1   | C     | 367 | TYR  | 5.2  |
| 1   | C     | 362 | LYS  | 4.9  |
| 1   | B     | 3   | ILE  | 4.4  |
| 1   | A     | 416 | THR  | 4.4  |
| 1   | C     | 368 | ILE  | 4.4  |
| 1   | C     | 373 | PHE  | 4.4  |
| 1   | C     | 255 | ARG  | 4.3  |
| 1   | C     | 252 | GLU  | 4.2  |
| 1   | C     | 359 | GLN  | 4.2  |
| 1   | A     | 91  | ARG  | 4.1  |
| 1   | C     | 345 | ARG  | 4.0  |
| 1   | C     | 342 | LYS  | 4.0  |
| 1   | A     | 420 | LEU  | 3.9  |
| 1   | A     | 3   | ILE  | 3.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 192 | ARG  | 3.9  |
| 1   | C     | 375 | ILE  | 3.8  |
| 1   | B     | 236 | ARG  | 3.8  |
| 1   | B     | 341 | ALA  | 3.8  |
| 1   | C     | 343 | PRO  | 3.8  |
| 1   | B     | 343 | PRO  | 3.8  |
| 1   | B     | 420 | LEU  | 3.7  |
| 1   | C     | 236 | ARG  | 3.6  |
| 1   | B     | 132 | TYR  | 3.5  |
| 1   | B     | 359 | GLN  | 3.4  |
| 1   | C     | 365 | ILE  | 3.2  |
| 1   | C     | 222 | PHE  | 3.2  |
| 1   | C     | 3   | ILE  | 3.1  |
| 1   | C     | 371 | ASN  | 3.1  |
| 1   | C     | 420 | LEU  | 3.1  |
| 1   | C     | 341 | ALA  | 3.0  |
| 1   | B     | 342 | LYS  | 3.0  |
| 1   | C     | 250 | GLN  | 3.0  |
| 1   | B     | 192 | ARG  | 2.9  |
| 1   | C     | 279 | ALA  | 2.9  |
| 1   | A     | 414 | LEU  | 2.8  |
| 1   | C     | 248 | GLY  | 2.8  |
| 1   | C     | 284 | GLN  | 2.8  |
| 1   | C     | 378 | ASP  | 2.8  |
| 1   | B     | 419 | GLU  | 2.8  |
| 1   | C     | 196 | TRP  | 2.8  |
| 1   | C     | 191 | GLY  | 2.7  |
| 1   | B     | 357 | ALA  | 2.7  |
| 1   | C     | 364 | PRO  | 2.7  |
| 1   | B     | 358 | ASN  | 2.7  |
| 1   | B     | 279 | ALA  | 2.6  |
| 1   | B     | 298 | LEU  | 2.6  |
| 1   | C     | 360 | GLU  | 2.6  |
| 1   | C     | 285 | ALA  | 2.6  |
| 1   | A     | 284 | GLN  | 2.6  |
| 1   | C     | 340 | GLN  | 2.6  |
| 1   | B     | 345 | ARG  | 2.5  |
| 1   | B     | 284 | GLN  | 2.5  |
| 1   | C     | 344 | TYR  | 2.5  |
| 1   | C     | 366 | HIS  | 2.5  |
| 1   | B     | 256 | PHE  | 2.5  |
| 1   | C     | 221 | PRO  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 370 | ASP  | 2.5  |
| 1   | B     | 33  | PRO  | 2.5  |
| 1   | B     | 251 | TYR  | 2.4  |
| 1   | B     | 34  | ASP  | 2.4  |
| 1   | C     | 403 | ALA  | 2.4  |
| 1   | B     | 222 | PHE  | 2.4  |
| 1   | C     | 193 | HIS  | 2.4  |
| 1   | C     | 414 | LEU  | 2.4  |
| 1   | B     | 229 | GLU  | 2.4  |
| 1   | C     | 132 | TYR  | 2.4  |
| 1   | C     | 206 | GLN  | 2.4  |
| 1   | C     | 278 | LEU  | 2.4  |
| 1   | C     | 301 | ALA  | 2.3  |
| 1   | A     | 236 | ARG  | 2.3  |
| 1   | B     | 327 | ALA  | 2.3  |
| 1   | B     | 104 | ASP  | 2.3  |
| 1   | B     | 32  | HIS  | 2.3  |
| 1   | A     | 192 | ARG  | 2.3  |
| 1   | C     | 207 | SER  | 2.2  |
| 1   | A     | 357 | ALA  | 2.2  |
| 1   | C     | 376 | THR  | 2.2  |
| 1   | A     | 251 | TYR  | 2.2  |
| 1   | A     | 419 | GLU  | 2.2  |
| 1   | A     | 292 | TRP  | 2.2  |
| 1   | C     | 280 | ASN  | 2.2  |
| 1   | B     | 365 | ILE  | 2.2  |
| 1   | B     | 15  | THR  | 2.2  |
| 1   | C     | 277 | ALA  | 2.2  |
| 1   | C     | 256 | PHE  | 2.2  |
| 1   | B     | 228 | LEU  | 2.2  |
| 1   | C     | 361 | LYS  | 2.1  |
| 1   | C     | 91  | ARG  | 2.1  |
| 1   | B     | 37  | GLY  | 2.1  |
| 1   | A     | 356 | VAL  | 2.1  |
| 1   | B     | 82  | LYS  | 2.1  |
| 1   | C     | 275 | ALA  | 2.1  |
| 1   | A     | 417 | GLU  | 2.1  |
| 1   | A     | 345 | ARG  | 2.1  |
| 1   | A     | 415 | ARG  | 2.1  |
| 1   | A     | 342 | LYS  | 2.0  |
| 1   | B     | 356 | VAL  | 2.0  |
| 1   | B     | 348 | ILE  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 343 | PRO  | 2.0  |
| 1   | C     | 419 | GLU  | 2.0  |
| 1   | B     | 149 | PHE  | 2.0  |
| 1   | C     | 404 | LYS  | 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | NA   | A     | 421 | 1/1   | 0.94 | 0.23 | 6,6,6,6                     | 0     |
| 2   | NA   | C     | 421 | 1/1   | 0.96 | 0.18 | 8,8,8,8                     | 0     |
| 2   | NA   | B     | 421 | 1/1   | 0.97 | 0.18 | 1,1,1,1                     | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.