



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:39 PM UTC

PDB ID : 1U76 / pdb\_00001u76  
Title : Crystal structure of hPCNA bound to residues 452-466 of the DNA polymerase-delta-p66 subunit  
Authors : Bruning, J.B.; Shamoo, Y.  
Deposited on : 2004-08-02  
Resolution : 2.60 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                                                             |

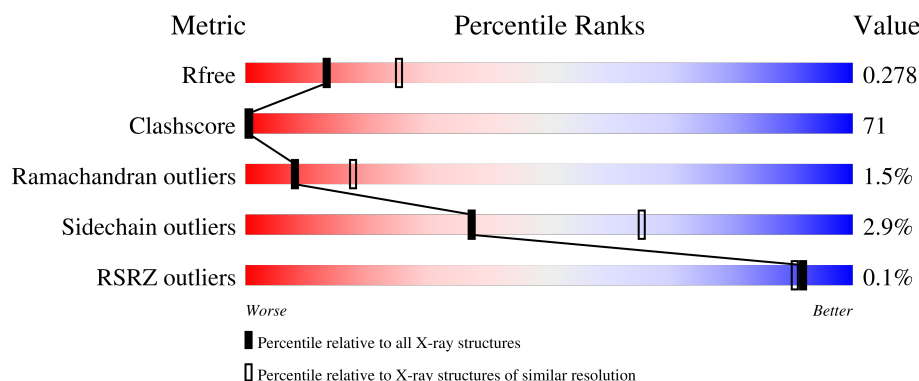
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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                      | 4008 (2.60-2.60)                                      |
| Clashscore            | 190562                      | 4347 (2.60-2.60)                                      |
| Ramachandran outliers | 187476                      | 4277 (2.60-2.60)                                      |
| Sidechain outliers    | 187428                      | 4277 (2.60-2.60)                                      |
| RSRZ outliers         | 180081                      | 4008 (2.60-2.60)                                      |

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     | 261    |                  |
| 1   | C     | 261    |                  |
| 1   | E     | 261    |                  |
| 2   | B     | 15     |                  |
| 2   | D     | 15     |                  |

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| Mol | Chain | Length | Quality of chain                                                                                                                                    |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------|
| 2   | F     | 15     | <div><div></div><div></div><div></div><div></div><div></div></div> <div><div>7%</div><div>20%</div><div>47%</div><div>20%</div><div>13%</div></div> |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6701 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 Proliferating cell nuclear antigen.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 253      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1934  | 1217 | 316 | 385 | 16 |         |         |       |
| 1   | C     | 251      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1923  | 1211 | 314 | 382 | 16 |         |         |       |
| 1   | E     | 253      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1933  | 1216 | 318 | 383 | 16 |         |         |       |

- Molecule 2 is a protein called KANRQVSITGFFQRK peptide from DNA polymerase delta subunit 3.

| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 2   | B     | 12       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 96    | 61 | 18 | 17 |         |         |       |
| 2   | D     | 13       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 107   | 67 | 22 | 18 |         |         |       |
| 2   | F     | 13       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 107   | 67 | 22 | 18 |         |         |       |

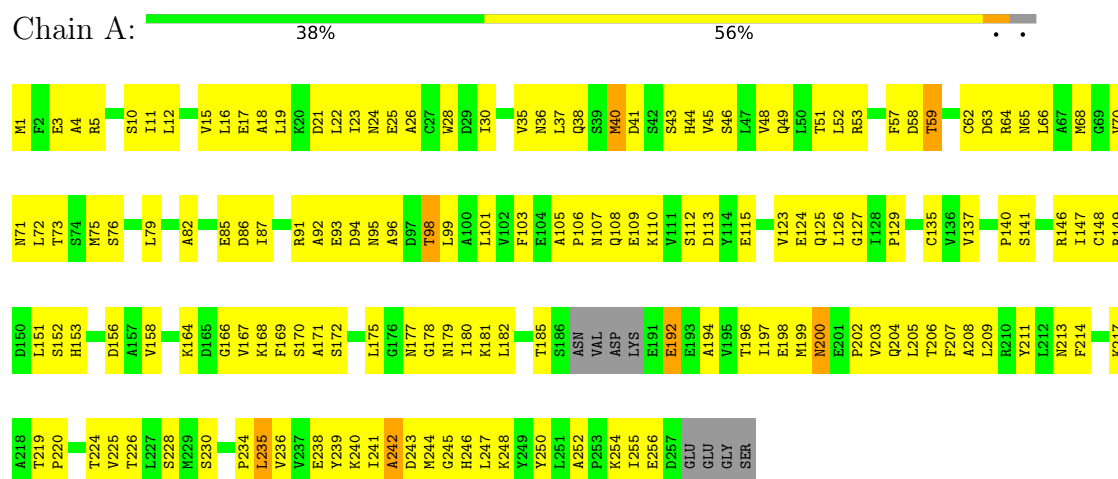
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3   | A     | 181      | Total | O   | 0       | 0       |
|     |       |          | 181   | 181 |         |         |
| 3   | B     | 10       | Total | O   | 0       | 0       |
|     |       |          | 10    | 10  |         |         |
| 3   | C     | 197      | Total | O   | 0       | 0       |
|     |       |          | 197   | 197 |         |         |
| 3   | D     | 11       | Total | O   | 0       | 0       |
|     |       |          | 11    | 11  |         |         |
| 3   | E     | 187      | Total | O   | 0       | 0       |
|     |       |          | 187   | 187 |         |         |
| 3   | F     | 15       | Total | O   | 0       | 0       |
|     |       |          | 15    | 15  |         |         |

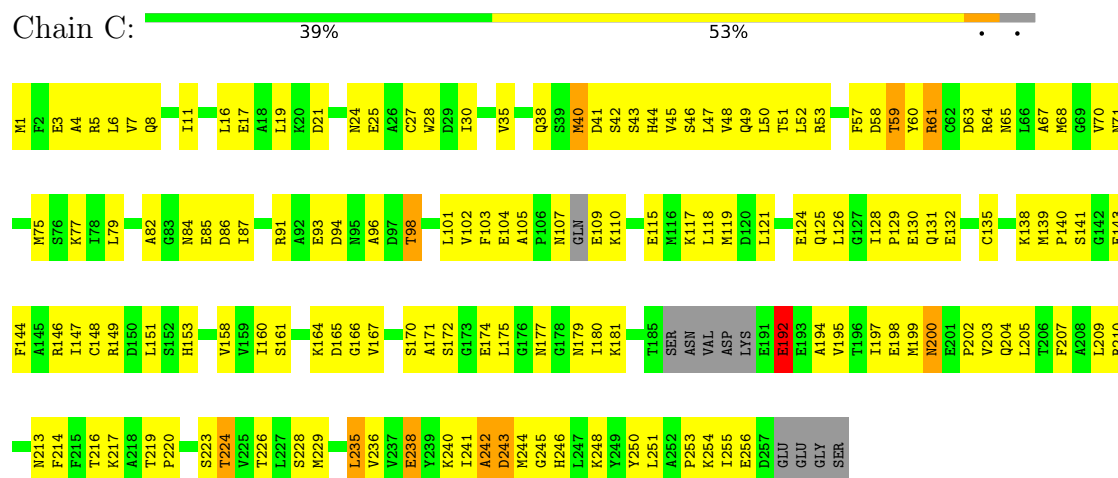
### 3 Residue-property plots

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: Proliferating cell nuclear antigen

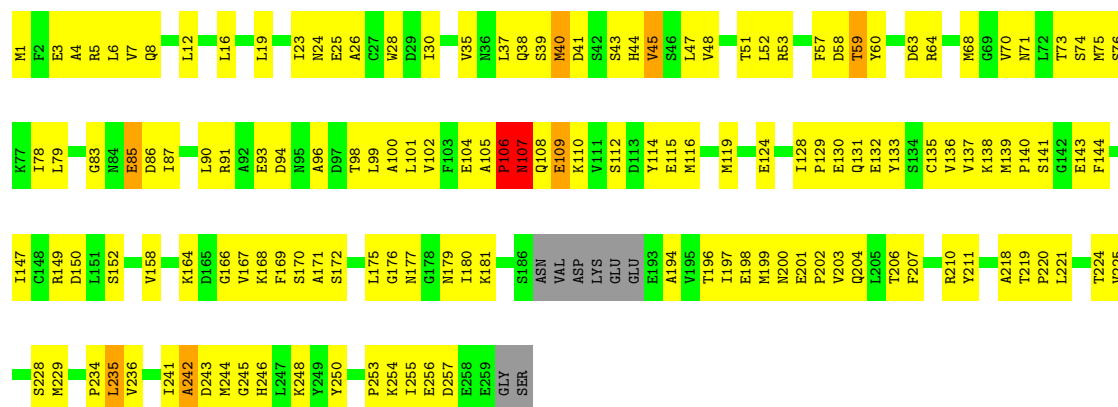


#### • Molecule 1: Proliferating cell nuclear antigen



#### • Molecule 1: Proliferating cell nuclear antigen





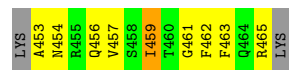
- Molecule 2: KANRQVSITGFFQRK peptide from DNA polymerase delta subunit 3

Chain B: 13% 53% 13% 20%



- Molecule 2: KANRQVSITGFFQRK peptide from DNA polymerase delta subunit 3

Chain D: 27% 53% 7% 13%



- Molecule 2: KANRQVSITGFFQRK peptide from DNA polymerase delta subunit 3

Chain F: 7% 20% 47% 20% 13%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 32 2 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 82.48Å 82.48Å 203.80Å<br>90.00° 90.00° 120.00°              | Depositor        |
| Resolution (Å)                                                          | 10.00 – 2.60<br>10.00 – 2.60                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 94.0 (10.00-2.60)<br>93.6 (10.00-2.60)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.08                                                        | Depositor        |
| $R_{sym}$                                                               | 0.08                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.50 (at 2.61Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.240 , 0.278<br>0.241 , 0.278                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1150 reflections (4.70%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 58.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.391                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.41 , 77.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$ | Xtriage          |
| Estimated twinning fraction                                             | 0.000 for -h,-k,l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 6701                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 65.0                                                        | 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 25.58 % 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 3.0861e-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     | 0.48         | 0/1959  | 0.92        | 4/2646 (0.2%)  |
| 1   | C     | 0.46         | 0/1947  | 0.93        | 4/2628 (0.2%)  |
| 1   | E     | 0.46         | 0/1958  | 0.93        | 5/2645 (0.2%)  |
| 2   | B     | 0.50         | 0/97    | 0.86        | 0/129          |
| 2   | D     | 0.48         | 0/108   | 0.84        | 0/143          |
| 2   | F     | 0.48         | 0/108   | 0.80        | 0/143          |
| All | All   | 0.47         | 0/6177  | 0.92        | 13/8334 (0.2%) |

There are no bond length outliers.

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | E     | 107 | ASN  | N-CA-C | -7.40 | 98.86       | 109.96   |
| 1   | E     | 200 | ASN  | N-CA-C | -6.78 | 105.14      | 113.41   |
| 1   | A     | 200 | ASN  | N-CA-C | -6.67 | 105.28      | 113.41   |
| 1   | C     | 200 | ASN  | N-CA-C | -6.56 | 105.41      | 113.41   |
| 1   | C     | 40  | MET  | N-CA-C | -6.13 | 102.44      | 110.53   |
| 1   | E     | 40  | MET  | N-CA-C | -5.86 | 102.80      | 110.53   |
| 1   | E     | 109 | GLU  | N-CA-C | -5.70 | 105.66      | 113.30   |
| 1   | A     | 40  | MET  | N-CA-C | -5.67 | 103.04      | 110.53   |
| 1   | A     | 109 | GLU  | N-CA-C | -5.67 | 106.02      | 113.17   |
| 1   | A     | 238 | GLU  | N-CA-C | 5.48  | 118.01      | 108.76   |
| 1   | C     | 238 | GLU  | N-CA-C | 5.25  | 117.64      | 108.76   |
| 1   | E     | 45  | VAL  | N-CA-C | -5.15 | 107.82      | 113.43   |
| 1   | C     | 192 | GLU  | N-CA-C | -5.08 | 106.93      | 112.72   |

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     | 1934  | 0        | 1934     | 272     | 0            |
| 1   | C     | 1923  | 0        | 1926     | 275     | 0            |
| 1   | E     | 1933  | 0        | 1936     | 275     | 1            |
| 2   | B     | 96    | 0        | 92       | 23      | 0            |
| 2   | D     | 107   | 0        | 105      | 30      | 0            |
| 2   | F     | 107   | 0        | 105      | 26      | 0            |
| 3   | A     | 181   | 0        | 0        | 166     | 0            |
| 3   | B     | 10    | 0        | 0        | 11      | 0            |
| 3   | C     | 197   | 0        | 0        | 207     | 0            |
| 3   | D     | 11    | 0        | 0        | 12      | 0            |
| 3   | E     | 187   | 0        | 0        | 197     | 1            |
| 3   | F     | 15    | 0        | 0        | 10      | 0            |
| All | All   | 6701  | 0        | 6098     | 864     | 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 71.

