



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:20 AM UTC

PDB ID : 3DPQ / pdb\_00003dpq  
Title : Crystal structure of the substrate binding domain of E. coli DnaK in complex with a long pyrrolic acid-derived inhibitor peptide (form B)  
Authors : Roujeinikova, A.  
Deposited on : 2008-07-09  
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:

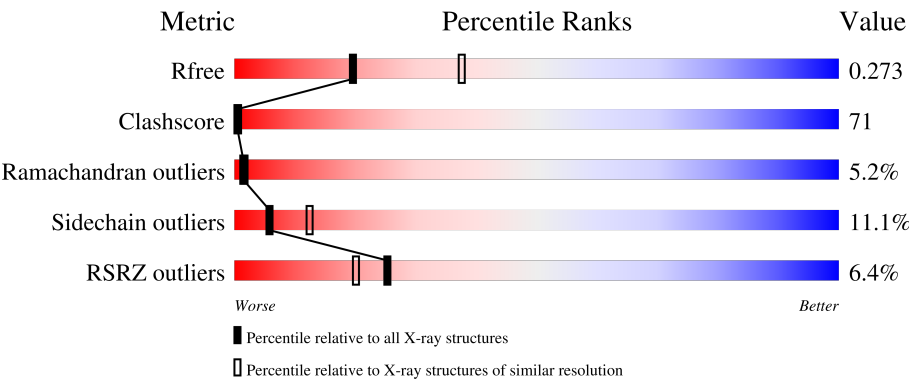
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| 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 i

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     | 219    | <div><div>3%</div><div>37%</div><div>47%</div><div>13%</div><div>.</div></div>               |
| 1   | B     | 219    | <div><div>7%</div><div>22%</div><div>60%</div><div>12%</div><div>..</div></div>              |
| 1   | E     | 219    | <div><div>5%</div><div>26%</div><div>53%</div><div>14%</div><div>7%</div></div>              |
| 1   | F     | 219    | <div><div>8%</div><div>26%</div><div>53%</div><div>17%</div><div>..</div></div>              |
| 2   | C     | 20     | <div><div>5%</div><div>40%</div><div>10%</div><div>5%</div><div>5%</div><div>40%</div></div> |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 2   | D     | 20     | <div><div></div><div></div><div></div><div></div></div> <div>20%25%55%</div>       |
| 2   | G     | 20     | <div><div></div><div></div><div></div><div></div></div> <div>15%15%25%20%40%</div> |
| 2   | H     | 20     | <div><div></div><div></div><div></div><div></div></div> <div>5%10%20%15%55%</div>  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8427 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 Chaperone protein dnaK.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 212      | Total | C    | N   | O   | S | 9       | 5       | 0     |
|     |       |          | 1644  | 1012 | 288 | 338 | 6 |         |         |       |
| 1   | B     | 212      | Total | C    | N   | O   | S | 9       | 5       | 0     |
|     |       |          | 1654  | 1018 | 293 | 337 | 6 |         |         |       |
| 1   | E     | 203      | Total | C    | N   | O   | S | 0       | 9       | 0     |
|     |       |          | 1626  | 999  | 292 | 329 | 6 |         |         |       |
| 1   | F     | 214      | Total | C    | N   | O   | S | 0       | 4       | 0     |
|     |       |          | 1647  | 1015 | 287 | 339 | 6 |         |         |       |

- Molecule 2 is a protein called inhibitor peptide.

| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 2   | C     | 12       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 105   | 72 | 19 | 14 |         |         |       |
| 2   | D     | 9        | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 80    | 56 | 13 | 11 |         |         |       |
| 2   | G     | 12       | Total | C  | N  | O  | 0       | 1       | 0     |
|     |       |          | 109   | 74 | 21 | 14 |         |         |       |
| 2   | H     | 9        | Total | C  | N  | O  | 11      | 1       | 0     |
|     |       |          | 91    | 62 | 17 | 12 |         |         |       |

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

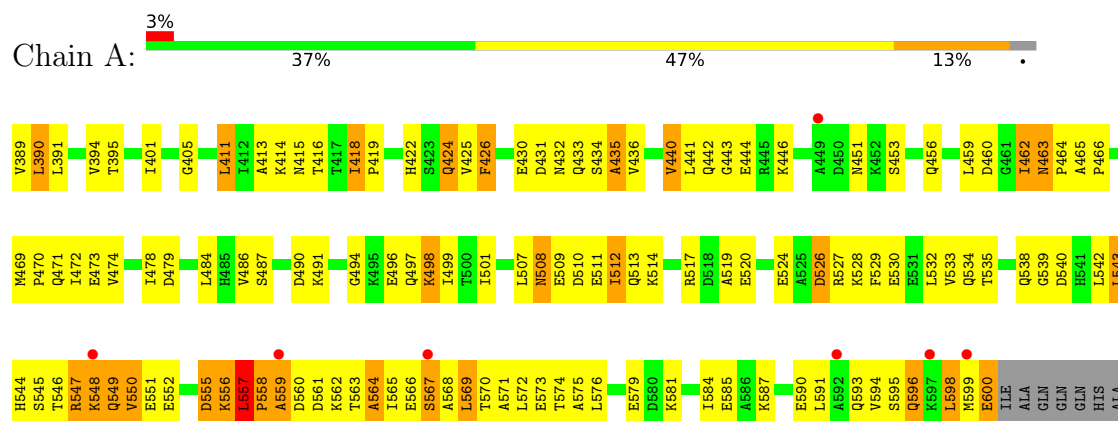
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4   | A     | 352      | Total | O   | 0       | 0       |
|     |       |          | 352   | 352 |         |         |
| 4   | B     | 308      | Total | O   | 0       | 0       |
|     |       |          | 308   | 308 |         |         |
| 4   | E     | 334      | Total | O   | 0       | 0       |
|     |       |          | 334   | 334 |         |         |
| 4   | F     | 334      | Total | O   | 0       | 0       |
|     |       |          | 334   | 334 |         |         |
| 4   | C     | 27       | Total | O   | 0       | 0       |
|     |       |          | 27    | 27  |         |         |
| 4   | D     | 36       | Total | O   | 0       | 0       |
|     |       |          | 36    | 36  |         |         |
| 4   | G     | 50       | Total | O   | 0       | 0       |
|     |       |          | 50    | 50  |         |         |
| 4   | H     | 25       | Total | O   | 0       | 0       |
|     |       |          | 25    | 25  |         |         |

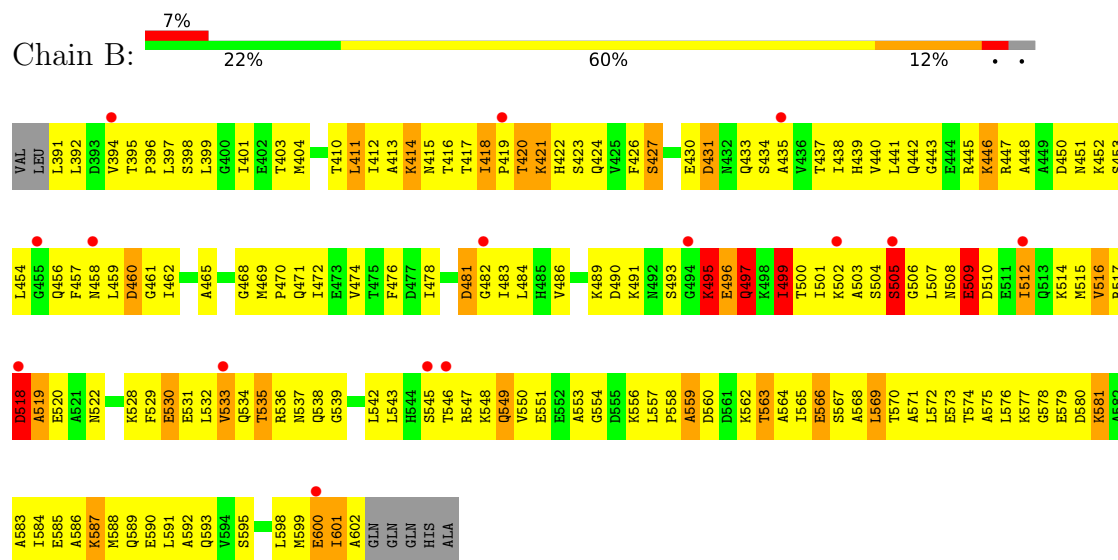
### 3 Residue-property plots

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.

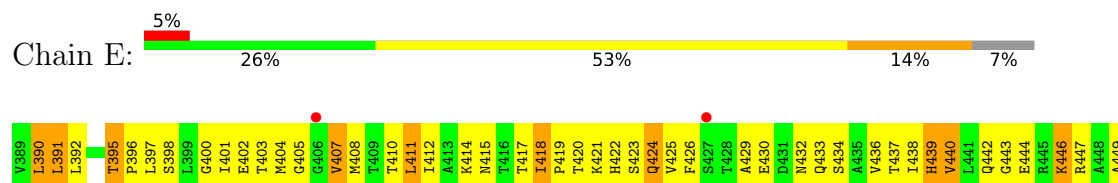
#### • Molecule 1: Chaperone protein dnaK