All (864) 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:E:64:ARG:HA    | 3:E:444:HOH:O | 1.33                     | 1.27              |
| 1:E:236:VAL:HA   | 3:E:420:HOH:O | 1.35                     | 1.26              |
| 1:A:40:MET:HB3   | 3:A:351:HOH:O | 1.37                     | 1.24              |
| 1:E:73:THR:HB    | 3:E:395:HOH:O | 1.30                     | 1.23              |
| 2:F:456:GLN:HG3  | 3:F:540:HOH:O | 1.38                     | 1.21              |
| 1:C:194:ALA:HB1  | 3:C:343:HOH:O | 1.45                     | 1.14              |
| 2:B:460:THR:HA   | 3:B:525:HOH:O | 1.48                     | 1.13              |
| 1:A:126:LEU:HB3  | 3:A:366:HOH:O | 1.47                     | 1.12              |
| 1:E:152:SER:HA   | 3:E:443:HOH:O | 1.49                     | 1.11              |
| 1:E:133:TYR:HA   | 3:E:448:HOH:O | 1.47                     | 1.11              |
| 1:E:171:ALA:HB2  | 3:E:349:HOH:O | 1.48                     | 1.11              |
| 1:A:23:ILE:HA    | 3:A:343:HOH:O | 1.49                     | 1.11              |
| 1:C:102:VAL:HG23 | 3:C:368:HOH:O | 1.50                     | 1.10              |
| 1:A:217:LYS:HG3  | 3:A:339:HOH:O | 1.51                     | 1.09              |
| 1:E:45:VAL:HB    | 3:E:376:HOH:O | 1.53                     | 1.09              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:73:THR:HA    | 3:A:402:HOH:O    | 1.53                     | 1.08              |
| 1:A:203:VAL:HA   | 3:A:422:HOH:O    | 1.51                     | 1.08              |
| 1:A:49:GLN:HB2   | 3:A:439:HOH:O    | 1.54                     | 1.07              |
| 1:E:105:ALA:HB3  | 3:E:348:HOH:O    | 1.53                     | 1.07              |
| 3:C:385:HOH:O    | 2:D:454:ASN:HB3  | 1.53                     | 1.06              |
| 1:A:36:ASN:HB2   | 3:A:334:HOH:O    | 1.55                     | 1.06              |
| 1:C:131:GLN:HB2  | 3:C:426:HOH:O    | 1.56                     | 1.04              |
| 1:A:16:LEU:HD22  | 1:A:79:LEU:HD12  | 1.38                     | 1.04              |
| 1:E:108:GLN:HA   | 3:E:383:HOH:O    | 1.57                     | 1.04              |
| 1:A:203:VAL:HB   | 3:A:348:HOH:O    | 1.57                     | 1.04              |
| 1:A:58:ASP:HB3   | 3:A:338:HOH:O    | 1.57                     | 1.03              |
| 1:A:248:LYS:HD3  | 3:A:409:HOH:O    | 1.57                     | 1.03              |
| 1:E:16:LEU:HD22  | 1:E:79:LEU:HD12  | 1.41                     | 1.01              |
| 1:E:242:ALA:HB2  | 3:E:417:HOH:O    | 1.59                     | 1.01              |
| 1:C:24:ASN:HB3   | 3:C:374:HOH:O    | 1.58                     | 1.01              |
| 1:E:35:VAL:HB    | 3:E:398:HOH:O    | 1.56                     | 1.01              |
| 1:A:99:LEU:HA    | 3:A:357:HOH:O    | 1.61                     | 1.00              |
| 1:E:114:TYR:HA   | 3:E:340:HOH:O    | 1.60                     | 0.99              |
| 1:C:243:ASP:HB2  | 3:C:401:HOH:O    | 1.64                     | 0.97              |
| 1:E:73:THR:HA    | 3:E:406:HOH:O    | 1.63                     | 0.97              |
| 1:A:239:TYR:HB3  | 3:A:427:HOH:O    | 1.64                     | 0.97              |
| 1:A:252:ALA:HB3  | 3:A:346:HOH:O    | 1.63                     | 0.97              |
| 1:C:131:GLN:HB3  | 3:C:373:HOH:O    | 1.64                     | 0.97              |
| 1:C:194:ALA:HB3  | 3:C:377:HOH:O    | 1.65                     | 0.97              |
| 1:A:169:PHE:HB2  | 3:A:425:HOH:O    | 1.62                     | 0.96              |
| 1:A:101:LEU:HG   | 3:A:405:HOH:O    | 1.63                     | 0.96              |
| 1:E:23:ILE:HA    | 3:E:425:HOH:O    | 1.65                     | 0.96              |
| 1:C:124:GLU:HG3  | 2:D:465:ARG:HH21 | 1.28                     | 0.96              |
| 1:A:247:LEU:HD12 | 3:A:404:HOH:O    | 1.65                     | 0.95              |
| 1:E:85:GLU:HG2   | 3:E:360:HOH:O    | 1.66                     | 0.95              |
| 1:E:206:THR:OG1  | 2:F:453:ALA:HB2  | 1.65                     | 0.95              |
| 1:E:48:VAL:HG23  | 3:E:401:HOH:O    | 1.66                     | 0.95              |
| 1:A:103:PHE:HE2  | 3:A:377:HOH:O    | 1.50                     | 0.94              |
| 2:D:457:VAL:HA   | 3:D:272:HOH:O    | 1.65                     | 0.93              |
| 1:E:102:VAL:HG12 | 3:E:346:HOH:O    | 1.66                     | 0.93              |
| 1:C:170:SER:HB3  | 1:C:179:ASN:HB3  | 1.51                     | 0.93              |
| 1:A:44:HIS:HA    | 3:A:351:HOH:O    | 1.67                     | 0.93              |
| 1:A:103:PHE:CE2  | 3:A:377:HOH:O    | 2.21                     | 0.93              |
| 1:E:96:ALA:HB3   | 3:E:338:HOH:O    | 1.67                     | 0.93              |
| 1:C:70:VAL:HG11  | 3:C:405:HOH:O    | 1.68                     | 0.92              |
| 1:C:130:GLU:HG3  | 3:C:389:HOH:O    | 1.69                     | 0.92              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:153:HIS:HE1  | 3:A:431:HOH:O   | 1.54                     | 0.91              |
| 1:E:225:VAL:HG22 | 3:E:385:HOH:O   | 1.67                     | 0.91              |
| 1:A:76:SER:HB3   | 3:A:402:HOH:O   | 1.72                     | 0.90              |
| 1:E:170:SER:HB3  | 1:E:179:ASN:HB3 | 1.54                     | 0.88              |
| 1:C:240:LYS:HE2  | 3:C:439:HOH:O   | 1.71                     | 0.88              |
| 1:E:25:GLU:HG2   | 3:E:370:HOH:O   | 1.74                     | 0.88              |
| 1:A:94:ASP:HB3   | 3:A:365:HOH:O   | 1.73                     | 0.87              |
| 1:E:52:LEU:HB2   | 3:E:398:HOH:O   | 1.72                     | 0.87              |
| 1:C:117:LYS:HB3  | 3:C:421:HOH:O   | 1.73                     | 0.87              |
| 1:A:170:SER:HB3  | 1:A:179:ASN:HB3 | 1.55                     | 0.87              |
| 1:A:18:ALA:C     | 3:A:435:HOH:O   | 2.16                     | 0.87              |
| 1:E:76:SER:HB3   | 3:E:406:HOH:O   | 1.74                     | 0.87              |
| 1:C:153:HIS:CB   | 3:C:347:HOH:O   | 2.21                     | 0.86              |
| 1:C:52:LEU:HD22  | 1:C:244:MET:HE2 | 1.57                     | 0.86              |
| 1:A:48:VAL:HG12  | 3:A:404:HOH:O   | 1.75                     | 0.86              |
| 1:A:151:LEU:HB2  | 3:A:437:HOH:O   | 1.75                     | 0.85              |
| 1:E:167:VAL:HG22 | 3:E:367:HOH:O   | 1.76                     | 0.85              |
| 1:C:16:LEU:HD22  | 1:C:79:LEU:HD12 | 1.55                     | 0.85              |
| 1:A:197:ILE:HG22 | 3:A:396:HOH:O   | 1.76                     | 0.84              |
| 1:A:167:VAL:HG22 | 3:A:378:HOH:O   | 1.78                     | 0.84              |
| 1:C:160:ILE:HG22 | 3:C:408:HOH:O   | 1.76                     | 0.84              |
| 1:C:91:ARG:HB2   | 3:C:397:HOH:O   | 1.76                     | 0.83              |
| 1:C:224:THR:HB   | 3:C:386:HOH:O   | 1.76                     | 0.83              |
| 1:A:239:TYR:C    | 3:A:427:HOH:O   | 2.21                     | 0.83              |
| 1:E:139:MET:HG2  | 3:E:426:HOH:O   | 1.78                     | 0.83              |
| 1:A:199:MET:HB2  | 3:A:396:HOH:O   | 1.77                     | 0.82              |
| 1:A:213:ASN:C    | 3:A:434:HOH:O   | 2.21                     | 0.82              |
| 1:E:150:ASP:N    | 3:E:433:HOH:O   | 2.11                     | 0.82              |
| 1:A:203:VAL:CA   | 3:A:422:HOH:O   | 2.17                     | 0.82              |
| 1:A:219:THR:HA   | 3:A:354:HOH:O   | 1.79                     | 0.82              |
| 1:C:181:LYS:HG3  | 3:C:348:HOH:O   | 1.78                     | 0.82              |
| 1:C:194:ALA:C    | 3:C:403:HOH:O   | 2.23                     | 0.82              |
| 1:A:169:PHE:HD1  | 3:A:425:HOH:O   | 1.62                     | 0.82              |
| 1:C:75:MET:SD    | 3:C:405:HOH:O   | 2.36                     | 0.81              |
| 1:C:214:PHE:HA   | 3:C:330:HOH:O   | 1.79                     | 0.81              |
| 1:E:107:ASN:HB2  | 3:E:342:HOH:O   | 1.79                     | 0.81              |
| 1:E:52:LEU:HD22  | 1:E:244:MET:HE2 | 1.62                     | 0.81              |
| 1:E:225:VAL:HG13 | 3:E:385:HOH:O   | 1.81                     | 0.81              |
| 1:E:5:ARG:HB3    | 1:E:59:THR:HB   | 1.63                     | 0.81              |
| 1:E:149:ARG:HB3  | 3:E:433:HOH:O   | 1.81                     | 0.81              |
| 1:E:43:SER:HB3   | 3:E:364:HOH:O   | 1.80                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:48:VAL:N     | 3:E:401:HOH:O    | 2.14                     | 0.80              |
| 1:E:94:ASP:N     | 3:E:439:HOH:O    | 2.15                     | 0.80              |
| 1:A:103:PHE:CB   | 3:A:412:HOH:O    | 2.29                     | 0.80              |
| 1:C:91:ARG:HD3   | 3:C:397:HOH:O    | 1.81                     | 0.80              |
| 1:C:148:CYS:SG   | 3:C:444:HOH:O    | 2.40                     | 0.80              |
| 1:A:254:LYS:HE2  | 3:B:271:HOH:O    | 1.82                     | 0.80              |
| 1:A:52:LEU:HD22  | 1:A:244:MET:HE2  | 1.61                     | 0.79              |
| 1:A:167:VAL:C    | 3:A:378:HOH:O    | 2.26                     | 0.79              |
| 1:C:57:PHE:HB3   | 3:C:455:HOH:O    | 1.82                     | 0.79              |
| 1:C:61:ARG:HG2   | 3:C:396:HOH:O    | 1.81                     | 0.79              |
| 1:E:201:GLU:HA   | 3:E:388:HOH:O    | 1.83                     | 0.79              |
| 1:A:169:PHE:CD1  | 3:A:425:HOH:O    | 2.33                     | 0.79              |
| 1:C:6:LEU:C      | 3:C:422:HOH:O    | 2.25                     | 0.79              |
| 1:A:156:ASP:HB3  | 3:A:423:HOH:O    | 1.82                     | 0.78              |
| 1:C:58:ASP:HA    | 3:C:356:HOH:O    | 1.84                     | 0.78              |
| 2:B:464:GLN:NE2  | 2:B:464:GLN:H    | 1.80                     | 0.78              |
| 1:E:106:PRO:HB2  | 3:E:350:HOH:O    | 1.84                     | 0.78              |
| 2:F:456:GLN:C    | 3:F:540:HOH:O    | 2.26                     | 0.78              |
| 1:A:182:LEU:N    | 3:A:393:HOH:O    | 2.16                     | 0.78              |
| 1:E:211:TYR:CE1  | 3:F:449:HOH:O    | 2.35                     | 0.78              |
| 1:A:5:ARG:HB3    | 1:A:59:THR:HB    | 1.64                     | 0.77              |
| 1:C:194:ALA:HA   | 3:C:403:HOH:O    | 1.83                     | 0.77              |
| 1:C:5:ARG:HB3    | 1:C:59:THR:HB    | 1.66                     | 0.77              |
| 1:E:59:THR:C     | 3:E:381:HOH:O    | 2.27                     | 0.77              |
| 1:E:254:LYS:HG3  | 3:E:358:HOH:O    | 1.84                     | 0.77              |
| 1:E:201:GLU:CA   | 3:E:388:HOH:O    | 2.33                     | 0.77              |
| 1:A:110:LYS:HE2  | 3:A:420:HOH:O    | 1.84                     | 0.77              |
| 1:A:225:VAL:C    | 3:A:406:HOH:O    | 2.28                     | 0.76              |
| 1:E:90:LEU:HA    | 3:E:405:HOH:O    | 1.83                     | 0.76              |
| 1:A:203:VAL:CB   | 3:A:348:HOH:O    | 2.21                     | 0.76              |
| 1:E:196:THR:HG23 | 3:E:434:HOH:O    | 1.85                     | 0.76              |
| 1:E:256:GLU:HA   | 3:E:374:HOH:O    | 1.85                     | 0.76              |
| 1:C:50:LEU:HA    | 3:C:431:HOH:O    | 1.85                     | 0.76              |
| 1:C:5:ARG:N      | 3:C:455:HOH:O    | 2.17                     | 0.76              |
| 1:C:42:SER:HA    | 3:C:355:HOH:O    | 1.87                     | 0.75              |
| 1:C:192:GLU:HB2  | 3:C:338:HOH:O    | 1.85                     | 0.75              |
| 1:C:94:ASP:N     | 3:C:415:HOH:O    | 2.19                     | 0.75              |
| 1:C:242:ALA:O    | 3:C:401:HOH:O    | 2.04                     | 0.75              |
| 1:A:156:ASP:N    | 3:A:423:HOH:O    | 2.20                     | 0.75              |
| 1:C:40:MET:HE3   | 2:D:459:ILE:HD13 | 1.69                     | 0.75              |
| 1:C:146:ARG:CZ   | 3:C:400:HOH:O    | 2.35                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:225:VAL:CA   | 3:A:358:HOH:O    | 2.34                     | 0.74              |
| 1:A:63:ASP:C     | 3:A:359:HOH:O    | 2.31                     | 0.74              |
| 1:A:147:ILE:HG23 | 1:A:180:ILE:HD12 | 1.69                     | 0.74              |
| 1:A:207:PHE:HA   | 3:A:428:HOH:O    | 1.88                     | 0.74              |
| 1:C:253:PRO:C    | 3:C:372:HOH:O    | 2.31                     | 0.74              |
| 1:A:92:ALA:HA    | 3:A:357:HOH:O    | 1.87                     | 0.74              |
| 1:E:139:MET:N    | 3:E:426:HOH:O    | 2.19                     | 0.74              |
| 1:C:70:VAL:C     | 3:C:381:HOH:O    | 2.30                     | 0.74              |
| 1:E:5:ARG:HB2    | 3:E:422:HOH:O    | 1.87                     | 0.74              |
| 1:E:138:LYS:C    | 3:E:426:HOH:O    | 2.31                     | 0.73              |
| 1:A:203:VAL:HG13 | 3:A:422:HOH:O    | 1.88                     | 0.73              |
| 1:E:60:TYR:C     | 3:E:381:HOH:O    | 2.31                     | 0.73              |
| 1:E:114:TYR:CA   | 3:E:340:HOH:O    | 2.24                     | 0.73              |
| 1:C:124:GLU:HG3  | 2:D:465:ARG:NH2  | 2.02                     | 0.73              |
| 1:A:244:MET:C    | 3:A:382:HOH:O    | 2.30                     | 0.73              |
| 1:C:175:LEU:HG   | 3:C:360:HOH:O    | 1.89                     | 0.73              |
| 3:C:372:HOH:O    | 2:D:456:GLN:NE2  | 2.20                     | 0.73              |
| 1:E:137:VAL:HG23 | 3:E:347:HOH:O    | 1.88                     | 0.73              |
| 1:E:255:ILE:HD13 | 2:F:457:VAL:HG21 | 1.69                     | 0.73              |
| 1:A:254:LYS:HB3  | 3:B:271:HOH:O    | 1.89                     | 0.73              |
| 1:E:58:ASP:C     | 3:E:341:HOH:O    | 2.32                     | 0.73              |
| 1:E:5:ARG:CG     | 3:E:422:HOH:O    | 2.36                     | 0.72              |
| 2:D:454:ASN:N    | 3:D:393:HOH:O    | 2.20                     | 0.72              |
| 1:A:123:VAL:HG12 | 3:A:370:HOH:O    | 1.88                     | 0.72              |
| 1:E:199:MET:HG2  | 3:E:396:HOH:O    | 1.89                     | 0.72              |
| 1:A:49:GLN:HG2   | 3:A:386:HOH:O    | 1.87                     | 0.72              |
| 1:E:202:PRO:HD2  | 3:E:388:HOH:O    | 1.88                     | 0.72              |
| 1:C:64:ARG:HG2   | 3:C:351:HOH:O    | 1.89                     | 0.72              |
| 1:A:181:LYS:C    | 3:A:393:HOH:O    | 2.33                     | 0.72              |
| 1:C:58:ASP:HB2   | 3:C:328:HOH:O    | 1.89                     | 0.72              |
| 1:E:94:ASP:HB3   | 3:E:375:HOH:O    | 1.90                     | 0.72              |
| 1:A:203:VAL:N    | 3:A:348:HOH:O    | 2.22                     | 0.71              |
| 1:A:180:ILE:HD11 | 3:E:421:HOH:O    | 1.89                     | 0.71              |
| 1:E:3:GLU:HG2    | 3:E:368:HOH:O    | 1.90                     | 0.71              |
| 1:A:18:ALA:HB3   | 3:A:435:HOH:O    | 1.90                     | 0.71              |
| 1:A:22:LEU:HD21  | 3:A:356:HOH:O    | 1.90                     | 0.71              |
| 1:C:6:LEU:N      | 3:C:422:HOH:O    | 2.22                     | 0.71              |
| 2:F:464:GLN:HG2  | 3:F:303:HOH:O    | 1.90                     | 0.71              |
| 1:A:112:SER:HB3  | 3:C:458:HOH:O    | 1.91                     | 0.71              |
| 1:C:118:LEU:HB3  | 3:C:345:HOH:O    | 1.90                     | 0.71              |
| 1:C:194:ALA:CA   | 3:C:403:HOH:O    | 2.38                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:224:THR:CB   | 3:C:386:HOH:O    | 2.34                     | 0.71              |
| 1:E:130:GLU:HA   | 3:E:399:HOH:O    | 1.89                     | 0.71              |
| 1:E:168:LYS:C    | 3:E:367:HOH:O    | 2.33                     | 0.70              |
| 1:C:238:GLU:CD   | 3:C:439:HOH:O    | 2.34                     | 0.70              |
| 1:E:175:LEU:HG   | 3:E:294:HOH:O    | 1.91                     | 0.70              |
| 1:E:58:ASP:HB2   | 3:E:341:HOH:O    | 1.90                     | 0.70              |
| 1:A:18:ALA:CB    | 3:A:435:HOH:O    | 2.39                     | 0.70              |
| 1:A:200:ASN:N    | 3:A:436:HOH:O    | 2.23                     | 0.70              |
| 1:E:35:VAL:CB    | 3:E:398:HOH:O    | 2.25                     | 0.70              |
| 1:E:101:LEU:HD12 | 3:E:392:HOH:O    | 1.90                     | 0.70              |
| 1:C:151:LEU:HD21 | 3:C:362:HOH:O    | 1.91                     | 0.70              |
| 1:E:78:ILE:CG2   | 3:E:442:HOH:O    | 2.39                     | 0.70              |
| 1:E:119:MET:SD   | 3:E:370:HOH:O    | 2.49                     | 0.70              |
| 1:E:199:MET:CG   | 3:E:396:HOH:O    | 2.39                     | 0.70              |
| 1:C:153:HIS:ND1  | 3:C:347:HOH:O    | 2.23                     | 0.70              |
| 1:E:3:GLU:OE2    | 1:E:91:ARG:HD3   | 1.92                     | 0.70              |
| 1:A:66:LEU:HD23  | 3:A:400:HOH:O    | 1.92                     | 0.69              |
| 1:A:214:PHE:HA   | 3:A:434:HOH:O    | 1.91                     | 0.69              |
| 1:A:225:VAL:HA   | 3:A:358:HOH:O    | 1.90                     | 0.69              |
| 1:C:50:LEU:CA    | 3:C:431:HOH:O    | 2.39                     | 0.69              |
| 1:A:180:ILE:HG13 | 3:E:421:HOH:O    | 1.92                     | 0.69              |
| 1:A:243:ASP:C    | 3:A:382:HOH:O    | 2.35                     | 0.69              |
| 1:E:255:ILE:HD12 | 3:E:296:HOH:O    | 1.90                     | 0.69              |
| 1:A:126:LEU:HD21 | 3:B:525:HOH:O    | 1.93                     | 0.69              |
| 1:A:168:LYS:N    | 3:A:378:HOH:O    | 2.25                     | 0.69              |
| 1:E:53:ARG:NE    | 3:E:365:HOH:O    | 2.25                     | 0.69              |
| 1:E:135:CYS:SG   | 3:E:396:HOH:O    | 2.50                     | 0.69              |
| 2:F:465:ARG:HG2  | 2:F:465:ARG:HH11 | 1.56                     | 0.69              |
| 1:C:255:ILE:HD13 | 2:D:457:VAL:HG21 | 1.75                     | 0.69              |
| 1:E:254:LYS:HG2  | 2:F:456:GLN:HA   | 1.74                     | 0.69              |
| 1:C:138:LYS:HG3  | 3:C:369:HOH:O    | 1.92                     | 0.68              |
| 1:C:144:PHE:CD1  | 3:C:444:HOH:O    | 2.46                     | 0.68              |
| 1:E:47:LEU:C     | 3:E:401:HOH:O    | 2.36                     | 0.68              |
| 1:E:37:LEU:HD23  | 3:E:404:HOH:O    | 1.93                     | 0.68              |
| 1:A:66:LEU:HA    | 3:A:400:HOH:O    | 1.93                     | 0.68              |
| 3:C:385:HOH:O    | 2:D:454:ASN:CB   | 2.26                     | 0.68              |
| 1:E:3:GLU:CG     | 3:E:368:HOH:O    | 2.41                     | 0.68              |
| 1:C:41:ASP:O     | 3:C:355:HOH:O    | 2.12                     | 0.68              |
| 1:E:60:TYR:CA    | 3:E:381:HOH:O    | 2.42                     | 0.67              |
| 1:E:133:TYR:CD1  | 3:E:371:HOH:O    | 2.46                     | 0.67              |
| 1:E:158:VAL:HA   | 3:E:349:HOH:O    | 1.95                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:3:GLU:OE2    | 1:A:91:ARG:HD3   | 1.95                     | 0.67              |
| 1:A:214:PHE:N    | 3:A:434:HOH:O    | 2.24                     | 0.67              |
| 1:A:180:ILE:CG1  | 3:E:421:HOH:O    | 2.42                     | 0.67              |
| 1:A:64:ARG:HD2   | 3:A:365:HOH:O    | 1.93                     | 0.67              |
| 1:A:103:PHE:HB3  | 3:A:412:HOH:O    | 1.92                     | 0.67              |
| 1:A:180:ILE:HB   | 3:A:425:HOH:O    | 1.94                     | 0.67              |
| 1:C:30:ILE:HD12  | 1:C:35:VAL:HG22  | 1.76                     | 0.67              |
| 1:E:202:PRO:HG3  | 3:E:366:HOH:O    | 1.95                     | 0.67              |
| 2:B:461:GLY:N    | 3:B:471:HOH:O    | 2.19                     | 0.67              |
| 1:C:126:LEU:C    | 3:C:412:HOH:O    | 2.37                     | 0.67              |
| 1:E:5:ARG:CB     | 3:E:422:HOH:O    | 2.42                     | 0.67              |
| 1:E:7:VAL:O      | 3:E:354:HOH:O    | 2.13                     | 0.67              |
| 1:E:30:ILE:HD12  | 1:E:35:VAL:HG22  | 1.76                     | 0.67              |
| 1:E:253:PRO:HB2  | 3:E:296:HOH:O    | 1.94                     | 0.67              |
| 1:C:254:LYS:HE2  | 3:D:393:HOH:O    | 1.92                     | 0.67              |
| 1:A:225:VAL:HG22 | 3:A:406:HOH:O    | 1.95                     | 0.67              |
| 1:E:175:LEU:C    | 3:E:379:HOH:O    | 2.38                     | 0.67              |
| 1:A:87:ILE:CG1   | 3:A:417:HOH:O    | 2.43                     | 0.67              |
| 1:A:169:PHE:CB   | 3:A:425:HOH:O    | 2.30                     | 0.67              |
| 1:E:139:MET:SD   | 3:E:427:HOH:O    | 2.53                     | 0.67              |
| 1:C:254:LYS:HG2  | 2:D:456:GLN:HA   | 1.77                     | 0.66              |
| 1:E:5:ARG:HG3    | 3:E:422:HOH:O    | 1.94                     | 0.66              |
| 1:C:195:VAL:HG23 | 3:C:403:HOH:O    | 1.93                     | 0.66              |
| 3:C:359:HOH:O    | 2:D:463:PHE:HA   | 1.95                     | 0.66              |
| 2:D:461:GLY:C    | 3:D:254:HOH:O    | 2.38                     | 0.66              |
| 1:A:172:SER:HB3  | 1:A:177:ASN:HB3  | 1.78                     | 0.66              |
| 1:E:94:ASP:CB    | 3:E:439:HOH:O    | 2.42                     | 0.66              |
| 1:E:35:VAL:C     | 3:E:398:HOH:O    | 2.38                     | 0.66              |
| 1:E:207:PHE:HA   | 3:E:358:HOH:O    | 1.95                     | 0.66              |
| 1:A:182:LEU:HG   | 3:A:393:HOH:O    | 1.96                     | 0.66              |
| 1:E:138:LYS:HE3  | 3:E:434:HOH:O    | 1.95                     | 0.66              |
| 1:A:180:ILE:CD1  | 3:E:421:HOH:O    | 2.43                     | 0.66              |
| 1:C:103:PHE:O    | 3:C:380:HOH:O    | 2.14                     | 0.66              |
| 1:C:144:PHE:CE1  | 3:C:444:HOH:O    | 2.48                     | 0.66              |
| 1:E:59:THR:HG22  | 3:E:381:HOH:O    | 1.95                     | 0.66              |
| 1:A:10:SER:N     | 3:A:362:HOH:O    | 2.28                     | 0.65              |
| 1:E:201:GLU:CB   | 3:E:388:HOH:O    | 2.44                     | 0.65              |
| 1:A:108:GLN:CB   | 3:A:341:HOH:O    | 2.44                     | 0.65              |
| 1:A:40:MET:HE3   | 2:B:459:ILE:HD13 | 1.77                     | 0.65              |
| 1:C:6:LEU:HG     | 3:C:414:HOH:O    | 1.96                     | 0.65              |
| 1:C:11:ILE:HG13  | 3:C:388:HOH:O    | 1.97                     | 0.65              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:41:ASP:OD2  | 1:E:43:SER:HB2   | 1.97                     | 0.65              |
| 1:A:226:THR:N   | 3:A:406:HOH:O    | 2.29                     | 0.65              |
| 1:C:165:ASP:HA  | 3:C:402:HOH:O    | 1.96                     | 0.65              |
| 1:E:5:ARG:HB3   | 3:E:341:HOH:O    | 1.96                     | 0.65              |
| 1:E:133:TYR:CE1 | 3:E:371:HOH:O    | 2.48                     | 0.65              |
| 1:A:24:ASN:N    | 3:A:343:HOH:O    | 2.29                     | 0.65              |
| 1:A:214:PHE:CA  | 3:A:434:HOH:O    | 2.45                     | 0.65              |
| 1:E:57:PHE:CE1  | 1:E:244:MET:HE1  | 2.32                     | 0.65              |
| 1:C:250:TYR:N   | 3:C:429:HOH:O    | 2.23                     | 0.65              |
| 1:E:229:MET:N   | 3:E:409:HOH:O    | 2.23                     | 0.65              |
| 1:A:252:ALA:N   | 3:A:346:HOH:O    | 2.29                     | 0.65              |
| 1:C:102:VAL:N   | 3:C:368:HOH:O    | 2.29                     | 0.65              |
| 1:C:121:LEU:HA  | 3:C:437:HOH:O    | 1.95                     | 0.65              |
| 1:C:214:PHE:CD1 | 3:C:330:HOH:O    | 2.50                     | 0.65              |
| 1:C:229:MET:HA  | 3:C:315:HOH:O    | 1.97                     | 0.64              |
| 1:A:26:ALA:HA   | 3:A:394:HOH:O    | 1.97                     | 0.64              |
| 1:C:153:HIS:CG  | 3:C:347:HOH:O    | 2.47                     | 0.64              |
| 1:C:51:THR:N    | 3:C:431:HOH:O    | 2.31                     | 0.64              |
| 1:C:5:ARG:HD3   | 3:C:328:HOH:O    | 1.96                     | 0.64              |
| 1:E:39:SER:N    | 3:E:404:HOH:O    | 2.30                     | 0.64              |
| 1:A:53:ARG:HB2  | 3:A:408:HOH:O    | 1.97                     | 0.64              |
| 1:C:8:GLN:N     | 3:C:414:HOH:O    | 2.30                     | 0.64              |
| 1:C:11:ILE:CG1  | 3:C:388:HOH:O    | 2.45                     | 0.64              |
| 1:E:170:SER:CB  | 1:E:179:ASN:HB3  | 2.28                     | 0.64              |
| 1:E:172:SER:HB3 | 1:E:177:ASN:HB3  | 1.78                     | 0.64              |
| 1:A:19:LEU:HG   | 3:A:435:HOH:O    | 1.96                     | 0.64              |
| 1:A:64:ARG:N    | 3:A:359:HOH:O    | 2.30                     | 0.64              |
| 1:C:58:ASP:C    | 3:C:328:HOH:O    | 2.40                     | 0.64              |
| 1:A:151:LEU:N   | 3:A:437:HOH:O    | 2.31                     | 0.64              |
| 1:A:252:ALA:CB  | 3:A:346:HOH:O    | 2.33                     | 0.64              |
| 2:B:464:GLN:H   | 2:B:464:GLN:CD   | 2.05                     | 0.64              |
| 1:E:43:SER:CB   | 3:E:364:HOH:O    | 2.44                     | 0.64              |
| 1:C:216:THR:HB  | 3:C:413:HOH:O    | 1.96                     | 0.63              |
| 1:E:40:MET:HE3  | 2:F:459:ILE:HD13 | 1.79                     | 0.63              |
| 1:E:57:PHE:HE1  | 1:E:244:MET:HE1  | 1.63                     | 0.63              |
| 1:E:94:ASP:CA   | 3:E:375:HOH:O    | 2.46                     | 0.63              |
| 1:A:170:SER:CB  | 1:A:179:ASN:HB3  | 2.27                     | 0.63              |
| 1:C:47:LEU:O    | 3:C:429:HOH:O    | 2.16                     | 0.63              |
| 1:C:77:LYS:HE3  | 3:C:353:HOH:O    | 1.98                     | 0.63              |
| 1:A:226:THR:C   | 3:A:406:HOH:O    | 2.40                     | 0.63              |
| 1:C:126:LEU:CA  | 3:C:412:HOH:O    | 2.45                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:140:PRO:HB3  | 3:E:429:HOH:O    | 1.98                     | 0.63              |
| 1:A:124:GLU:HB3  | 3:A:332:HOH:O    | 1.97                     | 0.63              |
| 1:E:225:VAL:C    | 3:E:385:HOH:O    | 2.40                     | 0.63              |
| 1:C:172:SER:HB3  | 1:C:177:ASN:HB3  | 1.80                     | 0.62              |
| 1:C:110:LYS:CE   | 3:C:354:HOH:O    | 2.47                     | 0.62              |
| 1:A:30:ILE:HD12  | 1:A:35:VAL:HG22  | 1.80                     | 0.62              |
| 1:C:101:LEU:C    | 3:C:368:HOH:O    | 2.41                     | 0.62              |
| 1:C:40:MET:HE3   | 2:D:459:ILE:CD1  | 2.28                     | 0.62              |
| 1:A:40:MET:HE2   | 1:A:44:HIS:CG    | 2.35                     | 0.62              |
| 1:C:149:ARG:NH1  | 3:C:371:HOH:O    | 2.32                     | 0.62              |
| 1:E:87:ILE:HG12  | 3:E:354:HOH:O    | 1.99                     | 0.62              |
| 1:E:210:ARG:NH1  | 3:E:382:HOH:O    | 2.32                     | 0.62              |
| 1:E:107:ASN:C    | 3:E:342:HOH:O    | 2.42                     | 0.62              |
| 1:E:168:LYS:CD   | 3:E:430:HOH:O    | 2.47                     | 0.62              |
| 1:A:204:GLN:N    | 3:A:422:HOH:O    | 2.30                     | 0.62              |
| 1:C:164:LYS:O    | 3:C:402:HOH:O    | 2.16                     | 0.62              |
| 1:C:216:THR:CB   | 3:C:413:HOH:O    | 2.46                     | 0.62              |
| 1:E:78:ILE:HG22  | 3:E:442:HOH:O    | 1.96                     | 0.62              |
| 1:E:257:ASP:N    | 3:E:374:HOH:O    | 2.33                     | 0.62              |
| 1:A:40:MET:HG3   | 3:A:383:HOH:O    | 1.98                     | 0.62              |
| 1:C:57:PHE:CE1   | 1:C:244:MET:HE1  | 2.35                     | 0.61              |
| 1:A:87:ILE:HG12  | 3:A:417:HOH:O    | 1.99                     | 0.61              |
| 1:C:207:PHE:HA   | 3:C:288:HOH:O    | 1.99                     | 0.61              |
| 1:E:181:LYS:HE2  | 3:E:430:HOH:O    | 2.00                     | 0.61              |
| 2:D:465:ARG:N    | 3:D:246:HOH:O    | 2.33                     | 0.61              |
| 2:D:459:ILE:N    | 2:D:459:ILE:HD12 | 2.15                     | 0.61              |
| 1:E:171:ALA:O    | 1:E:177:ASN:HB2  | 2.01                     | 0.61              |
| 1:C:77:LYS:HD3   | 3:C:441:HOH:O    | 2.00                     | 0.61              |
| 2:D:456:GLN:O    | 3:D:272:HOH:O    | 2.16                     | 0.61              |
| 1:E:202:PRO:CD   | 3:E:403:HOH:O    | 2.49                     | 0.61              |
| 1:C:103:PHE:CE2  | 3:C:432:HOH:O    | 2.51                     | 0.61              |
| 1:E:229:MET:CA   | 3:E:409:HOH:O    | 2.49                     | 0.61              |
| 1:A:234:PRO:HD3  | 2:B:462:PHE:CD2  | 2.36                     | 0.61              |
| 1:C:40:MET:HE2   | 1:C:44:HIS:CG    | 2.35                     | 0.61              |
| 1:C:180:ILE:HG13 | 3:C:362:HOH:O    | 2.01                     | 0.61              |
| 1:A:246:HIS:NE2  | 3:A:407:HOH:O    | 2.31                     | 0.61              |
| 1:A:168:LYS:CA   | 3:A:378:HOH:O    | 2.49                     | 0.60              |
| 1:A:171:ALA:O    | 1:A:177:ASN:HB2  | 2.02                     | 0.60              |
| 1:E:131:GLN:HB3  | 3:E:264:HOH:O    | 2.00                     | 0.60              |
| 1:A:48:VAL:C     | 3:A:439:HOH:O    | 2.43                     | 0.60              |
| 1:C:174:GLU:N    | 3:C:433:HOH:O    | 2.33                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:57:PHE:HD2   | 3:C:455:HOH:O    | 1.84                     | 0.60              |
| 1:E:94:ASP:CA    | 3:E:439:HOH:O    | 2.50                     | 0.60              |
| 1:A:245:GLY:N    | 3:A:382:HOH:O    | 2.34                     | 0.60              |