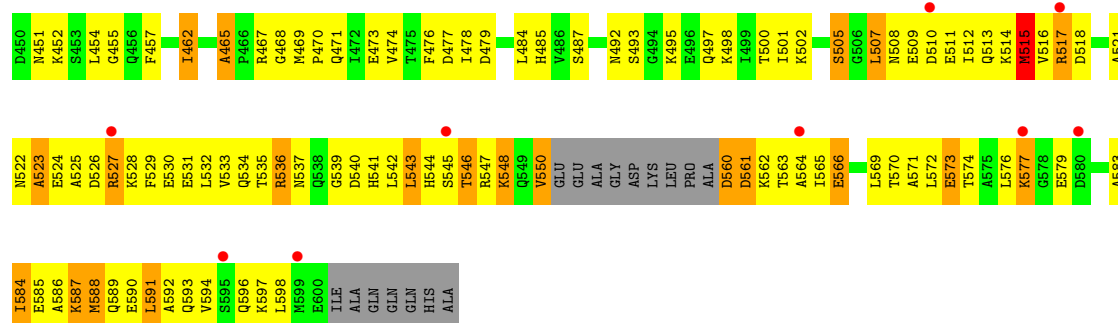


#### • Molecule 1: Chaperone protein dnaK

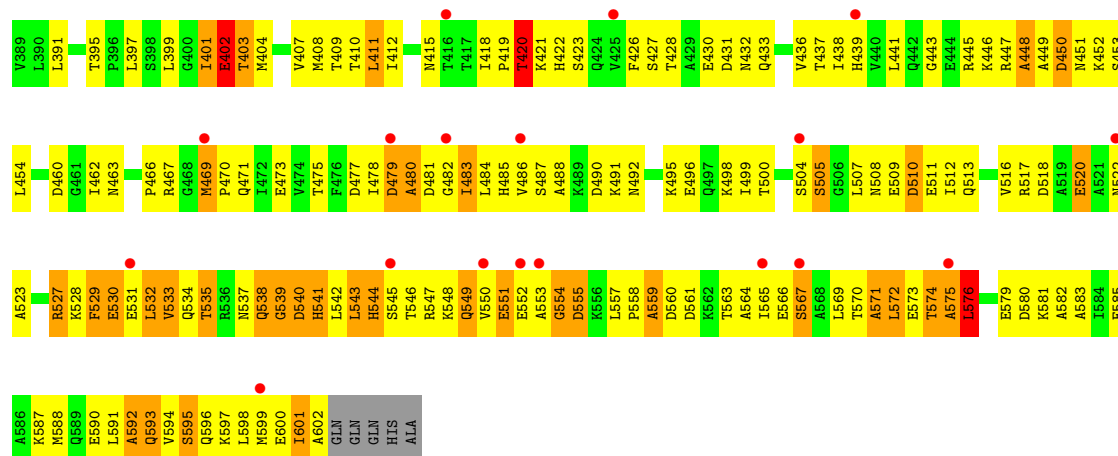


#### • Molecule 1: Chaperone protein dnaK





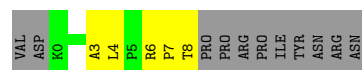
• Molecule 1: Chaperone protein dnaK



• Molecule 2: inhibitor peptide



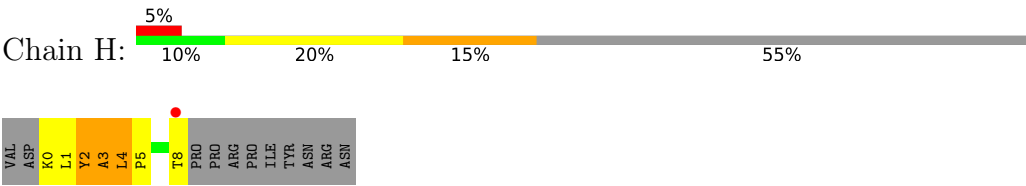
• Molecule 2: inhibitor peptide



• Molecule 2: inhibitor peptide



● Molecule 2: inhibitor peptide



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 77.71Å 91.65Å 154.80Å<br>90.00° 90.00° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 8.00 – 2.60<br>8.00 – 2.60                                  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 82.0 (8.00-2.60)<br>79.2 (8.00-2.60)                        | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.08                                                        | Depositor        |
| $R_{sym}$                                                               | 0.08                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.60 (at 1.94Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.4.0073                                             | Depositor        |
| R, $R_{free}$                                                           | 0.254 , 0.319<br>0.266 , 0.273                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3491 reflections (4.28%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 24.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.554                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.59 , 164.9                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.84                                                        | EDS              |
| Total number of atoms                                                   | 8427                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 24.0                                                        | 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 22.01 % 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 6.2189e-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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ALC

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     | 0.92         | 3/1658 (0.2%) | 1.30        | 15/2236 (0.7%) |
| 1   | B     | 0.81         | 0/1668        | 1.28        | 14/2243 (0.6%) |
| 1   | E     | 0.79         | 0/1638        | 1.28        | 13/2202 (0.6%) |
| 1   | F     | 0.78         | 0/1673        | 1.28        | 14/2253 (0.6%) |
| 2   | C     | 0.56         | 0/97          | 1.11        | 0/131          |
| 2   | D     | 0.74         | 0/70          | 1.14        | 2/93 (2.2%)    |
| 2   | G     | 0.62         | 0/104         | 2.34        | 5/142 (3.5%)   |
| 2   | H     | 0.68         | 0/81          | 1.44        | 2/108 (1.9%)   |
| All | All   | 0.82         | 3/6989 (0.0%) | 1.30        | 65/9408 (0.7%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 1                   | 0                   |
| 1   | B     | 0                   | 2                   |
| 2   | C     | 0                   | 1                   |
| 2   | G     | 0                   | 1                   |
| 2   | H     | 0                   | 1                   |
| All | All   | 1                   | 5                   |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 547 | ARG  | CA-C  | -5.36 | 1.46        | 1.53     |
| 1   | A     | 508 | ASN  | N-CA  | 5.20  | 1.51        | 1.46     |
| 1   | A     | 426 | PHE  | CA-C  | -5.12 | 1.46        | 1.52     |

All (65) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 2   | G     | 9   | PRO  | CA-C-N    | 16.43  | 140.38      | 119.84   |
| 2   | G     | 9   | PRO  | C-N-CA    | 16.43  | 140.38      | 119.84   |
| 1   | B     | 497 | GLN  | N-CA-C    | 11.05  | 125.38      | 110.35   |
| 1   | A     | 547 | ARG  | N-CA-C    | -10.34 | 97.15       | 112.04   |
| 1   | B     | 496 | GLU  | N-CA-C    | 9.51   | 125.77      | 111.04   |
| 1   | F     | 539 | GLY  | N-CA-C    | -9.11  | 104.64      | 114.67   |
| 2   | H     | 4   | LEU  | CA-C-N    | -8.42  | 109.32      | 119.84   |
| 2   | H     | 4   | LEU  | C-N-CA    | -8.42  | 109.32      | 119.84   |
| 1   | A     | 598 | LEU  | N-CA-C    | -8.08  | 102.05      | 112.23   |
| 1   | B     | 518 | ASP  | CB-CG-OD2 | 7.46   | 135.56      | 118.40   |
| 1   | A     | 463 | ASN  | CA-C-N    | -7.27  | 112.15      | 119.93   |
| 1   | A     | 463 | ASN  | C-N-CA    | -7.27  | 112.15      | 119.93   |
| 1   | E     | 395 | THR  | CA-C-N    | 7.17   | 126.81      | 119.56   |
| 1   | E     | 395 | THR  | C-N-CA    | 7.17   | 126.81      | 119.56   |
| 1   | B     | 505 | SER  | N-CA-C    | 7.14   | 120.93      | 109.86   |
| 1   | A     | 560 | ASP  | N-CA-C    | -7.14  | 104.45      | 113.02   |
| 1   | E     | 591 | LEU  | N-CA-C    | -7.05  | 103.60      | 111.71   |
| 1   | E     | 536 | ARG  | N-CA-C    | -6.93  | 103.66      | 111.07   |
| 1   | A     | 569 | LEU  | N-CA-C    | -6.82  | 104.44      | 112.89   |
| 1   | E     | 527 | ARG  | N-CA-C    | -6.78  | 104.98      | 113.18   |
| 1   | E     | 566 | GLU  | N-CA-C    | -6.73  | 104.33      | 112.54   |
| 1   | E     | 594 | VAL  | N-CA-C    | -6.54  | 106.31      | 113.43   |
| 1   | F     | 576 | LEU  | N-CA-C    | -6.47  | 104.96      | 112.92   |
| 1   | B     | 569 | LEU  | N-CA-C    | -6.46  | 104.16      | 111.14   |
| 1   | B     | 518 | ASP  | CB-CG-OD1 | -6.36  | 103.77      | 118.40   |
| 1   | A     | 494 | GLY  | N-CA-C    | -6.35  | 106.47      | 115.30   |
| 2   | G     | 4   | LEU  | CA-C-N    | -6.33  | 113.76      | 120.66   |
| 2   | G     | 4   | LEU  | C-N-CA    | -6.33  | 113.76      | 120.66   |
| 1   | F     | 527 | ARG  | N-CA-C    | -6.30  | 105.55      | 113.18   |
| 1   | B     | 481 | ASP  | N-CA-C    | -6.18  | 105.50      | 113.16   |
| 1   | B     | 587 | LYS  | N-CA-C    | -6.13  | 104.90      | 112.38   |
| 1   | A     | 456 | GLN  | N-CA-C    | 6.08   | 118.03      | 108.96   |
| 1   | F     | 410 | THR  | N-CA-C    | 6.04   | 118.24      | 108.34   |
| 1   | E     | 390 | LEU  | N-CA-C    | -5.86  | 106.30      | 113.50   |
| 1   | B     | 512 | ILE  | N-CA-C    | -5.84  | 105.04      | 110.53   |
| 1   | F     | 549 | GLN  | N-CA-C    | -5.84  | 105.25      | 112.38   |
| 1   | A     | 512 | ILE  | N-CA-C    | -5.81  | 105.14      | 110.78   |
| 1   | E     | 571 | ALA  | N-CA-C    | -5.77  | 106.41      | 113.50   |
| 1   | E     | 465 | ALA  | N-CA-C    | 5.73   | 113.29      | 108.13   |
| 2   | D     | 4   | LEU  | CA-C-N    | 5.73   | 125.71      | 120.21   |
| 2   | D     | 4   | LEU  | C-N-CA    | 5.73   | 125.71      | 120.21   |
| 1   | F     | 402 | GLU  | N-CA-C    | 5.57   | 115.63      | 108.34   |
| 1   | F     | 480 | ALA  | N-CA-C    | -5.51  | 105.66      | 112.38   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 435 | ALA  | N-CA-C   | 5.42  | 116.69      | 108.07   |
| 1   | F     | 535 | THR  | N-CA-C   | -5.42 | 105.48      | 111.71   |
| 1   | E     | 587 | LYS  | N-CA-C   | -5.32 | 105.64      | 111.82   |
| 1   | A     | 585 | GLU  | N-CA-C   | -5.31 | 105.66      | 111.82   |
| 1   | A     | 547 | ARG  | O-C-N    | 5.25  | 129.39      | 122.30   |
| 1   | F     | 567 | SER  | N-CA-C   | -5.23 | 106.76      | 112.72   |
| 1   | F     | 510 | ASP  | N-CA-C   | -5.23 | 105.75      | 111.82   |
| 2   | G     | 9   | PRO  | C-N-CD   | -5.20 | 103.67      | 125.00   |
| 1   | B     | 519 | ALA  | N-CA-C   | -5.20 | 105.30      | 111.69   |
| 1   | A     | 440 | VAL  | CB-CA-C  | -5.17 | 103.98      | 111.68   |
| 1   | B     | 422 | HIS  | N-CA-C   | 5.15  | 116.89      | 108.55   |
| 1   | B     | 518 | ASP  | CA-CB-CG | -5.15 | 107.45      | 112.60   |
| 1   | A     | 555 | ASP  | N-CA-C   | -5.13 | 104.19      | 110.65   |
| 1   | F     | 540 | ASP  | N-CA-C   | -5.11 | 106.13      | 112.93   |
| 1   | A     | 568 | ALA  | N-CA-C   | -5.09 | 105.82      | 112.23   |
| 1   | F     | 450 | ASP  | N-CA-C   | -5.09 | 107.05      | 114.12   |
| 1   | E     | 577 | LYS  | N-CA-C   | -5.07 | 107.05      | 113.18   |
| 1   | B     | 548 | LYS  | N-CA-C   | -5.05 | 105.85      | 111.36   |
| 1   | F     | 582 | ALA  | N-CA-C   | -5.04 | 105.97      | 111.82   |
| 1   | F     | 420 | THR  | N-CA-C   | 5.04  | 116.47      | 108.96   |
| 1   | E     | 515 | MET  | N-CA-C   | -5.03 | 105.88      | 111.36   |
| 1   | B     | 499 | ILE  | N-CA-C   | 5.02  | 114.66      | 108.53   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | A     | 548 | LYS  | CA   |

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | B     | 495 | LYS  | Peptide   |
| 1   | B     | 496 | GLU  | Peptide   |
| 2   | C     | 3   | ALC  | Mainchain |
| 2   | G     | 2   | TYR  | Mainchain |
| 2   | H     | 2   | TYR  | Mainchain |

## 5.2 Too-close contacts [i](#)

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     | 1644  | 0        | 1651     | 198     | 0            |
| 1   | B     | 1654  | 0        | 1679     | 264     | 1            |
| 1   | E     | 1626  | 0        | 1649     | 257     | 1            |
| 1   | F     | 1647  | 0        | 1673     | 257     | 0            |
| 2   | C     | 105   | 0        | 121      | 6       | 0            |
| 2   | D     | 80    | 0        | 94       | 4       | 0            |
| 2   | G     | 109   | 0        | 123      | 15      | 0            |
| 2   | H     | 91    | 0        | 106      | 6       | 0            |
| 3   | E     | 5     | 0        | 0        | 0       | 0            |
| 4   | A     | 352   | 0        | 0        | 10      | 0            |
| 4   | B     | 308   | 0        | 0        | 12      | 0            |
| 4   | C     | 27    | 0        | 0        | 0       | 0            |
| 4   | D     | 36    | 0        | 0        | 2       | 0            |
| 4   | E     | 334   | 0        | 0        | 13      | 0            |
| 4   | F     | 334   | 0        | 0        | 6       | 0            |
| 4   | G     | 50    | 0        | 0        | 1       | 0            |
| 4   | H     | 25    | 0        | 0        | 0       | 0            |
| All | All   | 8427  | 0        | 7096     | 991     | 1            |