| 1:C:58:ASP:CA    | 3:C:356:HOH:O    | 2.46                     | 0.60              |
| 1:A:53:ARG:NH2   | 3:A:270:HOH:O    | 2.29                     | 0.60              |
| 1:A:57:PHE:HE1   | 1:A:244:MET:HE1  | 1.67                     | 0.60              |
| 1:A:178:GLY:HA2  | 3:E:340:HOH:O    | 2.01                     | 0.60              |
| 1:C:214:PHE:CA   | 3:C:330:HOH:O    | 2.42                     | 0.60              |
| 1:A:57:PHE:CE1   | 1:A:244:MET:HE1  | 2.37                     | 0.60              |
| 1:C:170:SER:CB   | 1:C:179:ASN:HB3  | 2.28                     | 0.60              |
| 1:C:226:THR:HG22 | 3:C:369:HOH:O    | 2.01                     | 0.60              |
| 1:C:42:SER:CA    | 3:C:355:HOH:O    | 2.49                     | 0.59              |
| 1:C:195:VAL:N    | 3:C:403:HOH:O    | 2.33                     | 0.59              |
| 1:E:202:PRO:N    | 3:E:403:HOH:O    | 2.34                     | 0.59              |
| 1:C:161:SER:N    | 3:C:408:HOH:O    | 2.35                     | 0.59              |
| 1:E:40:MET:HE2   | 1:E:44:HIS:CG    | 2.36                     | 0.59              |
| 1:E:250:TYR:HA   | 3:E:420:HOH:O    | 2.01                     | 0.59              |
| 2:B:464:GLN:CD   | 2:B:464:GLN:N    | 2.61                     | 0.59              |
| 1:C:254:LYS:HG3  | 3:C:288:HOH:O    | 2.01                     | 0.59              |
| 1:E:64:ARG:HD2   | 1:E:94:ASP:HB3   | 1.84                     | 0.59              |
| 1:E:3:GLU:CD     | 3:E:368:HOH:O    | 2.45                     | 0.59              |
| 1:A:40:MET:HE3   | 2:B:459:ILE:CD1  | 2.32                     | 0.59              |
| 1:C:135:CYS:SG   | 1:C:199:MET:HG2  | 2.42                     | 0.59              |
| 1:A:252:ALA:CA   | 3:A:346:HOH:O    | 2.50                     | 0.59              |
| 1:E:115:GLU:HG3  | 3:E:304:HOH:O    | 2.02                     | 0.59              |
| 1:E:115:GLU:N    | 3:E:340:HOH:O    | 2.36                     | 0.59              |
| 1:C:224:THR:CG2  | 3:C:386:HOH:O    | 2.51                     | 0.59              |
| 1:C:87:ILE:HG23  | 3:C:422:HOH:O    | 2.02                     | 0.58              |
| 1:A:70:VAL:HB    | 3:A:399:HOH:O    | 2.02                     | 0.58              |
| 1:E:40:MET:HE3   | 2:F:459:ILE:CD1  | 2.33                     | 0.58              |
| 1:E:202:PRO:HD2  | 3:E:403:HOH:O    | 2.02                     | 0.58              |
| 1:A:255:ILE:HD13 | 2:B:457:VAL:HG21 | 1.85                     | 0.58              |
| 1:E:70:VAL:HB    | 3:E:353:HOH:O    | 2.04                     | 0.58              |
| 1:C:30:ILE:HG13  | 1:C:68:MET:CE    | 2.33                     | 0.58              |
| 2:D:462:PHE:N    | 3:D:254:HOH:O    | 2.36                     | 0.58              |
| 1:E:12:LEU:CA    | 3:E:344:HOH:O    | 2.52                     | 0.58              |
| 1:E:254:LYS:HE3  | 3:F:132:HOH:O    | 2.04                     | 0.58              |
| 1:C:3:GLU:OE2    | 1:C:91:ARG:HD3   | 2.03                     | 0.58              |
| 1:E:4:ALA:HB1    | 1:E:57:PHE:CD2   | 2.38                     | 0.58              |
| 1:E:78:ILE:HG23  | 3:E:442:HOH:O    | 2.03                     | 0.58              |
| 1:E:229:MET:C    | 3:E:409:HOH:O    | 2.46                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:105:ALA:N    | 3:C:380:HOH:O    | 2.37                     | 0.58              |
| 1:C:8:GLN:C      | 3:C:414:HOH:O    | 2.46                     | 0.58              |
| 1:C:149:ARG:HG2  | 1:C:149:ARG:HH11 | 1.68                     | 0.57              |
| 1:A:141:SER:HB2  | 1:A:219:THR:HG23 | 1.86                     | 0.57              |
| 1:A:175:LEU:HG   | 3:A:316:HOH:O    | 2.04                     | 0.57              |
| 1:C:61:ARG:NH2   | 3:C:451:HOH:O    | 2.37                     | 0.57              |
| 1:C:57:PHE:HE1   | 1:C:244:MET:HE1  | 1.69                     | 0.57              |
| 1:E:202:PRO:CD   | 3:E:388:HOH:O    | 2.50                     | 0.57              |
| 1:E:176:GLY:HA3  | 3:E:379:HOH:O    | 2.04                     | 0.57              |
| 1:A:113:ASP:N    | 3:C:458:HOH:O    | 2.37                     | 0.57              |
| 1:A:244:MET:N    | 3:A:382:HOH:O    | 2.37                     | 0.57              |
| 1:C:51:THR:O     | 1:C:245:GLY:HA3  | 2.03                     | 0.57              |
| 1:C:124:GLU:HB2  | 3:C:435:HOH:O    | 2.03                     | 0.57              |
| 1:E:28:TRP:HE3   | 1:E:35:VAL:HG11  | 1.70                     | 0.57              |
| 1:E:86:ASP:OD1   | 1:E:105:ALA:HA   | 2.04                     | 0.57              |
| 1:A:49:GLN:N     | 3:A:439:HOH:O    | 2.37                     | 0.57              |
| 1:A:196:THR:C    | 3:A:397:HOH:O    | 2.48                     | 0.57              |
| 2:B:459:ILE:HD12 | 2:B:459:ILE:N    | 2.20                     | 0.57              |
| 1:C:50:LEU:C     | 3:C:431:HOH:O    | 2.48                     | 0.57              |
| 1:C:153:HIS:HB2  | 3:C:347:HOH:O    | 1.93                     | 0.57              |
| 1:E:94:ASP:HB2   | 3:E:439:HOH:O    | 2.03                     | 0.57              |
| 1:E:51:THR:O     | 1:E:245:GLY:HA3  | 2.05                     | 0.57              |
| 1:A:226:THR:CA   | 3:A:406:HOH:O    | 2.53                     | 0.56              |
| 1:C:144:PHE:CG   | 3:C:444:HOH:O    | 2.57                     | 0.56              |
| 1:A:156:ASP:CB   | 3:A:423:HOH:O    | 2.46                     | 0.56              |
| 1:A:37:LEU:O     | 3:A:386:HOH:O    | 2.18                     | 0.56              |
| 1:A:91:ARG:NH1   | 3:A:432:HOH:O    | 2.37                     | 0.56              |
| 1:C:144:PHE:CZ   | 3:C:444:HOH:O    | 2.58                     | 0.56              |
| 1:E:53:ARG:NH2   | 3:E:278:HOH:O    | 2.36                     | 0.56              |
| 2:F:464:GLN:N    | 3:F:303:HOH:O    | 2.38                     | 0.56              |
| 2:B:460:THR:HG22 | 3:B:525:HOH:O    | 2.05                     | 0.56              |
| 1:C:16:LEU:HD13  | 1:C:79:LEU:CD1   | 2.35                     | 0.56              |
| 1:E:107:ASN:O    | 1:E:109:GLU:OE1  | 2.23                     | 0.56              |
| 1:E:168:LYS:CA   | 3:E:367:HOH:O    | 2.53                     | 0.56              |
| 1:C:210:ARG:HB3  | 3:C:367:HOH:O    | 2.05                     | 0.56              |
| 1:E:43:SER:CA    | 3:E:364:HOH:O    | 2.52                     | 0.56              |
| 1:C:129:PRO:HD3  | 3:C:359:HOH:O    | 2.05                     | 0.56              |
| 1:A:208:ALA:HB2  | 3:B:50:HOH:O     | 2.05                     | 0.56              |
| 1:C:64:ARG:HD2   | 1:C:94:ASP:HB3   | 1.88                     | 0.56              |
| 1:C:171:ALA:O    | 1:C:177:ASN:HB2  | 2.05                     | 0.56              |
| 1:C:194:ALA:CB   | 3:C:377:HOH:O    | 2.39                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:87:ILE:HG22  | 3:E:292:HOH:O    | 2.04                     | 0.56              |
| 1:A:211:TYR:HB3  | 3:A:289:HOH:O    | 2.05                     | 0.56              |
| 2:F:457:VAL:N    | 3:F:540:HOH:O    | 2.37                     | 0.56              |
| 1:A:200:ASN:CG   | 3:A:436:HOH:O    | 2.49                     | 0.55              |
| 2:D:462:PHE:C    | 3:D:254:HOH:O    | 2.49                     | 0.55              |
| 1:E:90:LEU:HD22  | 3:E:405:HOH:O    | 2.07                     | 0.55              |
| 1:A:16:LEU:HD21  | 1:A:75:MET:CG    | 2.37                     | 0.55              |
| 1:A:49:GLN:CA    | 3:A:439:HOH:O    | 2.54                     | 0.55              |
| 1:A:240:LYS:N    | 3:A:427:HOH:O    | 2.38                     | 0.55              |
| 1:C:8:GLN:CA     | 3:C:414:HOH:O    | 2.55                     | 0.55              |
| 1:C:19:LEU:CD2   | 1:C:48:VAL:HG11  | 2.37                     | 0.55              |
| 1:E:100:ALA:HA   | 3:E:392:HOH:O    | 2.06                     | 0.55              |
| 1:C:141:SER:HB2  | 1:C:219:THR:HG23 | 1.89                     | 0.55              |
| 1:C:161:SER:C    | 3:C:408:HOH:O    | 2.49                     | 0.55              |
| 1:E:132:GLU:O    | 3:E:448:HOH:O    | 2.18                     | 0.55              |
| 1:A:86:ASP:OD1   | 1:A:105:ALA:HA   | 2.07                     | 0.55              |
| 1:A:112:SER:CA   | 3:C:458:HOH:O    | 2.54                     | 0.55              |
| 1:C:53:ARG:NH2   | 3:C:266:HOH:O    | 2.37                     | 0.55              |
| 1:C:93:GLU:HB2   | 1:C:96:ALA:HB3   | 1.89                     | 0.55              |
| 1:C:167:VAL:HG23 | 3:C:408:HOH:O    | 2.07                     | 0.55              |
| 1:A:93:GLU:HB2   | 1:A:96:ALA:HB3   | 1.89                     | 0.55              |
| 1:A:135:CYS:SG   | 1:A:199:MET:HG2  | 2.46                     | 0.55              |
| 1:A:151:LEU:HD21 | 3:E:421:HOH:O    | 2.06                     | 0.55              |
| 1:A:254:LYS:HG2  | 2:B:456:GLN:HA   | 1.89                     | 0.55              |
| 1:C:174:GLU:CG   | 3:C:433:HOH:O    | 2.55                     | 0.55              |
| 1:E:139:MET:HG3  | 3:E:427:HOH:O    | 2.05                     | 0.54              |
| 1:C:194:ALA:CA   | 3:C:377:HOH:O    | 2.54                     | 0.54              |
| 1:E:19:LEU:CD2   | 1:E:48:VAL:HG11  | 2.38                     | 0.54              |
| 1:E:135:CYS:HB3  | 3:E:347:HOH:O    | 2.05                     | 0.54              |
| 1:E:99:LEU:O     | 3:E:392:HOH:O    | 2.18                     | 0.54              |
| 1:A:219:THR:CA   | 3:A:354:HOH:O    | 2.44                     | 0.54              |
| 1:C:30:ILE:CD1   | 1:C:35:VAL:HG22  | 2.37                     | 0.54              |
| 1:C:132:GLU:N    | 3:C:426:HOH:O    | 2.40                     | 0.54              |
| 1:A:51:THR:O     | 1:A:245:GLY:HA3  | 2.07                     | 0.54              |
| 2:F:462:PHE:C    | 2:F:463:PHE:HD2  | 2.16                     | 0.54              |
| 1:A:26:ALA:CA    | 3:A:394:HOH:O    | 2.54                     | 0.54              |
| 1:A:49:GLN:CB    | 3:A:439:HOH:O    | 2.30                     | 0.54              |
| 2:B:461:GLY:CA   | 3:B:471:HOH:O    | 2.56                     | 0.54              |
| 1:E:6:LEU:HD12   | 3:E:378:HOH:O    | 2.07                     | 0.54              |
| 2:D:463:PHE:N    | 3:D:254:HOH:O    | 2.40                     | 0.54              |
| 1:E:139:MET:CG   | 3:E:427:HOH:O    | 2.56                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:28:TRP:HE3   | 1:A:35:VAL:HG11  | 1.73                     | 0.54              |
| 1:C:119:MET:CE   | 3:C:337:HOH:O    | 2.56                     | 0.53              |
| 1:E:236:VAL:HG22 | 3:E:420:HOH:O    | 2.07                     | 0.53              |
| 1:C:65:ASN:N     | 3:C:351:HOH:O    | 2.38                     | 0.53              |
| 1:C:224:THR:HG21 | 3:C:386:HOH:O    | 2.08                     | 0.53              |
| 1:A:25:GLU:O     | 3:A:394:HOH:O    | 2.19                     | 0.53              |
| 1:A:203:VAL:CG1  | 3:A:422:HOH:O    | 2.52                     | 0.53              |
| 1:A:239:TYR:CB   | 3:A:427:HOH:O    | 2.37                     | 0.53              |
| 1:C:82:ALA:HA    | 3:C:430:HOH:O    | 2.07                     | 0.53              |
| 1:E:37:LEU:CD2   | 3:E:404:HOH:O    | 2.54                     | 0.53              |
| 2:B:454:ASN:N    | 3:B:271:HOH:O    | 2.41                     | 0.53              |
| 1:C:77:LYS:CD    | 3:C:441:HOH:O    | 2.55                     | 0.53              |
| 1:E:147:ILE:HG23 | 1:E:180:ILE:HD12 | 1.91                     | 0.53              |
| 1:A:30:ILE:HG13  | 1:A:68:MET:CE    | 2.39                     | 0.53              |
| 2:B:461:GLY:HA3  | 3:B:471:HOH:O    | 2.09                     | 0.53              |
| 1:E:199:MET:HG3  | 3:E:396:HOH:O    | 2.06                     | 0.53              |
| 2:F:459:ILE:N    | 2:F:459:ILE:HD12 | 2.23                     | 0.53              |
| 1:A:45:VAL:HG13  | 3:A:346:HOH:O    | 2.08                     | 0.53              |
| 1:C:98:THR:HG22  | 3:C:276:HOH:O    | 2.09                     | 0.53              |
| 1:E:1:MET:H3     | 1:E:63:ASP:HB2   | 1.73                     | 0.53              |
| 1:E:143:GLU:HB3  | 3:E:427:HOH:O    | 2.08                     | 0.53              |
| 1:A:94:ASP:CA    | 3:A:365:HOH:O    | 2.56                     | 0.53              |
| 1:A:151:LEU:CA   | 3:A:437:HOH:O    | 2.57                     | 0.53              |
| 1:C:179:ASN:HA   | 3:C:362:HOH:O    | 2.09                     | 0.53              |
| 2:D:454:ASN:CA   | 3:D:393:HOH:O    | 2.57                     | 0.53              |
| 1:E:108:GLN:N    | 3:E:342:HOH:O    | 2.42                     | 0.53              |
| 1:E:229:MET:O    | 3:E:409:HOH:O    | 2.18                     | 0.53              |
| 1:A:246:HIS:CD2  | 3:A:407:HOH:O    | 2.61                     | 0.53              |
| 1:C:205:LEU:HD23 | 3:C:268:HOH:O    | 2.09                     | 0.52              |
| 1:E:30:ILE:HG13  | 1:E:68:MET:CE    | 2.39                     | 0.52              |
| 1:C:204:GLN:HG2  | 3:C:285:HOH:O    | 2.09                     | 0.52              |
| 1:C:140:PRO:HD3  | 3:C:457:HOH:O    | 2.10                     | 0.52              |
| 1:C:174:GLU:HG2  | 3:C:433:HOH:O    | 2.10                     | 0.52              |
| 1:E:16:LEU:HD13  | 1:E:79:LEU:CD1   | 2.40                     | 0.52              |
| 1:A:16:LEU:HD21  | 1:A:75:MET:HG2   | 1.90                     | 0.52              |
| 1:A:170:SER:HB3  | 1:A:179:ASN:CB   | 2.34                     | 0.52              |
| 1:C:254:LYS:HG3  | 3:C:372:HOH:O    | 2.08                     | 0.52              |
| 1:E:60:TYR:N     | 3:E:381:HOH:O    | 2.39                     | 0.52              |
| 1:E:135:CYS:HA   | 1:E:198:GLU:O    | 2.09                     | 0.52              |
| 1:E:194:ALA:HA   | 3:E:318:HOH:O    | 2.09                     | 0.52              |
| 1:C:217:LYS:HG3  | 3:C:387:HOH:O    | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:168:LYS:NZ   | 3:E:430:HOH:O    | 2.43                     | 0.52              |
| 1:C:248:LYS:HE3  | 3:C:341:HOH:O    | 2.08                     | 0.52              |
| 1:E:94:ASP:CB    | 3:E:375:HOH:O    | 2.54                     | 0.52              |
| 1:E:256:GLU:CA   | 3:E:374:HOH:O    | 2.51                     | 0.52              |
| 1:E:104:GLU:HG3  | 3:E:346:HOH:O    | 2.09                     | 0.52              |
| 1:A:4:ALA:HB1    | 1:A:57:PHE:CD2   | 2.44                     | 0.51              |
| 1:C:147:ILE:HG23 | 1:C:180:ILE:HD12 | 1.92                     | 0.51              |
| 1:C:16:LEU:HD21  | 1:C:75:MET:CG    | 2.40                     | 0.51              |
| 1:C:21:ASP:HA    | 3:C:322:HOH:O    | 2.10                     | 0.51              |
| 1:C:126:LEU:N    | 3:C:412:HOH:O    | 2.44                     | 0.51              |
| 1:E:45:VAL:HG13  | 2:F:456:GLN:NE2  | 2.25                     | 0.51              |
| 2:F:457:VAL:C    | 3:F:540:HOH:O    | 2.54                     | 0.51              |
| 1:E:107:ASN:CB   | 3:E:342:HOH:O    | 2.50                     | 0.51              |
| 1:A:16:LEU:HD13  | 1:A:79:LEU:CD1   | 2.41                     | 0.51              |
| 1:A:92:ALA:HA    | 3:A:323:HOH:O    | 2.10                     | 0.51              |
| 1:A:254:LYS:NZ   | 3:A:315:HOH:O    | 2.41                     | 0.51              |
| 1:C:28:TRP:HE3   | 1:C:35:VAL:HG11  | 1.75                     | 0.51              |
| 1:C:44:HIS:C     | 2:D:459:ILE:HD11 | 2.35                     | 0.51              |
| 1:E:85:GLU:CG    | 3:E:360:HOH:O    | 2.38                     | 0.51              |
| 1:A:64:ARG:C     | 3:A:359:HOH:O    | 2.54                     | 0.51              |
| 1:C:214:PHE:N    | 3:C:330:HOH:O    | 2.43                     | 0.51              |
| 3:C:350:HOH:O    | 2:D:462:PHE:CE2  | 2.64                     | 0.51              |
| 1:E:16:LEU:HD21  | 1:E:75:MET:CG    | 2.41                     | 0.51              |
| 1:E:59:THR:O     | 3:E:381:HOH:O    | 2.18                     | 0.51              |
| 1:E:107:ASN:CA   | 3:E:342:HOH:O    | 2.58                     | 0.51              |
| 3:E:374:HOH:O    | 2:F:454:ASN:CB   | 2.59                     | 0.51              |
| 1:E:52:LEU:HB3   | 1:E:244:MET:HE1  | 1.92                     | 0.51              |
| 1:A:19:LEU:CD2   | 1:A:48:VAL:HG11  | 2.41                     | 0.51              |
| 1:E:110:LYS:HB3  | 3:E:348:HOH:O    | 2.10                     | 0.51              |
| 1:C:255:ILE:HD11 | 3:C:350:HOH:O    | 2.11                     | 0.51              |
| 1:E:93:GLU:HB2   | 1:E:96:ALA:HB3   | 1.92                     | 0.51              |
| 1:A:225:VAL:C    | 3:A:358:HOH:O    | 2.51                     | 0.50              |
| 1:C:1:MET:H3     | 1:C:63:ASP:HB2   | 1.76                     | 0.50              |
| 1:C:110:LYS:HE3  | 3:C:354:HOH:O    | 2.10                     | 0.50              |
| 1:C:172:SER:HB3  | 1:C:177:ASN:CB   | 2.41                     | 0.50              |
| 1:A:95:ASN:OD1   | 3:A:387:HOH:O    | 2.19                     | 0.50              |
| 1:A:112:SER:CB   | 3:C:458:HOH:O    | 2.56                     | 0.50              |
| 1:C:24:ASN:C     | 3:C:374:HOH:O    | 2.53                     | 0.50              |
| 1:C:146:ARG:NE   | 3:C:400:HOH:O    | 2.44                     | 0.50              |
| 1:C:174:GLU:CA   | 3:C:433:HOH:O    | 2.58                     | 0.50              |
| 1:E:24:ASN:OD1   | 3:E:397:HOH:O    | 2.19                     | 0.50              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:136:VAL:N   | 3:E:347:HOH:O    | 2.44                     | 0.50              |
| 1:A:107:ASN:CB  | 3:A:372:HOH:O    | 2.59                     | 0.50              |
| 1:A:151:LEU:CD2 | 3:E:421:HOH:O    | 2.59                     | 0.50              |
| 1:C:135:CYS:HA  | 1:C:198:GLU:O    | 2.10                     | 0.50              |
| 1:C:194:ALA:O   | 3:C:457:HOH:O    | 2.20                     | 0.50              |
| 1:A:254:LYS:HG3 | 3:A:428:HOH:O    | 2.11                     | 0.50              |
| 1:C:125:GLN:C   | 3:C:412:HOH:O    | 2.55                     | 0.50              |
| 1:A:72:LEU:HD21 | 3:A:399:HOH:O    | 2.10                     | 0.50              |
| 1:C:226:THR:CG2 | 3:C:369:HOH:O    | 2.58                     | 0.50              |
| 1:C:180:ILE:N   | 3:C:362:HOH:O    | 2.43                     | 0.50              |
| 1:C:86:ASP:OD1  | 1:C:105:ALA:HA   | 2.11                     | 0.50              |
| 1:E:168:LYS:N   | 3:E:367:HOH:O    | 2.45                     | 0.50              |
| 1:A:149:ARG:HG2 | 1:A:149:ARG:HH11 | 1.76                     | 0.50              |
| 1:E:170:SER:HB3 | 1:E:179:ASN:CB   | 2.33                     | 0.50              |
| 1:A:45:VAL:CG1  | 3:A:346:HOH:O    | 2.59                     | 0.49              |
| 1:C:8:GLN:HB2   | 3:C:414:HOH:O    | 2.11                     | 0.49              |
| 1:C:45:VAL:HG13 | 2:D:456:GLN:NE2  | 2.26                     | 0.49              |
| 1:E:47:LEU:CA   | 3:E:401:HOH:O    | 2.58                     | 0.49              |
| 1:A:49:GLN:HA   | 3:A:386:HOH:O    | 2.12                     | 0.49              |
| 1:C:28:TRP:NE1  | 3:C:405:HOH:O    | 2.45                     | 0.49              |
| 1:E:143:GLU:O   | 1:E:147:ILE:HG13 | 2.12                     | 0.49              |
| 1:C:70:VAL:CG1  | 3:C:405:HOH:O    | 2.41                     | 0.49              |
| 1:E:52:LEU:HB3  | 1:E:244:MET:CE   | 2.42                     | 0.49              |
| 1:E:228:SER:HB2 | 1:E:236:VAL:HB   | 1.94                     | 0.49              |
| 1:A:28:TRP:CE3  | 1:A:35:VAL:HG11  | 2.47                     | 0.49              |
| 1:A:207:PHE:CA  | 3:A:428:HOH:O    | 2.54                     | 0.49              |
| 1:E:141:SER:HB2 | 1:E:219:THR:HG23 | 1.93                     | 0.49              |
| 1:E:225:VAL:CG2 | 3:E:385:HOH:O    | 2.43                     | 0.49              |
| 1:C:143:GLU:O   | 1:C:147:ILE:HG13 | 2.12                     | 0.49              |
| 1:A:40:MET:CG   | 3:A:383:HOH:O    | 2.59                     | 0.49              |
| 1:C:139:MET:HA  | 3:C:457:HOH:O    | 2.11                     | 0.49              |
| 1:E:131:GLN:N   | 3:E:399:HOH:O    | 2.44                     | 0.49              |
| 1:C:5:ARG:HB3   | 3:C:328:HOH:O    | 2.11                     | 0.49              |
| 1:E:12:LEU:HA   | 3:E:344:HOH:O    | 2.13                     | 0.49              |
| 1:E:94:ASP:HA   | 3:E:375:HOH:O    | 2.10                     | 0.49              |
| 3:A:366:HOH:O   | 2:B:463:PHE:HD1  | 1.96                     | 0.48              |
| 1:C:213:ASN:C   | 3:C:330:HOH:O    | 2.55                     | 0.48              |
| 1:E:166:GLY:HA2 | 1:E:197:ILE:CD1  | 2.43                     | 0.48              |
| 1:A:103:PHE:CG  | 3:A:412:HOH:O    | 2.61                     | 0.48              |
| 1:C:63:ASP:CG   | 3:C:396:HOH:O    | 2.56                     | 0.48              |
| 1:C:107:ASN:O   | 1:C:109:GLU:OE1  | 2.32                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:172:SER:HB3  | 1:E:177:ASN:CB   | 2.43                     | 0.48              |
| 1:C:38:GLN:HA    | 1:C:48:VAL:O     | 2.14                     | 0.48              |
| 1:E:30:ILE:CD1   | 1:E:35:VAL:HG22  | 2.43                     | 0.48              |
| 1:C:255:ILE:HG23 | 3:C:286:HOH:O    | 2.13                     | 0.48              |
| 1:E:149:ARG:HG2  | 1:E:149:ARG:HH11 | 1.79                     | 0.48              |
| 1:E:248:LYS:NZ   | 3:E:408:HOH:O    | 2.46                     | 0.48              |
| 1:A:172:SER:HB3  | 1:A:177:ASN:CB   | 2.42                     | 0.48              |
| 1:E:28:TRP:CE3   | 1:E:35:VAL:HG11  | 2.46                     | 0.48              |
| 1:E:225:VAL:CG1  | 3:E:385:HOH:O    | 2.52                     | 0.48              |
| 1:A:87:ILE:HG13  | 3:A:417:HOH:O    | 2.13                     | 0.48              |
| 2:D:454:ASN:C    | 2:D:454:ASN:HD22 | 2.22                     | 0.48              |
| 1:A:30:ILE:CD1   | 1:A:35:VAL:HG22  | 2.43                     | 0.48              |
| 1:C:153:HIS:CD2  | 3:C:298:HOH:O    | 2.66                     | 0.48              |
| 1:C:7:VAL:HG13   | 3:C:420:HOH:O    | 2.14                     | 0.48              |
| 1:C:21:ASP:HB2   | 3:C:277:HOH:O    | 2.13                     | 0.48              |
| 1:C:166:GLY:HA2  | 1:C:197:ILE:HD12 | 1.96                     | 0.48              |
| 1:E:105:ALA:O    | 1:E:106:PRO:C    | 2.57                     | 0.48              |
| 2:B:457:VAL:HG11 | 2:B:462:PHE:HE1  | 1.79                     | 0.47              |
| 1:C:28:TRP:CE3   | 1:C:35:VAL:HG11  | 2.49                     | 0.47              |
| 1:C:144:PHE:CD2  | 3:C:444:HOH:O    | 2.66                     | 0.47              |
| 2:D:453:ALA:C    | 3:D:393:HOH:O    | 2.53                     | 0.47              |
| 1:A:68:MET:O     | 1:A:70:VAL:HG23  | 2.14                     | 0.47              |
| 1:C:124:GLU:N    | 3:C:435:HOH:O    | 2.33                     | 0.47              |
| 1:E:168:LYS:HD3  | 3:E:430:HOH:O    | 2.11                     | 0.47              |
| 1:E:203:VAL:HG12 | 1:E:204:GLN:N    | 2.28                     | 0.47              |
| 1:A:23:ILE:HG21  | 3:A:394:HOH:O    | 2.15                     | 0.47              |
| 1:C:16:LEU:HD21  | 1:C:75:MET:HG2   | 1.97                     | 0.47              |
| 1:E:63:ASP:O     | 3:E:444:HOH:O    | 2.20                     | 0.47              |
| 1:E:254:LYS:HG2  | 2:F:456:GLN:CA   | 2.44                     | 0.47              |
| 1:A:135:CYS:HA   | 1:A:198:GLU:O    | 2.14                     | 0.47              |
| 1:E:207:PHE:CZ   | 1:E:235:LEU:HB2  | 2.49                     | 0.47              |
| 1:C:64:ARG:HB3   | 1:C:94:ASP:OD1   | 2.15                     | 0.47              |
| 1:C:241:ILE:O    | 1:C:244:MET:HB2  | 2.15                     | 0.47              |
| 1:E:199:MET:HE2  | 1:E:202:PRO:HG3  | 1.95                     | 0.47              |
| 1:A:73:THR:CA    | 3:A:402:HOH:O    | 2.34                     | 0.47              |
| 1:C:172:SER:CB   | 1:C:177:ASN:HB3  | 2.44                     | 0.47              |
| 1:E:16:LEU:HD21  | 1:E:75:MET:HG2   | 1.97                     | 0.47              |
| 1:E:124:GLU:OE2  | 2:F:465:ARG:NH1  | 2.48                     | 0.47              |
| 1:E:196:THR:HA   | 3:E:355:HOH:O    | 2.14                     | 0.47              |
| 1:E:234:PRO:HD3  | 2:F:462:PHE:CD2  | 2.50                     | 0.47              |
| 1:A:129:PRO:HD3  | 2:B:463:PHE:CG   | 2.49                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:4:ALA:HB1    | 1:C:57:PHE:CD2   | 2.50                     | 0.47              |
| 1:C:24:ASN:CA    | 3:C:374:HOH:O    | 2.61                     | 0.47              |
| 1:A:95:ASN:HB2   | 3:A:297:HOH:O    | 2.13                     | 0.47              |
| 1:E:236:VAL:CA   | 3:E:420:HOH:O    | 2.20                     | 0.47              |
| 1:E:175:LEU:HD12 | 1:E:175:LEU:O    | 2.15                     | 0.47              |
| 1:C:52:LEU:HB3   | 1:C:244:MET:HE1  | 1.97                     | 0.46              |
| 1:C:110:LYS:HE3  | 1:E:180:ILE:HG21 | 1.96                     | 0.46              |
| 1:C:144:PHE:CE2  | 3:C:444:HOH:O    | 2.67                     | 0.46              |
| 1:C:160:ILE:C    | 3:C:408:HOH:O    | 2.58                     | 0.46              |
| 1:A:52:LEU:HB3   | 1:A:244:MET:HE1  | 1.96                     | 0.46              |
| 1:A:152:SER:N    | 3:A:437:HOH:O    | 2.44                     | 0.46              |
| 1:A:166:GLY:HA2  | 1:A:197:ILE:CD1  | 2.45                     | 0.46              |
| 1:C:194:ALA:C    | 3:C:377:HOH:O    | 2.59                     | 0.46              |
| 1:E:166:GLY:HA2  | 1:E:197:ILE:HD12 | 1.97                     | 0.46              |
| 1:A:26:ALA:HB2   | 3:A:394:HOH:O    | 2.15                     | 0.46              |
| 1:C:24:ASN:CB    | 3:C:374:HOH:O    | 2.36                     | 0.46              |
| 1:C:27:CYS:SG    | 3:C:449:HOH:O    | 2.61                     | 0.46              |
| 1:E:5:ARG:HD3    | 3:E:341:HOH:O    | 2.15                     | 0.46              |
| 1:E:110:LYS:HG2  | 3:E:314:HOH:O    | 2.15                     | 0.46              |
| 1:A:211:TYR:HD2  | 3:A:289:HOH:O    | 1.97                     | 0.46              |
| 1:C:41:ASP:OD2   | 1:C:43:SER:HB2   | 2.15                     | 0.46              |
| 1:C:153:HIS:HB3  | 3:C:347:HOH:O    | 2.03                     | 0.46              |
| 1:C:104:GLU:CA   | 3:C:380:HOH:O    | 2.64                     | 0.46              |
| 1:C:200:ASN:HB2  | 3:C:274:HOH:O    | 2.16                     | 0.46              |
| 1:E:74:SER:N     | 3:E:395:HOH:O    | 2.48                     | 0.46              |
| 1:C:207:PHE:CZ   | 1:C:235:LEU:HB2  | 2.51                     | 0.46              |
| 1:C:254:LYS:NZ   | 3:C:335:HOH:O    | 2.44                     | 0.46              |
| 1:A:44:HIS:C     | 2:B:459:ILE:HD11 | 2.40                     | 0.46              |
| 1:A:199:MET:HE2  | 1:A:202:PRO:HG3  | 1.96                     | 0.46              |
| 1:A:219:THR:C    | 3:A:354:HOH:O    | 2.59                     | 0.46              |
| 1:C:170:SER:HB3  | 1:C:179:ASN:CB   | 2.34                     | 0.46              |
| 1:A:52:LEU:HB3   | 1:A:244:MET:CE   | 2.46                     | 0.45              |
| 1:A:110:LYS:HE3  | 1:C:180:ILE:HG21 | 1.97                     | 0.45              |
| 1:A:166:GLY:HA2  | 1:A:197:ILE:HD12 | 1.98                     | 0.45              |
| 2:F:465:ARG:HG2  | 2:F:465:ARG:NH1  | 2.28                     | 0.45              |
| 1:E:23:ILE:C     | 3:E:397:HOH:O    | 2.60                     | 0.45              |
| 1:E:164:LYS:HA   | 1:E:199:MET:HE3  | 1.97                     | 0.45              |
| 1:A:1:MET:H3     | 1:A:63:ASP:HB2   | 1.82                     | 0.45              |
| 1:A:19:LEU:N     | 3:A:435:HOH:O    | 2.45                     | 0.45              |
| 1:A:62:CYS:C     | 3:A:359:HOH:O    | 2.58                     | 0.45              |
| 1:A:82:ALA:HA    | 3:A:412:HOH:O    | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:206:THR:OG1  | 2:B:453:ALA:HB2  | 2.16                     | 0.45              |
| 1:C:45:VAL:C     | 2:D:459:ILE:HG13 | 2.41                     | 0.45              |
| 1:C:128:ILE:HA   | 1:C:129:PRO:HD3  | 1.85                     | 0.45              |
| 1:E:71:ASN:C     | 1:E:71:ASN:HD22  | 2.23                     | 0.45              |
| 2:F:463:PHE:C    | 3:F:303:HOH:O    | 2.60                     | 0.45              |
| 1:C:119:MET:HE1  | 3:C:337:HOH:O    | 2.17                     | 0.45              |
| 1:E:38:GLN:HA    | 1:E:48:VAL:O     | 2.17                     | 0.45              |
| 1:E:149:ARG:O    | 1:E:152:SER:HB2  | 2.16                     | 0.45              |
| 1:E:170:SER:CB   | 3:E:387:HOH:O    | 2.64                     | 0.45              |
| 1:A:127:GLY:N    | 3:A:366:HOH:O    | 2.49                     | 0.45              |
| 1:C:166:GLY:HA2  | 1:C:197:ILE:CD1  | 2.46                     | 0.45              |
| 1:E:241:ILE:HG22 | 1:E:244:MET:HB2  | 1.99                     | 0.45              |
| 1:C:149:ARG:NH1  | 3:C:456:HOH:O    | 2.48                     | 0.45              |
| 1:E:246:HIS:HD2  | 1:E:248:LYS:HG3  | 1.81                     | 0.45              |
| 1:A:64:ARG:HD2   | 1:A:94:ASP:HB3   | 1.99                     | 0.45              |
| 1:A:45:VAL:HG13  | 2:B:456:GLN:NE2  | 2.32                     | 0.45              |
| 1:A:207:PHE:C    | 3:A:428:HOH:O    | 2.59                     | 0.45              |
| 1:C:61:ARG:NH1   | 3:C:396:HOH:O    | 2.49                     | 0.45              |
| 1:E:138:LYS:CA   | 3:E:426:HOH:O    | 2.63                     | 0.45              |
| 1:C:67:ALA:HA    | 3:C:449:HOH:O    | 2.16                     | 0.45              |
| 1:C:217:LYS:CG   | 3:C:387:HOH:O    | 2.64                     | 0.45              |
| 1:C:255:ILE:HD13 | 2:D:457:VAL:CG2  | 2.45                     | 0.45              |
| 1:E:71:ASN:ND2   | 3:E:395:HOH:O    | 2.50                     | 0.45              |