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 (991) 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:438[B]:ILE:HG21 | 1:E:457:PHE:CE1    | 1.32                     | 1.63              |
| 1:E:438[B]:ILE:CG2  | 1:E:457:PHE:CE1    | 1.94                     | 1.45              |
| 1:E:438[B]:ILE:HG21 | 1:E:457:PHE:CZ     | 1.53                     | 1.41              |
| 1:E:434:SER:O       | 1:E:462:ILE:HG22   | 1.26                     | 1.30              |
| 1:B:536:ARG:NH2     | 1:B:578:GLY:O      | 1.73                     | 1.20              |
| 1:B:484:LEU:HD23    | 1:B:501:ILE:HD12   | 1.21                     | 1.17              |
| 1:E:414:LYS:HD3     | 1:E:444:GLU:OE1    | 1.43                     | 1.16              |
| 1:E:408:MET:SD      | 1:E:451:ASN:ND2    | 2.20                     | 1.14              |
| 1:F:531[B]:GLU:OE1  | 1:F:534:GLN:NE2    | 1.81                     | 1.14              |
| 1:B:584:ILE:HG22    | 1:B:588:MET:HE3    | 1.28                     | 1.14              |
| 1:B:499:ILE:HG13    | 1:B:500:THR:H      | 0.99                     | 1.13              |
| 1:E:402:GLU:HB3     | 1:E:439:HIS:ND1    | 1.64                     | 1.11              |
| 1:E:513:GLN:O       | 1:E:517[B]:ARG:HD2 | 1.49                     | 1.11              |
| 1:F:520:GLU:OE1     | 1:F:520:GLU:O      | 1.68                     | 1.11              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:F:572:LEU:O      | 1:F:572:LEU:HD12   | 1.48                     | 1.09              |
| 1:A:557:LEU:HB3    | 1:A:558:PRO:HD2    | 1.28                     | 1.09              |
| 1:A:559:ALA:HA     | 1:A:562:LYS:CG     | 1.81                     | 1.09              |
| 1:F:553:ALA:HB1    | 1:F:601:ILE:CG2    | 1.80                     | 1.09              |
| 1:E:434:SER:C      | 1:E:462:ILE:HG22   | 1.77                     | 1.09              |
| 1:A:564:ALA:HB1    | 1:A:594:VAL:HB     | 1.35                     | 1.08              |
| 1:A:559:ALA:HA     | 1:A:562:LYS:HG2    | 1.28                     | 1.07              |
| 2:G:6[A]:ARG:HH22  | 2:G:9:PRO:HB3      | 1.14                     | 1.07              |
| 1:A:563:THR:HG23   | 1:A:564:ALA:N      | 1.66                     | 1.07              |
| 1:F:437:THR:HG21   | 1:F:439:HIS:CE1    | 1.89                     | 1.06              |
| 1:A:600:GLU:OE1    | 1:A:600:GLU:HA     | 1.53                     | 1.06              |
| 1:B:571:ALA:HB1    | 1:B:587:LYS:HD2    | 1.33                     | 1.05              |
| 1:A:508:ASN:O      | 1:A:512:ILE:HG13   | 1.55                     | 1.04              |
| 1:A:547:ARG:O      | 1:A:550:VAL:HB     | 1.55                     | 1.04              |
| 1:F:539:GLY:O      | 1:F:543:LEU:HB3    | 1.56                     | 1.04              |
| 1:A:564:ALA:CB     | 1:A:594:VAL:HB     | 1.87                     | 1.04              |
| 1:F:466:PRO:HD2    | 1:F:469:MET:SD     | 1.97                     | 1.03              |
| 1:E:543:LEU:O      | 1:E:547:ARG:HG3    | 1.59                     | 1.02              |
| 1:A:563:THR:CG2    | 1:A:564:ALA:H      | 1.72                     | 1.02              |
| 1:E:513:GLN:O      | 1:E:517[A]:ARG:HD3 | 1.60                     | 1.01              |
| 1:A:559:ALA:HB2    | 1:A:562:LYS:HE2    | 1.38                     | 1.01              |
| 1:E:438[B]:ILE:CG2 | 1:E:457:PHE:CD1    | 2.42                     | 1.01              |
| 1:F:553:ALA:HB1    | 1:F:601:ILE:HG22   | 1.39                     | 1.01              |
| 1:B:550:VAL:HG13   | 1:B:557:LEU:CD2    | 1.90                     | 1.01              |
| 1:B:499:ILE:CG1    | 1:B:500:THR:H      | 1.74                     | 1.00              |
| 1:F:543:LEU:HG     | 1:F:543:LEU:O      | 1.54                     | 1.00              |
| 1:B:584:ILE:HG22   | 1:B:588:MET:CE     | 1.92                     | 1.00              |
| 1:E:550:VAL:HG13   | 1:E:598:LEU:HD21   | 1.42                     | 0.99              |
| 1:B:442:GLN:OE1    | 1:B:506:GLY:HA3    | 1.61                     | 0.98              |
| 1:A:557:LEU:HB3    | 1:A:558:PRO:CD     | 1.92                     | 0.98              |
| 1:F:542:LEU:HD23   | 1:F:591:LEU:HD23   | 1.42                     | 0.97              |
| 1:A:595:SER:O      | 1:A:596:GLN:C      | 2.07                     | 0.97              |
| 1:B:569:LEU:HD12   | 1:B:591:LEU:CD1    | 1.94                     | 0.97              |
| 1:A:559:ALA:HB2    | 1:A:562:LYS:CE     | 1.95                     | 0.96              |
| 1:F:446[B]:LYS:CE  | 1:F:530:GLU:OE1    | 2.13                     | 0.96              |
| 1:F:574:THR:HG22   | 1:F:575:ALA:N      | 1.81                     | 0.96              |
| 1:B:569:LEU:HD12   | 1:B:591:LEU:HD11   | 1.45                     | 0.96              |
| 1:B:572:LEU:HD11   | 1:B:588:MET:HE2    | 1.46                     | 0.95              |
| 1:A:559:ALA:CB     | 1:A:562:LYS:HE2    | 1.96                     | 0.95              |
| 1:E:443:GLY:HA3    | 1:E:515:MET:HE3    | 1.49                     | 0.95              |
| 1:B:499:ILE:HG13   | 1:B:500:THR:N      | 1.75                     | 0.94              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:B:550:VAL:HG13    | 1:B:557:LEU:HD22    | 1.47                     | 0.94              |
| 1:B:595:SER:HB3     | 1:B:599:MET:CE      | 1.97                     | 0.94              |
| 1:F:528:LYS:C       | 1:F:530:GLU:H       | 1.69                     | 0.94              |
| 1:B:535:THR:HA      | 1:B:538:GLN:OE1     | 1.68                     | 0.93              |
| 1:F:447:ARG:C       | 1:F:449:ALA:H       | 1.75                     | 0.92              |
| 1:B:546:THR:HG21    | 1:B:569:LEU:HD11    | 1.52                     | 0.92              |
| 1:B:502[C]:LYS:O    | 1:B:505:SER:HB2     | 1.69                     | 0.92              |
| 1:E:562:LYS:HA      | 1:E:565:ILE:HD12    | 1.52                     | 0.91              |
| 1:F:574:THR:C       | 1:F:576:LEU:H       | 1.76                     | 0.91              |
| 2:G:6[A]:ARG:NH2    | 2:G:9:PRO:HB3       | 1.85                     | 0.91              |
| 1:F:401:ILE:HG13    | 1:F:402:GLU:N       | 1.83                     | 0.91              |
| 1:B:502[B]:LYS:O    | 1:B:505:SER:HB2     | 1.69                     | 0.91              |
| 2:G:6[A]:ARG:HH12   | 2:G:9:PRO:HD3       | 1.36                     | 0.91              |
| 1:F:553:ALA:CB      | 1:F:601:ILE:HG22    | 1.99                     | 0.90              |
| 1:E:507:LEU:HD13    | 1:E:511:GLU:HB3     | 1.53                     | 0.90              |
| 1:B:502[A]:LYS:O    | 1:B:505:SER:HB2     | 1.71                     | 0.90              |
| 1:B:572:LEU:HD11    | 1:B:588:MET:CE      | 2.01                     | 0.90              |
| 1:B:595:SER:HB3     | 1:B:599:MET:HE2     | 1.51                     | 0.90              |
| 1:E:497:GLN:HE21    | 1:E:498:LYS:H       | 1.15                     | 0.90              |
| 1:B:499:ILE:CG1     | 1:B:500:THR:N       | 2.33                     | 0.89              |
| 1:A:559:ALA:O       | 1:A:563:THR:HB      | 1.72                     | 0.89              |
| 1:B:472:ILE:HD11    | 4:B:784:HOH:O       | 1.71                     | 0.89              |
| 1:E:411[B]:LEU:HD13 | 1:E:476:PHE:CE1     | 2.08                     | 0.89              |
| 1:E:589:GLN:OE1     | 1:E:589:GLN:HA      | 1.72                     | 0.89              |
| 1:A:559:ALA:CB      | 1:A:562:LYS:CE      | 2.50                     | 0.89              |
| 1:E:405:GLY:HA3     | 1:E:533:VAL:CG1     | 2.02                     | 0.89              |
| 1:B:584:ILE:CG2     | 1:B:588:MET:HE3     | 2.03                     | 0.89              |
| 1:E:561:ASP:O       | 1:E:565:ILE:HG13    | 1.73                     | 0.89              |
| 1:F:430:GLU:OE1     | 1:F:544:HIS:CD2     | 2.25                     | 0.88              |
| 1:A:547:ARG:O       | 1:A:550:VAL:CB      | 2.21                     | 0.88              |
| 1:F:513:GLN:HG2     | 1:F:517:ARG:NH2     | 1.88                     | 0.88              |
| 1:F:401:ILE:HG13    | 1:F:402:GLU:H       | 1.36                     | 0.88              |
| 1:A:565:ILE:CD1     | 1:A:594:VAL:O       | 2.22                     | 0.87              |
| 1:A:459:LEU:HD23    | 1:A:472[B]:ILE:HD12 | 1.57                     | 0.87              |
| 1:E:418:ILE:HG22    | 1:E:420:THR:HG22    | 1.56                     | 0.87              |
| 1:E:584:ILE:HG22    | 1:E:588:MET:HE3     | 1.58                     | 0.86              |
| 1:A:564:ALA:HB1     | 1:A:594:VAL:CB      | 2.06                     | 0.86              |
| 1:E:434:SER:C       | 1:E:462:ILE:CG2     | 2.48                     | 0.86              |
| 1:E:438[B]:ILE:CG2  | 1:E:457:PHE:CZ      | 2.42                     | 0.86              |
| 1:F:443:GLY:HA3     | 1:F:451:ASN:OD1     | 1.76                     | 0.86              |
| 1:F:596:GLN:O       | 1:F:600:GLU:OE1     | 1.94                     | 0.86              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:E:539:GLY:HA3     | 1:E:588:MET:HE2     | 1.57                     | 0.85              |
| 1:F:542:LEU:CD2     | 1:F:591:LEU:HD23    | 2.05                     | 0.85              |
| 1:E:438[B]:ILE:HG23 | 1:E:457:PHE:CE1     | 2.12                     | 0.85              |
| 1:A:559:ALA:CA      | 1:A:562:LYS:HG2     | 2.06                     | 0.85              |
| 1:E:517[A]:ARG:HH11 | 1:E:517[A]:ARG:HB2  | 1.39                     | 0.85              |
| 1:F:528:LYS:C       | 1:F:530:GLU:N       | 2.33                     | 0.85              |
| 1:A:484:LEU:HD23    | 1:A:501[A]:ILE:HD12 | 1.58                     | 0.85              |
| 2:G:6[A]:ARG:HH22   | 2:G:9:PRO:CB        | 1.89                     | 0.84              |
| 1:E:401:ILE:HD11    | 1:E:426:PHE:CZ      | 2.11                     | 0.84              |
| 1:E:438[B]:ILE:HG22 | 1:E:457:PHE:CD1     | 2.12                     | 0.84              |
| 1:F:553:ALA:HB1     | 1:F:601:ILE:HG21    | 1.57                     | 0.84              |
| 1:F:576:LEU:HD13    | 1:F:576:LEU:O       | 1.77                     | 0.84              |
| 1:A:558:PRO:HG2     | 1:A:561:ASP:HB2     | 1.60                     | 0.84              |
| 1:E:433:GLN:HE21    | 1:E:436:VAL:HG12    | 1.42                     | 0.84              |
| 1:A:595:SER:O       | 1:A:596:GLN:O       | 1.93                     | 0.84              |
| 1:A:565:ILE:HD11    | 1:A:595:SER:HA      | 1.59                     | 0.84              |
| 1:F:574:THR:O       | 1:F:576:LEU:N       | 2.11                     | 0.84              |
| 1:A:559:ALA:CA      | 1:A:562:LYS:HE2     | 2.06                     | 0.84              |
| 1:F:402:GLU:HG3     | 1:F:403:THR:N       | 1.90                     | 0.83              |
| 1:A:563:THR:HG23    | 1:A:564:ALA:H       | 1.27                     | 0.83              |
| 1:A:543:LEU:HD13    | 1:A:572:LEU:HD23    | 1.60                     | 0.83              |
| 1:F:437:THR:CG2     | 1:F:439:HIS:CE1     | 2.60                     | 0.83              |
| 1:A:548:LYS:C       | 1:A:550:VAL:H       | 1.87                     | 0.83              |
| 1:A:529:PHE:O       | 1:A:533:VAL:HG23    | 1.79                     | 0.82              |
| 1:E:550:VAL:HG13    | 1:E:598:LEU:CD2     | 2.09                     | 0.82              |
| 1:F:532:LEU:O       | 1:F:534:GLN:N       | 2.12                     | 0.82              |
| 1:E:402:GLU:HG2     | 1:E:439:HIS:CE1     | 2.15                     | 0.82              |
| 1:F:446[B]:LYS:HE2  | 1:F:530:GLU:OE1     | 1.79                     | 0.82              |
| 1:F:588:MET:O       | 1:F:591:LEU:HB3     | 1.78                     | 0.82              |
| 1:F:570:THR:C       | 1:F:572:LEU:H       | 1.88                     | 0.82              |
| 2:C:10:PRO:HG2      | 2:C:11:ARG:HG2      | 1.62                     | 0.81              |
| 1:B:569:LEU:CD1     | 1:B:591:LEU:HD11    | 2.09                     | 0.81              |
| 1:B:554:GLY:C       | 1:B:556:LYS:H       | 1.86                     | 0.81              |
| 1:B:503:ALA:C       | 1:B:505:SER:H       | 1.88                     | 0.81              |
| 1:E:447[A]:ARG:HG2  | 1:E:529:PHE:CD2     | 2.16                     | 0.81              |
| 1:E:533:VAL:HG21    | 4:E:1169:HOH:O      | 1.80                     | 0.81              |
| 1:F:597:LYS:O       | 1:F:601:ILE:HG12    | 1.81                     | 0.80              |
| 1:A:559:ALA:HA      | 1:A:562:LYS:CE      | 2.12                     | 0.80              |
| 1:B:440:VAL:HG11    | 1:B:501:ILE:HD11    | 1.63                     | 0.80              |
| 1:F:531[B]:GLU:CD   | 1:F:534:GLN:HE22    | 1.88                     | 0.80              |
| 1:F:538:GLN:HA      | 1:F:541:HIS:CG      | 2.17                     | 0.80              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:F:549:GLN:OE1   | 1:F:598:LEU:CD2     | 2.29                     | 0.80              |
| 1:A:513[B]:GLN:O  | 1:A:517:ARG:HG3     | 1.82                     | 0.80              |
| 1:E:402:GLU:HG2   | 1:E:439:HIS:HE1     | 1.46                     | 0.80              |
| 1:E:405:GLY:HA3   | 1:E:533:VAL:HG11    | 1.63                     | 0.80              |
| 1:E:443:GLY:CA    | 1:E:515:MET:HE3     | 2.12                     | 0.80              |
| 1:E:543:LEU:O     | 1:E:547:ARG:CG      | 2.30                     | 0.80              |
| 1:B:602:ALA:HB1   | 1:F:495:LYS:HE3     | 1.64                     | 0.79              |
| 1:B:404:MET:HE1   | 2:C:3:ALC:HD22      | 1.63                     | 0.79              |
| 1:B:427:SER:HB3   | 1:B:468:GLY:HA2     | 1.65                     | 0.79              |
| 1:E:514:LYS:O     | 1:E:518:ASP:CG      | 2.26                     | 0.79              |
| 1:E:402:GLU:CG    | 1:E:439:HIS:CE1     | 2.65                     | 0.79              |
| 1:F:558:PRO:C     | 1:F:560:ASP:H       | 1.88                     | 0.78              |
| 1:E:562:LYS:C     | 1:E:564:ALA:H       | 1.91                     | 0.78              |
| 1:F:532:LEU:O     | 1:F:535:THR:N       | 2.17                     | 0.78              |
| 2:C:10:PRO:O      | 2:C:11:ARG:HB2      | 1.82                     | 0.78              |
| 1:F:572:LEU:HD12  | 1:F:572:LEU:C       | 2.09                     | 0.78              |
| 1:B:543:LEU:C     | 1:B:543:LEU:HD23    | 2.09                     | 0.77              |
| 1:A:548:LYS:O     | 1:A:550:VAL:N       | 2.16                     | 0.77              |
| 1:A:565:ILE:HD13  | 1:A:594:VAL:HG23    | 1.66                     | 0.77              |
| 1:F:446[B]:LYS:NZ | 1:F:530:GLU:OE1     | 2.17                     | 0.77              |
| 1:B:543:LEU:HD21  | 1:B:547:ARG:HH11    | 1.49                     | 0.77              |
| 1:F:508:ASN:OD1   | 1:F:511:GLU:HG3     | 1.85                     | 0.77              |
| 1:A:414:LYS:O     | 1:A:415:ASN:HB2     | 1.85                     | 0.76              |
| 1:A:513[A]:GLN:O  | 1:A:517:ARG:HG3     | 1.85                     | 0.76              |
| 1:B:438[B]:ILE:O  | 1:B:438[B]:ILE:HG13 | 1.85                     | 0.76              |
| 1:A:565:ILE:HD13  | 1:A:594:VAL:O       | 1.85                     | 0.76              |
| 1:F:542:LEU:O     | 1:F:544:HIS:N       | 2.19                     | 0.76              |
| 1:B:539:GLY:HA3   | 1:B:588:MET:CE      | 2.14                     | 0.76              |
| 1:B:565:ILE:HD13  | 1:B:598:LEU:HD22    | 1.67                     | 0.76              |
| 1:E:429:ALA:HB2   | 2:H:4:LEU:O         | 1.86                     | 0.76              |
| 1:F:404:MET:HE1   | 4:F:779:HOH:O       | 1.86                     | 0.76              |
| 1:A:556:LYS:HG3   | 1:A:562:LYS:CD      | 2.16                     | 0.75              |
| 1:B:394:VAL:HB    | 1:B:415:ASN:HA      | 1.67                     | 0.75              |
| 1:E:560:ASP:O     | 1:E:563:THR:N       | 2.20                     | 0.75              |
| 1:E:487:SER:OG    | 1:E:498:LYS:HG2     | 1.86                     | 0.75              |
| 1:F:537:ASN:O     | 1:F:539:GLY:N       | 2.19                     | 0.75              |
| 1:E:527:ARG:O     | 1:E:531:GLU:OE2     | 2.05                     | 0.75              |
| 1:B:484:LEU:CD2   | 1:B:501:ILE:HD12    | 2.10                     | 0.74              |
| 1:E:565:ILE:O     | 1:E:569:LEU:HG      | 1.87                     | 0.74              |
| 1:B:437:THR:HG23  | 1:B:458:ASN:ND2     | 2.03                     | 0.74              |
| 1:E:437:THR:O     | 1:E:439:HIS:CD2     | 2.40                     | 0.74              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:F:447:ARG:O      | 1:F:449:ALA:N       | 2.20                     | 0.74              |
| 1:F:532:LEU:HD22   | 1:F:579[B]:GLU:HG3  | 1.67                     | 0.74              |
| 1:E:408:MET:HE2    | 1:E:410:THR:CG2     | 2.17                     | 0.74              |
| 1:E:584:ILE:CG2    | 1:E:588:MET:HE3     | 2.16                     | 0.74              |
| 1:E:402:GLU:CB     | 1:E:439:HIS:ND1     | 2.49                     | 0.74              |
| 1:E:434:SER:O      | 1:E:462:ILE:CG2     | 2.22                     | 0.74              |
| 1:B:445:ARG:HD3    | 1:B:519:ALA:HA      | 1.68                     | 0.74              |
| 1:B:476:PHE:CE1    | 1:B:486:VAL:HG13    | 2.23                     | 0.74              |
| 1:F:538:GLN:HA     | 1:F:541:HIS:HB2     | 1.69                     | 0.74              |
| 1:B:471:GLN:OE1    | 1:B:491:LYS:HD2     | 1.88                     | 0.73              |
| 1:E:437:THR:O      | 1:E:439:HIS:NE2     | 2.20                     | 0.73              |
| 1:E:542:LEU:O      | 1:E:543:LEU:C       | 2.29                     | 0.73              |
| 1:F:532:LEU:HD21   | 1:F:579[A]:GLU:HA   | 1.71                     | 0.73              |
| 1:A:469:MET:O      | 4:A:615:HOH:O       | 2.05                     | 0.73              |
| 1:A:436:VAL:HG21   | 1:A:472[B]:ILE:HD13 | 1.70                     | 0.73              |
| 1:F:532:LEU:HD21   | 1:F:579[B]:GLU:HA   | 1.71                     | 0.73              |
| 1:A:557:LEU:CB     | 1:A:558:PRO:CD      | 2.66                     | 0.73              |
| 1:A:559:ALA:CA     | 1:A:562:LYS:CE      | 2.65                     | 0.73              |
| 1:E:411[B]:LEU:CD2 | 1:E:424:GLN:HB2     | 2.18                     | 0.73              |
| 1:F:513:GLN:HG2    | 1:F:517:ARG:HH21    | 1.53                     | 0.73              |
| 1:A:534:GLN:O      | 1:A:538:GLN:HG3     | 1.89                     | 0.73              |
| 1:A:564:ALA:HB3    | 1:A:594:VAL:HB      | 1.71                     | 0.73              |
| 1:F:463:ASN:OD1    | 1:F:492:ASN:ND2     | 2.19                     | 0.73              |
| 1:B:465:ALA:HB1    | 1:F:469:MET:HE1     | 1.69                     | 0.73              |
| 1:E:446[A]:LYS:CG  | 1:E:526:ASP:HB3     | 2.18                     | 0.73              |
| 1:B:572:LEU:HD13   | 1:B:588:MET:HG3     | 1.71                     | 0.72              |
| 1:B:482:GLY:O      | 1:B:503:ALA:HB2     | 1.88                     | 0.72              |
| 1:E:536:ARG:HA     | 1:E:576:LEU:CD2     | 2.20                     | 0.72              |
| 1:F:430:GLU:OE1    | 1:F:544:HIS:HD2     | 1.72                     | 0.72              |
| 1:E:532:LEU:HD21   | 1:E:579:GLU:HA      | 1.71                     | 0.72              |
| 1:F:571:ALA:O      | 1:F:587:LYS:HG3     | 1.90                     | 0.72              |
| 1:E:401:ILE:HD11   | 1:E:426:PHE:CE1     | 2.25                     | 0.72              |
| 1:E:533:VAL:HG22   | 4:E:1026:HOH:O      | 1.89                     | 0.72              |
| 1:F:487:SER:CB     | 1:F:498:LYS:HE2     | 2.19                     | 0.72              |
| 1:B:550:VAL:HG13   | 1:B:557:LEU:HD21    | 1.72                     | 0.71              |
| 1:A:559:ALA:CB     | 1:A:562:LYS:HE3     | 2.19                     | 0.71              |
| 1:E:562:LYS:C      | 1:E:564:ALA:N       | 2.42                     | 0.71              |
| 1:E:411[A]:LEU:CD1 | 1:E:424:GLN:HB2     | 2.20                     | 0.71              |
| 1:A:497:GLN:HG3    | 1:A:498:LYS:N       | 2.05                     | 0.71              |
| 1:A:565:ILE:HD11   | 1:A:594:VAL:O       | 1.90                     | 0.71              |
| 1:A:598:LEU:O      | 1:A:600:GLU:HB2     | 1.91                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:B:437:THR:HG23   | 1:B:458:ASN:HD21   | 1.55                     | 0.71              |
| 1:A:534:GLN:NE2    | 4:A:863:HOH:O      | 2.23                     | 0.71              |
| 1:F:487:SER:CB     | 1:F:498:LYS:HG2    | 2.20                     | 0.71              |
| 1:A:444:GLU:HA     | 1:A:444:GLU:OE1    | 1.90                     | 0.71              |
| 1:A:508:ASN:OD1    | 1:A:511:GLU:HG3    | 1.91                     | 0.71              |
| 1:E:443:GLY:HA3    | 1:E:515:MET:CE     | 2.20                     | 0.71              |
| 1:A:430:GLU:OE2    | 1:A:540:ASP:OD2    | 2.09                     | 0.70              |
| 1:E:411[B]:LEU:CD1 | 1:E:476:PHE:CE1    | 2.73                     | 0.70              |
| 1:B:539:GLY:HA3    | 1:B:588:MET:HE2    | 1.73                     | 0.70              |
| 1:A:547:ARG:C      | 1:A:550:VAL:HB     | 2.16                     | 0.70              |
| 1:F:452:LYS:HB2    | 1:F:507:LEU:HD21   | 1.73                     | 0.70              |
| 1:A:556:LYS:HB2    | 1:A:562:LYS:HB3    | 1.73                     | 0.70              |
| 1:E:434:SER:HA     | 1:E:462:ILE:HG23   | 1.74                     | 0.70              |
| 1:F:401:ILE:CG1    | 1:F:402:GLU:N      | 2.53                     | 0.69              |
| 1:F:558:PRO:O      | 1:F:560:ASP:N      | 2.25                     | 0.69              |
| 1:E:584:ILE:HG22   | 1:E:588:MET:CE     | 2.21                     | 0.69              |
| 1:B:484:LEU:HD23   | 1:B:501:ILE:CD1    | 2.12                     | 0.69              |
| 1:B:404:MET:O      | 4:B:941:HOH:O      | 2.09                     | 0.69              |
| 1:B:572:LEU:CD1    | 1:B:588:MET:HG3    | 2.23                     | 0.69              |
| 1:E:421:LYS:C      | 1:E:422:HIS:HD2    | 2.01                     | 0.69              |
| 1:E:446[B]:LYS:CG  | 1:E:526:ASP:HB3    | 2.22                     | 0.69              |
| 1:B:401:ILE:HD11   | 1:B:426:PHE:CZ     | 2.27                     | 0.69              |
| 1:F:487:SER:HA     | 1:F:498:LYS:HG2    | 1.72                     | 0.69              |
| 1:A:411:LEU:HD12   | 1:A:422:HIS:HD2    | 1.55                     | 0.69              |
| 1:A:563:THR:O      | 1:A:564:ALA:C      | 2.36                     | 0.69              |
| 1:B:430:GLU:O      | 1:B:431:ASP:C      | 2.36                     | 0.69              |
| 1:B:569:LEU:HD12   | 1:B:591:LEU:HD13   | 1.75                     | 0.69              |
| 1:E:462:ILE:HD11   | 1:E:470:PRO:CB     | 2.23                     | 0.69              |
| 1:B:584:ILE:CG2    | 1:B:588:MET:CE     | 2.65                     | 0.69              |
| 1:E:440:VAL:HG23   | 1:E:455:GLY:O      | 1.93                     | 0.69              |
| 1:E:589:GLN:O      | 1:E:592:ALA:HB3    | 1.93                     | 0.69              |
| 1:A:562:LYS:O      | 1:A:565:ILE:HB     | 1.92                     | 0.68              |
| 1:E:437:THR:HG23   | 1:E:439:HIS:HE2    | 1.56                     | 0.68              |
| 1:F:539:GLY:O      | 1:F:543:LEU:CB     | 2.38                     | 0.68              |
| 1:F:564:ALA:HB1    | 1:F:594:VAL:HG21   | 1.74                     | 0.68              |
| 1:B:438[B]:ILE:O   | 1:B:438[B]:ILE:CG1 | 2.40                     | 0.68              |
| 1:E:468:GLY:HA2    | 2:H:3:ALC:HE13     | 1.75                     | 0.68              |
| 1:F:409:THR:HG23   | 4:G:35:HOH:O       | 1.94                     | 0.68              |
| 1:F:427:SER:O      | 2:G:4:LEU:N        | 2.25                     | 0.68              |
| 1:E:587:LYS:HD2    | 1:E:587:LYS:N      | 2.06                     | 0.68              |
| 1:A:600:GLU:CD     | 1:A:600:GLU:C      | 2.61                     | 0.68              |