| 1:E:73:THR:CA    | 3:E:406:HOH:O    | 2.39                     | 0.45              |
| 1:C:91:ARG:CD    | 3:C:397:HOH:O    | 2.52                     | 0.44              |
| 1:C:235:LEU:HA   | 3:C:315:HOH:O    | 2.17                     | 0.44              |
| 1:E:26:ALA:HB3   | 3:E:353:HOH:O    | 2.16                     | 0.44              |
| 1:E:102:VAL:C    | 3:E:346:HOH:O    | 2.60                     | 0.44              |
| 1:C:217:LYS:CD   | 3:C:387:HOH:O    | 2.65                     | 0.44              |
| 1:E:12:LEU:CB    | 3:E:344:HOH:O    | 2.66                     | 0.44              |
| 1:E:176:GLY:CA   | 3:E:379:HOH:O    | 2.64                     | 0.44              |
| 1:A:41:ASP:OD2   | 1:A:43:SER:HB2   | 2.17                     | 0.44              |
| 1:A:246:HIS:HD2  | 1:A:248:LYS:HG3  | 1.82                     | 0.44              |
| 1:E:136:VAL:C    | 3:E:347:HOH:O    | 2.60                     | 0.44              |
| 1:E:137:VAL:CG1  | 1:E:139:MET:HE2  | 2.47                     | 0.44              |
| 1:A:205:LEU:HD11 | 1:A:230:SER:O    | 2.18                     | 0.44              |
| 1:C:158:VAL:HB   | 1:C:209:LEU:HD21 | 1.99                     | 0.44              |
| 1:C:164:LYS:HA   | 1:C:199:MET:HE3  | 1.98                     | 0.44              |
| 1:E:83:GLY:C     | 1:E:85:GLU:H     | 2.26                     | 0.44              |
| 1:E:105:ALA:O    | 3:E:383:HOH:O    | 2.21                     | 0.44              |
| 1:E:241:ILE:O    | 1:E:242:ALA:C    | 2.61                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:64:ARG:CG    | 3:C:351:HOH:O    | 2.54                     | 0.44              |
| 1:C:241:ILE:O    | 1:C:242:ALA:C    | 2.60                     | 0.44              |
| 1:E:255:ILE:HD13 | 2:F:457:VAL:CG2  | 2.44                     | 0.44              |
| 1:A:16:LEU:CD2   | 1:A:75:MET:HG2   | 2.48                     | 0.44              |
| 1:A:226:THR:HG21 | 3:A:410:HOH:O    | 2.17                     | 0.44              |
| 1:E:7:VAL:HG13   | 3:E:354:HOH:O    | 2.16                     | 0.44              |
| 1:A:140:PRO:HG3  | 1:A:192:GLU:O    | 2.17                     | 0.44              |
| 1:C:254:LYS:HB3  | 3:D:393:HOH:O    | 2.17                     | 0.44              |
| 1:E:246:HIS:CD2  | 1:E:248:LYS:HG3  | 2.53                     | 0.44              |
| 1:A:46:SER:HB2   | 1:A:250:TYR:O    | 2.18                     | 0.44              |
| 1:C:45:VAL:HG12  | 1:C:251:LEU:HD12 | 2.00                     | 0.44              |
| 1:A:26:ALA:CB    | 3:A:394:HOH:O    | 2.66                     | 0.44              |
| 1:A:228:SER:HB2  | 1:A:236:VAL:HB   | 1.98                     | 0.44              |
| 1:C:84:ASN:ND2   | 3:C:269:HOH:O    | 2.50                     | 0.44              |
| 1:C:140:PRO:CD   | 3:C:457:HOH:O    | 2.65                     | 0.44              |
| 1:A:21:ASP:HB2   | 3:A:388:HOH:O    | 2.17                     | 0.43              |
| 1:A:52:LEU:CD2   | 1:A:244:MET:HE2  | 2.42                     | 0.43              |
| 1:A:72:LEU:CD2   | 3:A:399:HOH:O    | 2.65                     | 0.43              |
| 1:A:158:VAL:HB   | 1:A:209:LEU:HD21 | 1.99                     | 0.43              |
| 1:A:164:LYS:HA   | 1:A:199:MET:HE3  | 1.99                     | 0.43              |
| 1:C:25:GLU:HG3   | 3:C:361:HOH:O    | 2.17                     | 0.43              |
| 1:E:176:GLY:N    | 3:E:379:HOH:O    | 2.49                     | 0.43              |
| 1:A:65:ASN:HB3   | 3:A:426:HOH:O    | 2.18                     | 0.43              |
| 1:C:115:GLU:HG2  | 3:C:376:HOH:O    | 2.18                     | 0.43              |
| 1:A:16:LEU:HD21  | 1:A:75:MET:SD    | 2.59                     | 0.43              |
| 1:A:38:GLN:HA    | 1:A:48:VAL:O     | 2.18                     | 0.43              |
| 1:A:197:ILE:CG2  | 3:A:396:HOH:O    | 2.47                     | 0.43              |
| 1:C:128:ILE:HG22 | 2:D:463:PHE:CE2  | 2.53                     | 0.43              |
| 2:D:454:ASN:C    | 2:D:454:ASN:ND2  | 2.77                     | 0.43              |
| 1:A:48:VAL:CG1   | 3:A:404:HOH:O    | 2.50                     | 0.43              |
| 1:A:146:ARG:HD3  | 1:A:149:ARG:NH2  | 2.33                     | 0.43              |
| 1:A:1:MET:H1     | 1:A:94:ASP:CG    | 2.26                     | 0.43              |
| 1:A:172:SER:CB   | 1:A:177:ASN:HB3  | 2.48                     | 0.43              |
| 1:A:246:HIS:CD2  | 1:A:248:LYS:HG3  | 2.53                     | 0.43              |
| 1:C:52:LEU:HB3   | 1:C:244:MET:CE   | 2.48                     | 0.43              |
| 1:C:16:LEU:HD21  | 1:C:75:MET:SD    | 2.59                     | 0.43              |
| 1:E:99:LEU:HD12  | 1:E:100:ALA:H    | 1.83                     | 0.43              |
| 1:E:108:GLN:O    | 1:E:108:GLN:HG3  | 2.18                     | 0.43              |
| 1:E:203:VAL:CG1  | 1:E:204:GLN:N    | 2.81                     | 0.43              |
| 1:A:16:LEU:CD2   | 1:A:79:LEU:HD12  | 2.28                     | 0.43              |
| 1:A:23:ILE:CA    | 3:A:343:HOH:O    | 2.28                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:225:VAL:HG13 | 3:A:406:HOH:O    | 2.19                     | 0.43              |
| 1:A:110:LYS:HA   | 1:C:181:LYS:O    | 2.18                     | 0.43              |
| 1:A:115:GLU:HG3  | 3:C:390:HOH:O    | 2.19                     | 0.43              |
| 1:C:11:ILE:HG12  | 3:C:388:HOH:O    | 2.12                     | 0.43              |
| 1:C:131:GLN:CB   | 3:C:426:HOH:O    | 2.35                     | 0.43              |
| 1:E:229:MET:HB2  | 3:E:409:HOH:O    | 2.18                     | 0.43              |
| 1:C:28:TRP:C     | 3:C:449:HOH:O    | 2.61                     | 0.43              |
| 1:C:199:MET:HE2  | 1:C:202:PRO:HG3  | 2.00                     | 0.43              |
| 1:A:207:PHE:CZ   | 1:A:235:LEU:HB2  | 2.54                     | 0.43              |
| 1:A:219:THR:N    | 1:A:220:PRO:HD2  | 2.33                     | 0.43              |
| 1:C:47:LEU:N     | 3:C:429:HOH:O    | 2.42                     | 0.43              |
| 1:C:160:ILE:CG2  | 3:C:408:HOH:O    | 2.51                     | 0.43              |
| 1:E:1:MET:N      | 1:E:94:ASP:OD2   | 2.50                     | 0.43              |
| 1:A:181:LYS:CA   | 3:A:393:HOH:O    | 2.67                     | 0.42              |
| 1:C:210:ARG:CB   | 3:C:367:HOH:O    | 2.65                     | 0.42              |
| 1:A:112:SER:HA   | 3:C:458:HOH:O    | 2.19                     | 0.42              |
| 1:C:219:THR:N    | 1:C:220:PRO:HD2  | 2.34                     | 0.42              |
| 1:C:253:PRO:O    | 3:C:372:HOH:O    | 2.20                     | 0.42              |
| 1:E:64:ARG:HD2   | 3:E:375:HOH:O    | 2.18                     | 0.42              |
| 1:E:135:CYS:SG   | 1:E:199:MET:HG2  | 2.59                     | 0.42              |
| 1:A:5:ARG:CB     | 1:A:59:THR:HB    | 2.42                     | 0.42              |
| 1:A:107:ASN:O    | 1:A:108:GLN:CB   | 2.66                     | 0.42              |
| 1:A:137:VAL:O    | 1:A:226:THR:HA   | 2.18                     | 0.42              |
| 1:A:241:ILE:O    | 1:A:244:MET:HB2  | 2.19                     | 0.42              |
| 1:C:129:PRO:HD2  | 3:C:309:HOH:O    | 2.18                     | 0.42              |
| 1:E:40:MET:HE1   | 1:E:44:HIS:ND1   | 2.35                     | 0.42              |
| 1:C:223:SER:HB3  | 3:C:338:HOH:O    | 2.19                     | 0.42              |
| 1:C:228:SER:HB2  | 1:C:236:VAL:HB   | 2.00                     | 0.42              |
| 1:E:64:ARG:HB3   | 1:E:94:ASP:OD1   | 2.19                     | 0.42              |
| 1:A:208:ALA:N    | 3:A:428:HOH:O    | 2.53                     | 0.42              |
| 1:C:246:HIS:CD2  | 1:C:248:LYS:HG3  | 2.55                     | 0.42              |
| 1:E:5:ARG:CB     | 1:E:59:THR:HB    | 2.42                     | 0.42              |
| 1:A:125:GLN:NE2  | 3:A:331:HOH:O    | 2.53                     | 0.42              |
| 1:A:199:MET:CE   | 1:A:202:PRO:HG3  | 2.50                     | 0.42              |
| 1:C:24:ASN:HB3   | 3:C:361:HOH:O    | 2.19                     | 0.42              |
| 1:C:203:VAL:HG12 | 1:C:204:GLN:N    | 2.33                     | 0.42              |
| 1:E:44:HIS:C     | 2:F:459:ILE:HD11 | 2.44                     | 0.42              |
| 1:E:116:MET:HG3  | 3:E:290:HOH:O    | 2.18                     | 0.42              |
| 1:C:103:PHE:CB   | 3:C:430:HOH:O    | 2.67                     | 0.42              |
| 1:C:110:LYS:HA   | 1:E:181:LYS:O    | 2.19                     | 0.42              |
| 1:C:217:LYS:HD2  | 3:C:387:HOH:O    | 2.20                     | 0.42              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:E:172:SER:CB   | 1:E:177:ASN:HB3 | 2.47                     | 0.42              |
| 1:A:12:LEU:HD12  | 1:A:12:LEU:HA   | 1.83                     | 0.42              |
| 1:A:25:GLU:HG3   | 3:A:352:HOH:O   | 2.19                     | 0.42              |
| 1:E:201:GLU:HG2  | 3:E:388:HOH:O   | 2.18                     | 0.42              |
| 1:A:64:ARG:HB3   | 1:A:94:ASP:OD1  | 2.19                     | 0.42              |
| 1:A:71:ASN:C     | 1:A:71:ASN:HD22 | 2.28                     | 0.42              |
| 1:A:96:ALA:HB1   | 1:A:98:THR:HG23 | 2.02                     | 0.42              |
| 1:A:203:VAL:CG1  | 1:A:204:GLN:N   | 2.83                     | 0.42              |
| 1:A:248:LYS:HB3  | 3:A:409:HOH:O   | 2.20                     | 0.42              |
| 1:C:60:TYR:O     | 1:C:61:ARG:HB2  | 2.19                     | 0.42              |
| 1:C:149:ARG:HD3  | 3:C:427:HOH:O   | 2.19                     | 0.42              |
| 1:E:106:PRO:HD2  | 3:E:350:HOH:O   | 2.19                     | 0.42              |
| 1:E:106:PRO:CB   | 3:E:350:HOH:O   | 2.57                     | 0.41              |
| 1:E:112:SER:HB3  | 1:E:114:TYR:HE1 | 1.86                     | 0.41              |
| 1:E:168:LYS:HD2  | 3:E:430:HOH:O   | 2.17                     | 0.41              |
| 1:A:11:ILE:O     | 1:A:15:VAL:HG23 | 2.21                     | 0.41              |
| 1:A:87:ILE:HG22  | 3:A:330:HOH:O   | 2.19                     | 0.41              |
| 1:E:169:PHE:CE1  | 3:E:367:HOH:O   | 2.73                     | 0.41              |
| 2:F:458:SER:HB3  | 3:F:517:HOH:O   | 2.20                     | 0.41              |
| 1:A:40:MET:N     | 3:A:383:HOH:O   | 2.38                     | 0.41              |
| 1:C:46:SER:HB2   | 3:C:429:HOH:O   | 2.20                     | 0.41              |
| 1:C:52:LEU:CD2   | 1:C:244:MET:HE2 | 2.38                     | 0.41              |
| 1:E:12:LEU:HD13  | 3:E:344:HOH:O   | 2.19                     | 0.41              |
| 1:A:164:LYS:HG2  | 3:A:328:HOH:O   | 2.21                     | 0.41              |
| 1:A:254:LYS:CB   | 3:B:271:HOH:O   | 2.61                     | 0.41              |
| 1:C:103:PHE:CD2  | 3:C:430:HOH:O   | 2.57                     | 0.41              |
| 1:E:68:MET:O     | 1:E:70:VAL:HG23 | 2.21                     | 0.41              |
| 1:E:128:ILE:HA   | 1:E:129:PRO:HD3 | 1.83                     | 0.41              |
| 1:E:144:PHE:N    | 3:E:427:HOH:O   | 2.53                     | 0.41              |
| 1:A:203:VAL:HG12 | 1:A:204:GLN:N   | 2.36                     | 0.41              |
| 1:A:241:ILE:O    | 1:A:242:ALA:C   | 2.63                     | 0.41              |
| 1:C:16:LEU:CD2   | 1:C:75:MET:HG2  | 2.50                     | 0.41              |
| 1:C:17:GLU:OE1   | 1:C:17:GLU:HA   | 2.20                     | 0.41              |
| 1:C:71:ASN:C     | 1:C:71:ASN:HD22 | 2.29                     | 0.41              |
| 1:C:131:GLN:CG   | 3:C:426:HOH:O   | 2.68                     | 0.41              |
| 1:A:64:ARG:NH1   | 3:A:365:HOH:O   | 2.53                     | 0.41              |
| 1:C:30:ILE:HG13  | 1:C:68:MET:HE3  | 2.02                     | 0.41              |
| 2:D:459:ILE:HD12 | 2:D:459:ILE:H   | 1.85                     | 0.41              |
| 1:E:1:MET:HB3    | 1:E:63:ASP:OD2  | 2.21                     | 0.41              |
| 1:E:256:GLU:C    | 3:E:374:HOH:O   | 2.64                     | 0.41              |
| 1:A:23:ILE:CG2   | 3:A:394:HOH:O   | 2.69                     | 0.41              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:17:GLU:HA   | 1:A:17:GLU:OE1  | 2.19                     | 0.41              |
| 1:A:148:CYS:C   | 3:A:437:HOH:O   | 2.63                     | 0.41              |
| 1:C:3:GLU:HB2   | 3:C:399:HOH:O   | 2.21                     | 0.41              |
| 1:C:131:GLN:CB  | 3:C:373:HOH:O   | 2.43                     | 0.41              |
| 1:C:248:LYS:CE  | 3:C:341:HOH:O   | 2.68                     | 0.41              |
| 1:E:115:GLU:HG2 | 3:E:340:HOH:O   | 2.21                     | 0.41              |
| 1:E:169:PHE:CD1 | 3:E:367:HOH:O   | 2.57                     | 0.41              |
| 1:C:203:VAL:HA  | 3:C:384:HOH:O   | 2.21                     | 0.41              |
| 1:E:218:ALA:O   | 1:E:221:LEU:HB2 | 2.21                     | 0.41              |
| 1:A:105:ALA:O   | 1:A:106:PRO:C   | 2.64                     | 0.40              |
| 1:C:205:LEU:CD2 | 3:C:391:HOH:O   | 2.68                     | 0.40              |
| 1:C:256:GLU:HA  | 3:C:385:HOH:O   | 2.20                     | 0.40              |
| 1:E:196:THR:N   | 3:E:434:HOH:O   | 2.54                     | 0.40              |
| 1:A:40:MET:HE1  | 1:A:44:HIS:ND1  | 2.37                     | 0.40              |
| 1:A:129:PRO:CG  | 2:B:463:PHE:HB3 | 2.51                     | 0.40              |
| 1:C:103:PHE:C   | 3:C:380:HOH:O   | 2.64                     | 0.40              |
| 1:E:12:LEU:HB2  | 3:E:344:HOH:O   | 2.21                     | 0.40              |
| 1:E:219:THR:N   | 1:E:220:PRO:HD2 | 2.35                     | 0.40              |
| 1:A:126:LEU:CD2 | 2:B:464:GLN:HA  | 2.52                     | 0.40              |
| 1:A:185:THR:OG1 | 1:A:194:ALA:HB1 | 2.21                     | 0.40              |
| 1:A:255:ILE:CG2 | 1:A:256:GLU:N   | 2.84                     | 0.40              |
| 1:E:112:SER:HB3 | 1:E:114:TYR:CE1 | 2.56                     | 0.40              |
| 1:E:202:PRO:CG  | 3:E:366:HOH:O   | 2.63                     | 0.40              |
| 1:C:49:GLN:O    | 3:C:431:HOH:O   | 2.22                     | 0.40              |
| 2:F:462:PHE:C   | 2:F:463:PHE:CD2 | 2.98                     | 0.40              |
| 1:A:124:GLU:C   | 3:A:370:HOH:O   | 2.64                     | 0.40              |
| 1:A:164:LYS:CG  | 3:A:328:HOH:O   | 2.69                     | 0.40              |
| 1:C:254:LYS:N   | 3:C:372:HOH:O   | 2.53                     | 0.40              |
| 2:F:465:ARG:NH1 | 2:F:465:ARG:CG  | 2.85                     | 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) |
|---------------|----------------------|--------------------------|-------------------|
| 1:E:8:GLN:NE2 | 1:E:8:GLN:NE2[5_674] | 1.61                     | 0.59              |
| 3:E:315:HOH:O | 3:E:360:HOH:O[5_674] | 2.17                     | 0.03              |