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| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 1:A:497:GLN:HG3     | 1:A:498:LYS:H    | 1.59                     | 0.68              |
| 1:E:420:THR:OG1     | 1:E:422:HIS:NE2  | 2.22                     | 0.68              |
| 1:E:421:LYS:C       | 1:E:422:HIS:CD2  | 2.72                     | 0.68              |
| 1:F:537:ASN:C       | 1:F:539:GLY:H    | 2.01                     | 0.68              |
| 1:B:546:THR:O       | 1:B:549:GLN:N    | 2.26                     | 0.68              |
| 1:F:542:LEU:CD2     | 1:F:591:LEU:CD2  | 2.71                     | 0.68              |
| 1:E:446[B]:LYS:HG2  | 1:E:526:ASP:HB3  | 1.76                     | 0.67              |
| 1:E:502:LYS:O       | 1:E:505:SER:OG   | 2.12                     | 0.67              |
| 1:A:545:SER:O       | 1:A:548:LYS:CA   | 2.43                     | 0.67              |
| 1:A:600:GLU:OE1     | 1:A:600:GLU:CA   | 2.29                     | 0.67              |
| 1:E:411[B]:LEU:HD13 | 1:E:476:PHE:CD1  | 2.29                     | 0.67              |
| 1:E:442:GLN:OE1     | 1:E:507:LEU:N    | 2.27                     | 0.67              |
| 1:E:546:THR:HG21    | 1:E:591:LEU:HD11 | 1.75                     | 0.67              |
| 1:F:404:MET:HE3     | 1:F:537:ASN:CG   | 2.20                     | 0.67              |
| 1:E:587:LYS:O       | 4:E:1045:HOH:O   | 2.12                     | 0.67              |
| 1:E:411[A]:LEU:HD11 | 1:E:424:GLN:HB2  | 1.77                     | 0.67              |
| 1:E:414:LYS:O       | 1:E:415:ASN:HB2  | 1.94                     | 0.67              |
| 1:F:549:GLN:O       | 1:F:552:GLU:HB3  | 1.95                     | 0.67              |
| 1:A:508:ASN:O       | 1:A:512:ILE:CG1  | 2.37                     | 0.66              |
| 1:B:542:LEU:HD23    | 1:B:588:MET:HG2  | 1.77                     | 0.66              |
| 1:F:466:PRO:CD      | 1:F:469:MET:SD   | 2.78                     | 0.66              |
| 1:F:549:GLN:OE1     | 1:F:598:LEU:HD23 | 1.94                     | 0.66              |
| 1:A:426:PHE:HE1     | 1:A:474:VAL:HB   | 1.61                     | 0.66              |
| 1:B:418:ILE:HB      | 1:B:419:PRO:HA   | 1.75                     | 0.66              |
| 1:F:574:THR:C       | 1:F:576:LEU:N    | 2.48                     | 0.66              |
| 1:B:438[B]:ILE:HG12 | 1:B:457:PHE:CE1  | 2.30                     | 0.66              |
| 1:B:558:PRO:C       | 1:B:560:ASP:H    | 2.02                     | 0.66              |
| 1:F:407:VAL:HG12    | 1:F:408:MET:N    | 2.10                     | 0.66              |
| 1:F:570:THR:C       | 1:F:572:LEU:N    | 2.49                     | 0.66              |
| 1:A:548:LYS:C       | 1:A:550:VAL:N    | 2.47                     | 0.66              |
| 1:F:574:THR:HG22    | 1:F:575:ALA:H    | 1.61                     | 0.66              |
| 1:B:476:PHE:HE1     | 1:B:486:VAL:CG1  | 2.08                     | 0.65              |
| 1:E:542:LEU:C       | 1:E:544:HIS:N    | 2.52                     | 0.65              |
| 1:F:520:GLU:O       | 1:F:520:GLU:CD   | 2.39                     | 0.65              |
| 1:B:396:PRO:HA      | 1:B:415:ASN:HD22 | 1.61                     | 0.65              |
| 1:B:532:LEU:HD12    | 1:B:581:LYS:HG3  | 1.78                     | 0.65              |
| 1:E:442:GLN:O       | 1:E:452:LYS:N    | 2.28                     | 0.65              |
| 1:E:566:GLU:HA      | 1:E:569:LEU:HD12 | 1.79                     | 0.65              |
| 1:B:442:GLN:NE2     | 4:B:705:HOH:O    | 2.28                     | 0.65              |
| 1:B:534:GLN:O       | 1:B:538:GLN:CD   | 2.40                     | 0.65              |
| 1:E:425[A]:VAL:HG23 | 1:E:473:GLU:OE1  | 1.96                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:B:451:ASN:O      | 4:B:701:HOH:O      | 2.15                     | 0.65              |
| 1:F:441:LEU:HD23   | 1:F:453:SER:HA     | 1.78                     | 0.65              |
| 1:A:543:LEU:HD22   | 1:A:576:LEU:CD1    | 2.27                     | 0.65              |
| 1:E:408:MET:HE2    | 1:E:410:THR:HG22   | 1.79                     | 0.65              |
| 1:E:573[B]:GLU:OE1 | 1:E:573[B]:GLU:HA  | 1.95                     | 0.65              |
| 1:A:556:LYS:HG3    | 1:A:562:LYS:HD2    | 1.77                     | 0.65              |
| 1:B:404:MET:HE2    | 2:C:3:ALC:HB3      | 1.79                     | 0.65              |
| 1:F:402:GLU:O      | 1:F:403:THR:HG22   | 1.96                     | 0.65              |
| 1:A:559:ALA:HA     | 1:A:562:LYS:CD     | 2.27                     | 0.65              |
| 1:E:572:LEU:HD12   | 1:E:572:LEU:O      | 1.97                     | 0.65              |
| 1:F:487:SER:CA     | 1:F:498:LYS:HG2    | 2.27                     | 0.64              |
| 1:F:550:VAL:O      | 1:F:551:GLU:C      | 2.40                     | 0.64              |
| 1:B:586:ALA:O      | 1:B:590:GLU:N      | 2.31                     | 0.64              |
| 1:A:564:ALA:HB1    | 1:A:594:VAL:CG1    | 2.28                     | 0.64              |
| 1:A:556:LYS:HG3    | 1:A:562:LYS:HD3    | 1.79                     | 0.64              |
| 1:B:440:VAL:HG11   | 1:B:501:ILE:CD1    | 2.28                     | 0.64              |
| 1:E:438[B]:ILE:CG2 | 1:E:438[B]:ILE:O   | 2.46                     | 0.64              |
| 1:E:469:MET:HB3    | 1:E:470:PRO:HD3    | 1.79                     | 0.64              |
| 1:F:538:GLN:HA     | 1:F:541:HIS:CB     | 2.27                     | 0.64              |
| 1:E:539:GLY:CA     | 1:E:588:MET:HE2    | 2.26                     | 0.64              |
| 1:F:592:ALA:O      | 1:F:594:VAL:N      | 2.31                     | 0.64              |
| 1:E:584:ILE:CG2    | 1:E:588:MET:CE     | 2.76                     | 0.64              |
| 1:F:391:LEU:HD23   | 1:F:391:LEU:C      | 2.22                     | 0.64              |
| 1:F:542:LEU:HG     | 1:F:591:LEU:HD21   | 1.80                     | 0.64              |
| 1:A:507:LEU:HD22   | 1:A:511:GLU:HB3    | 1.78                     | 0.64              |
| 1:A:459:LEU:HD23   | 1:A:472[B]:ILE:CD1 | 2.28                     | 0.64              |
| 1:A:590[B]:GLU:HA  | 1:A:593:GLN:HE21   | 1.62                     | 0.63              |
| 1:A:508:ASN:OD1    | 1:A:511:GLU:CG     | 2.45                     | 0.63              |
| 1:A:513[A]:GLN:NE2 | 1:A:517:ARG:HH21   | 1.96                     | 0.63              |
| 1:E:485:HIS:CE1    | 1:E:500:THR:HG23   | 2.33                     | 0.63              |
| 1:B:539:GLY:CA     | 1:B:588:MET:CE     | 2.76                     | 0.63              |
| 1:B:394:VAL:CB     | 1:B:415:ASN:HA     | 2.29                     | 0.63              |
| 1:A:548:LYS:O      | 1:A:551:GLU:N      | 2.21                     | 0.63              |
| 1:E:542:LEU:O      | 1:E:544:HIS:N      | 2.31                     | 0.63              |
| 1:F:574:THR:CG2    | 1:F:575:ALA:N      | 2.52                     | 0.63              |
| 1:E:391:LEU:O      | 1:E:392:LEU:HG     | 1.97                     | 0.63              |
| 1:F:395:THR:O      | 1:F:415:ASN:N      | 2.27                     | 0.63              |
| 1:F:402:GLU:C      | 1:F:403:THR:CG2    | 2.72                     | 0.63              |
| 2:C:10:PRO:O       | 2:C:11:ARG:CB      | 2.47                     | 0.63              |
| 2:G:2:TYR:O        | 2:G:3:ALC:HD12     | 1.99                     | 0.63              |
| 1:A:526:ASP:O      | 1:A:529:PHE:HB3    | 1.99                     | 0.63              |