## 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     | 249/261 (95%) | 226 (91%) | 21 (8%) | 2 (1%)   | 16          | 34  |
| 1   | C     | 245/261 (94%) | 226 (92%) | 15 (6%) | 4 (2%)   | 7           | 16  |
| 1   | E     | 249/261 (95%) | 228 (92%) | 17 (7%) | 4 (2%)   | 7           | 16  |
| 2   | B     | 10/15 (67%)   | 9 (90%)   | 0       | 1 (10%)  | 0           | 0   |
| 2   | D     | 11/15 (73%)   | 10 (91%)  | 1 (9%)  | 0        | 100         | 100 |
| 2   | F     | 11/15 (73%)   | 10 (91%)  | 0       | 1 (9%)   | 0           | 0   |
| All | All   | 775/828 (94%) | 709 (92%) | 54 (7%) | 12 (2%)  | 8           | 18  |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 242 | ALA  |
| 1   | C     | 242 | ALA  |
| 1   | E     | 242 | ALA  |
| 2   | F     | 454 | ASN  |
| 1   | A     | 59  | THR  |
| 1   | C     | 59  | THR  |
| 1   | C     | 61  | ARG  |
| 2   | B     | 454 | ASN  |
| 1   | E     | 106 | PRO  |
| 1   | C     | 243 | ASP  |
| 1   | E     | 59  | THR  |
| 1   | E     | 243 | ASP  |

### 5.3.2 Protein sidechains [i](#)

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     | 217/228 (95%) | 212 (98%) | 5 (2%)   | 44          | 71 |
| 1   | C     | 216/228 (95%) | 211 (98%) | 5 (2%)   | 44          | 71 |
| 1   | E     | 217/228 (95%) | 211 (97%) | 6 (3%)   | 38          | 66 |
| 2   | B     | 10/13 (77%)   | 9 (90%)   | 1 (10%)  | 7           | 16 |
| 2   | D     | 11/13 (85%)   | 10 (91%)  | 1 (9%)   | 9           | 19 |
| 2   | F     | 11/13 (85%)   | 9 (82%)   | 2 (18%)  | 2           | 3  |
| All | All   | 682/723 (94%) | 662 (97%) | 20 (3%)  | 37          | 65 |

All (20) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 85  | GLU  |
| 1   | A     | 98  | THR  |
| 1   | A     | 192 | GLU  |
| 1   | A     | 224 | THR  |
| 1   | A     | 235 | LEU  |
| 2   | B     | 459 | ILE  |
| 1   | C     | 85  | GLU  |
| 1   | C     | 98  | THR  |
| 1   | C     | 192 | GLU  |
| 1   | C     | 224 | THR  |
| 1   | C     | 235 | LEU  |
| 2   | D     | 459 | ILE  |
| 1   | E     | 85  | GLU  |
| 1   | E     | 98  | THR  |
| 1   | E     | 106 | PRO  |
| 1   | E     | 107 | ASN  |
| 1   | E     | 224 | THR  |
| 1   | E     | 235 | LEU  |
| 2   | F     | 459 | ILE  |
| 2   | F     | 465 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 65  | ASN  |
| 1   | A     | 71  | ASN  |
| 1   | A     | 179 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 213 | ASN  |
| 2   | B     | 454 | ASN  |
| 2   | B     | 456 | GLN  |
| 2   | B     | 464 | GLN  |
| 1   | C     | 65  | ASN  |
| 1   | C     | 71  | ASN  |
| 1   | C     | 179 | ASN  |
| 1   | C     | 184 | GLN  |
| 1   | C     | 213 | ASN  |
| 2   | D     | 454 | ASN  |
| 2   | D     | 456 | GLN  |
| 1   | E     | 65  | ASN  |
| 1   | E     | 71  | ASN  |
| 1   | E     | 179 | ASN  |
| 1   | E     | 184 | GLN  |
| 1   | E     | 213 | ASN  |
| 2   | F     | 456 | GLN  |
| 2   | F     | 464 | GLN  |

### 5.3.3 RNA [i](#)

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 ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 253/261 (96%) | -0.51  | 0 100 100    | 33, 59, 100, 122      | 0     |
| 1   | C     | 251/261 (96%) | -0.52  | 0 100 100    | 35, 58, 99, 124       | 0     |
| 1   | E     | 253/261 (96%) | -0.57  | 0 100 100    | 35, 59, 100, 122      | 0     |
| 2   | B     | 12/15 (80%)   | -0.27  | 0 100 100    | 41, 66, 90, 99        | 0     |
| 2   | D     | 13/15 (86%)   | -0.37  | 0 100 100    | 40, 60, 101, 109      | 0     |
| 2   | F     | 13/15 (86%)   | -0.12  | 1 (7%) 19 15 | 41, 58, 109, 118      | 0     |
| All | All   | 795/828 (96%) | -0.52  | 1 (0%) 92 90 | 33, 59, 100, 124      | 0     |

All (1) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | F     | 453 | ALA  | 3.8  |

### 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.