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| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 1:B:452:LYS:HB2     | 1:B:507:LEU:HG   | 1.80                     | 0.62              |
| 1:A:547:ARG:O       | 1:A:550:VAL:CG1  | 2.48                     | 0.62              |
| 1:B:448:ALA:C       | 1:B:450:ASP:H    | 2.06                     | 0.62              |
| 1:F:600:GLU:C       | 1:F:602:ALA:H    | 2.05                     | 0.62              |
| 1:A:508:ASN:OD1     | 1:A:511:GLU:CD   | 2.42                     | 0.62              |
| 1:B:427:SER:CB      | 1:B:468:GLY:HA2  | 2.29                     | 0.62              |
| 1:F:479:ASP:O       | 1:F:482:GLY:N    | 2.32                     | 0.62              |
| 1:E:530:GLU:OE2     | 4:E:1294:HOH:O   | 2.16                     | 0.62              |
| 1:F:558:PRO:HG2     | 1:F:561:ASP:OD2  | 2.00                     | 0.62              |
| 1:A:545:SER:O       | 1:A:549:GLN:N    | 2.32                     | 0.62              |
| 1:B:502[B]:LYS:O    | 1:B:505:SER:CB   | 2.47                     | 0.62              |
| 1:E:402:GLU:CB      | 1:E:439:HIS:CE1  | 2.83                     | 0.62              |
| 1:E:438[B]:ILE:HG23 | 1:E:438[B]:ILE:O | 1.98                     | 0.62              |
| 1:F:569:LEU:O       | 1:F:573:GLU:N    | 2.32                     | 0.62              |
| 1:F:538:GLN:CA      | 1:F:541:HIS:HB2  | 2.30                     | 0.62              |
| 1:A:563:THR:HG22    | 1:A:564:ALA:H    | 1.64                     | 0.61              |
| 1:B:458:ASN:O       | 1:B:497:GLN:HG3  | 2.00                     | 0.61              |
| 1:F:430:GLU:C       | 1:F:467:ARG:HB3  | 2.25                     | 0.61              |
| 1:B:502[C]:LYS:O    | 1:B:505:SER:CB   | 2.47                     | 0.61              |
| 1:E:562:LYS:O       | 1:E:564:ALA:N    | 2.34                     | 0.61              |
| 1:E:447[B]:ARG:HG2  | 1:E:529:PHE:CD2  | 2.34                     | 0.61              |
| 1:A:411:LEU:HD12    | 1:A:422:HIS:CD2  | 2.36                     | 0.61              |
| 1:E:433:GLN:NE2     | 1:E:436:VAL:HG12 | 2.12                     | 0.61              |
| 1:B:396:PRO:HA      | 1:B:415:ASN:ND2  | 2.15                     | 0.61              |
| 1:B:427:SER:OG      | 1:B:470:PRO:O    | 2.14                     | 0.61              |
| 1:F:527:ARG:O       | 1:F:530:GLU:CB   | 2.49                     | 0.61              |
| 1:B:586:ALA:HA      | 1:B:589:GLN:HB3  | 1.81                     | 0.61              |
| 1:F:527:ARG:O       | 1:F:530:GLU:HB3  | 2.01                     | 0.61              |
| 1:F:573:GLU:O       | 1:F:576:LEU:HB3  | 2.00                     | 0.61              |
| 1:B:558:PRO:O       | 1:B:560:ASP:N    | 2.34                     | 0.61              |
| 1:E:411[B]:LEU:HD23 | 1:E:424:GLN:HB2  | 1.82                     | 0.61              |
| 1:E:522:ASN:O       | 1:E:525:ALA:HB3  | 2.01                     | 0.61              |
| 1:F:550:VAL:O       | 1:F:553:ALA:N    | 2.34                     | 0.61              |
| 1:B:395:THR:O       | 1:B:415:ASN:N    | 2.34                     | 0.61              |
| 1:F:487:SER:HB2     | 1:F:498:LYS:HE2  | 1.81                     | 0.61              |
| 1:F:537:ASN:C       | 1:F:539:GLY:N    | 2.58                     | 0.61              |
| 1:F:544:HIS:C       | 1:F:546:THR:H    | 2.07                     | 0.61              |
| 1:F:564:ALA:CB      | 1:F:594:VAL:HG21 | 2.31                     | 0.61              |
| 1:E:407:VAL:HG13    | 4:E:1169:HOH:O   | 2.01                     | 0.60              |
| 1:E:418:ILE:HA      | 1:E:419:PRO:C    | 2.25                     | 0.60              |
| 1:E:462:ILE:HD11    | 1:E:470:PRO:CG   | 2.31                     | 0.60              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:A:465:ALA:O       | 1:A:466:PRO:C       | 2.42                     | 0.60              |
| 1:E:543:LEU:O       | 1:E:547:ARG:CD      | 2.49                     | 0.60              |
| 1:F:475:THR:HB      | 1:F:487:SER:OG      | 2.02                     | 0.60              |
| 1:F:487:SER:HB3     | 1:F:498:LYS:HG2     | 1.81                     | 0.60              |
| 1:F:597:LYS:HA      | 1:F:600:GLU:OE1     | 2.02                     | 0.60              |
| 1:A:424:GLN:NE2     | 4:A:613:HOH:O       | 2.31                     | 0.60              |
| 1:A:563:THR:O       | 1:A:566:GLU:N       | 2.35                     | 0.60              |
| 1:B:401:ILE:HG21    | 1:B:438[B]:ILE:HD12 | 1.83                     | 0.60              |
| 1:E:446[A]:LYS:HG3  | 1:E:526:ASP:O       | 2.01                     | 0.60              |
| 1:E:401:ILE:CD1     | 1:E:426:PHE:CZ      | 2.84                     | 0.60              |
| 1:E:423:SER:HB3     | 1:E:473:GLU:OE2     | 2.01                     | 0.60              |
| 1:A:464:PRO:HA      | 4:A:659:HOH:O       | 2.02                     | 0.60              |
| 1:F:601:ILE:HG22    | 1:F:601:ILE:O       | 2.02                     | 0.60              |
| 1:B:539:GLY:CA      | 1:B:588:MET:HE2     | 2.31                     | 0.60              |
| 1:B:562:LYS:O       | 1:B:563:THR:C       | 2.45                     | 0.60              |
| 1:B:600:GLU:O       | 1:B:601:ILE:C       | 2.45                     | 0.60              |
| 1:A:440:VAL:C       | 1:A:441:LEU:HG      | 2.26                     | 0.59              |
| 1:E:510:ASP:O       | 1:E:514:LYS:HG3     | 2.01                     | 0.59              |
| 1:E:570:THR:HG22    | 1:E:570:THR:O       | 2.02                     | 0.59              |
| 1:F:418:ILE:HB      | 1:F:419:PRO:HA      | 1.83                     | 0.59              |
| 1:B:502[A]:LYS:O    | 1:B:505:SER:CB      | 2.49                     | 0.59              |
| 1:E:401:ILE:HD11    | 1:E:426:PHE:CE2     | 2.36                     | 0.59              |
| 1:A:552:GLU:O       | 1:A:552:GLU:HG2     | 2.02                     | 0.59              |
| 1:E:402:GLU:HB3     | 1:E:439:HIS:CE1     | 2.35                     | 0.59              |
| 1:F:538:GLN:O       | 1:F:541:HIS:HB2     | 2.03                     | 0.59              |
| 1:A:462[B]:ILE:HG23 | 1:A:462[B]:ILE:O    | 2.03                     | 0.59              |
| 1:F:487:SER:HB3     | 1:F:498:LYS:HE2     | 1.82                     | 0.59              |
| 1:A:441:LEU:HD23    | 1:A:453:SER:HA      | 1.85                     | 0.59              |
| 1:B:553:ALA:O       | 1:B:556:LYS:HB2     | 2.01                     | 0.59              |
| 1:A:440:VAL:HG12    | 1:A:441:LEU:N       | 2.17                     | 0.58              |
| 1:A:394:VAL:O       | 1:A:418:ILE:HD11    | 2.03                     | 0.58              |
| 1:B:550:VAL:CG1     | 1:B:557:LEU:HD22    | 2.28                     | 0.58              |
| 1:E:397:LEU:HD11    | 1:E:512:ILE:HG12    | 1.84                     | 0.58              |
| 1:F:544:HIS:C       | 1:F:546:THR:N       | 2.60                     | 0.58              |
| 1:B:391:LEU:C       | 1:B:391:LEU:HD23    | 2.28                     | 0.58              |
| 1:B:543:LEU:CD2     | 1:B:547:ARG:HH11    | 2.15                     | 0.58              |
| 1:F:548:LYS:O       | 1:F:551:GLU:HB2     | 2.03                     | 0.58              |
| 2:D:8:THR:HG22      | 4:D:379:HOH:O       | 2.02                     | 0.58              |
| 1:B:476:PHE:CE1     | 1:B:486:VAL:CG1     | 2.85                     | 0.58              |
| 1:E:542:LEU:O       | 1:E:545:SER:N       | 2.36                     | 0.58              |
| 1:F:538:GLN:HA      | 1:F:541:HIS:CD2     | 2.38                     | 0.58              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:F:545:SER:O      | 1:F:549:GLN:HB2   | 2.04                     | 0.58              |
| 1:B:445:ARG:HH12   | 1:B:447:ARG:HD2   | 1.66                     | 0.58              |
| 1:E:398:SER:N      | 1:E:414:LYS:HB3   | 2.18                     | 0.58              |
| 1:E:479:ASP:OD1    | 1:E:479:ASP:C     | 2.46                     | 0.58              |
| 1:B:534:GLN:O      | 1:B:534:GLN:HG2   | 2.03                     | 0.58              |
| 1:A:510:ASP:O      | 1:A:514:LYS:HG3   | 2.04                     | 0.58              |
| 1:A:563:THR:O      | 1:A:565:ILE:N     | 2.36                     | 0.58              |
| 1:B:536:ARG:O      | 1:B:576:LEU:HD22  | 2.04                     | 0.58              |
| 1:F:594:VAL:O      | 1:F:594:VAL:HG22  | 2.03                     | 0.58              |
| 1:E:429:ALA:CB     | 2:H:4:LEU:O       | 2.52                     | 0.58              |
| 1:E:522:ASN:HB3    | 1:E:525:ALA:HB3   | 1.85                     | 0.58              |
| 1:F:549:GLN:OE1    | 1:F:598:LEU:HD22  | 2.04                     | 0.58              |
| 1:F:558:PRO:C      | 1:F:560:ASP:N     | 2.59                     | 0.58              |
| 1:F:570:THR:O      | 1:F:572:LEU:N     | 2.37                     | 0.58              |
| 1:B:517:ARG:O      | 1:B:520:GLU:CB    | 2.51                     | 0.58              |
| 1:E:440:VAL:HG21   | 1:E:501:ILE:HD11  | 1.85                     | 0.58              |
| 1:A:563:THR:C      | 1:A:565:ILE:N     | 2.59                     | 0.57              |
| 1:B:394:VAL:CG2    | 1:B:415:ASN:HA    | 2.34                     | 0.57              |
| 1:B:502[A]:LYS:CB  | 1:B:502[A]:LYS:NZ | 2.67                     | 0.57              |
| 1:F:528:LYS:O      | 1:F:530:GLU:N     | 2.36                     | 0.57              |
| 1:B:534:GLN:O      | 1:B:538:GLN:HG3   | 2.04                     | 0.57              |
| 1:F:538:GLN:C      | 1:F:540:ASP:H     | 2.12                     | 0.57              |
| 1:F:447:ARG:O      | 1:F:450:ASP:N     | 2.35                     | 0.57              |
| 1:F:540:ASP:O      | 1:F:541:HIS:C     | 2.47                     | 0.57              |
| 1:E:446[B]:LYS:HG3 | 1:E:526:ASP:O     | 2.05                     | 0.57              |
| 1:E:447[A]:ARG:HG2 | 1:E:529:PHE:CE2   | 2.39                     | 0.57              |
| 1:F:532:LEU:CD2    | 1:F:579[A]:GLU:HA | 2.35                     | 0.57              |
| 1:A:539:GLY:O      | 1:A:543:LEU:HB2   | 2.05                     | 0.57              |
| 1:F:430:GLU:CD     | 1:F:544:HIS:CD2   | 2.82                     | 0.57              |
| 1:A:590[B]:GLU:HA  | 1:A:593:GLN:NE2   | 2.19                     | 0.57              |
| 1:B:517:ARG:O      | 1:B:520:GLU:HB3   | 2.04                     | 0.57              |
| 1:B:571:ALA:CB     | 1:B:587:LYS:HD2   | 2.21                     | 0.57              |
| 1:B:575:ALA:C      | 1:B:577:LYS:H     | 2.13                     | 0.57              |
| 1:E:405:GLY:HA3    | 1:E:533:VAL:HG13  | 1.87                     | 0.57              |
| 1:F:520:GLU:CD     | 1:F:520:GLU:C     | 2.73                     | 0.57              |
| 1:F:555:ASP:C      | 1:F:557:LEU:H     | 2.12                     | 0.57              |
| 1:B:580:ASP:O      | 1:B:581:LYS:C     | 2.48                     | 0.56              |
| 1:E:527:ARG:NH1    | 1:E:531:GLU:OE2   | 2.38                     | 0.56              |
| 1:E:597:LYS:O      | 1:E:598:LEU:HD12  | 2.05                     | 0.56              |
| 1:F:477:ASP:O      | 1:F:485:HIS:N     | 2.38                     | 0.56              |
| 1:F:538:GLN:C      | 1:F:540:ASP:N     | 2.61                     | 0.56              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:A:405:GLY:HA3     | 1:A:533:VAL:CG1     | 2.35                     | 0.56              |
| 1:F:513:GLN:CG      | 1:F:517:ARG:HH21    | 2.16                     | 0.56              |
| 1:A:472[A]:ILE:CD1  | 1:A:490:ASP:HB2     | 2.36                     | 0.56              |
| 1:A:543:LEU:O       | 1:A:547:ARG:HG3     | 2.05                     | 0.56              |
| 1:F:532:LEU:CD2     | 1:F:579[B]:GLU:HA   | 2.36                     | 0.56              |
| 1:B:469:MET:N       | 1:B:470:PRO:CD      | 2.68                     | 0.56              |
| 1:B:481:ASP:OD1     | 1:B:481:ASP:O       | 2.23                     | 0.56              |
| 1:E:401:ILE:CD1     | 1:E:426:PHE:CE1     | 2.88                     | 0.56              |
| 1:A:527:ARG:C       | 1:A:529:PHE:N       | 2.62                     | 0.56              |
| 1:B:503:ALA:C       | 1:B:505:SER:N       | 2.56                     | 0.56              |
| 1:B:512:ILE:O       | 1:B:516:VAL:HG23    | 2.06                     | 0.56              |
| 1:F:441:LEU:CD1     | 1:F:448:ALA:HB1     | 2.35                     | 0.56              |
| 1:A:571:ALA:O       | 1:A:574:THR:HB      | 2.05                     | 0.56              |
| 1:B:598:LEU:O       | 1:B:599:MET:C       | 2.48                     | 0.56              |
| 1:F:431:ASP:O       | 1:F:432:ASN:HB2     | 2.04                     | 0.56              |
| 1:B:543:LEU:C       | 1:B:543:LEU:CD2     | 2.78                     | 0.56              |
| 1:B:547:ARG:HG3     | 1:B:569:LEU:HD22    | 1.88                     | 0.56              |
| 1:F:549:GLN:HG2     | 1:F:598:LEU:HD21    | 1.88                     | 0.56              |
| 1:E:411[B]:LEU:HD21 | 1:E:424:GLN:HB2     | 1.89                     | 0.56              |
| 1:F:447:ARG:C       | 1:F:449:ALA:N       | 2.47                     | 0.56              |
| 1:B:401:ILE:HD11    | 1:B:426:PHE:CE2     | 2.40                     | 0.55              |
| 1:A:558:PRO:O       | 1:A:559:ALA:CB      | 2.54                     | 0.55              |
| 1:A:426:PHE:CE1     | 1:A:474:VAL:HB      | 2.42                     | 0.55              |
| 1:E:462:ILE:HD11    | 1:E:470:PRO:HB3     | 1.88                     | 0.55              |
| 1:B:420:THR:OG1     | 1:B:421[B]:LYS:N    | 2.38                     | 0.55              |
| 1:E:446[B]:LYS:HA   | 1:E:446[B]:LYS:HZ3  | 1.70                     | 0.55              |
| 1:F:404:MET:HE3     | 1:F:537:ASN:OD1     | 2.06                     | 0.55              |
| 1:E:507:LEU:HD13    | 1:E:511:GLU:CB      | 2.33                     | 0.55              |
| 1:F:545:SER:O       | 1:F:549:GLN:CB      | 2.55                     | 0.55              |
| 1:B:442:GLN:HB2     | 1:B:454:LEU:HD11    | 1.88                     | 0.55              |
| 1:B:459:LEU:HD11    | 1:B:495:LYS:HB3     | 1.89                     | 0.55              |
| 1:B:484:LEU:HB3     | 1:B:501:ILE:HB      | 1.88                     | 0.55              |
| 1:B:599:MET:O       | 1:B:602:ALA:O       | 2.24                     | 0.55              |
| 1:B:546:THR:CG2     | 1:B:569:LEU:HD11    | 2.31                     | 0.55              |
| 1:E:400:GLY:HA3     | 1:E:410:THR:HA      | 1.89                     | 0.55              |
| 1:E:527:ARG:CZ      | 1:E:531:GLU:OE2     | 2.55                     | 0.55              |
| 1:E:446[A]:LYS:HG3  | 1:E:526:ASP:HB3     | 1.89                     | 0.55              |
| 1:E:446[B]:LYS:HA   | 1:E:446[B]:LYS:NZ   | 2.22                     | 0.55              |
| 1:A:484:LEU:CD2     | 1:A:501[A]:ILE:HD12 | 2.33                     | 0.54              |
| 1:E:411[A]:LEU:HD13 | 1:E:424:GLN:HB2     | 1.88                     | 0.54              |
| 1:A:472[A]:ILE:HD13 | 1:A:490:ASP:HA      | 1.88                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:E:446[A]:LYS:HE3 | 1:E:446[A]:LYS:HA  | 1.88                     | 0.54              |
| 1:E:513:GLN:HG2    | 1:E:517[B]:ARG:HD3 | 1.88                     | 0.54              |
| 1:F:478:ILE:HG12   | 1:F:484:LEU:HD13   | 1.90                     | 0.54              |
| 1:F:585:GLU:HG2    | 1:F:588:MET:CE     | 2.38                     | 0.54              |
| 1:B:478:ILE:HG12   | 1:B:484:LEU:HA     | 1.87                     | 0.54              |
| 1:A:559:ALA:O      | 1:A:563:THR:CB     | 2.50                     | 0.54              |
| 1:A:567:SER:O      | 1:A:570:THR:HB     | 2.08                     | 0.54              |
| 1:B:539:GLY:HA3    | 1:B:588:MET:HE1    | 1.86                     | 0.54              |
| 1:F:520:GLU:OE1    | 1:F:520:GLU:C      | 2.46                     | 0.54              |
| 1:A:389:VAL:HG13   | 4:A:781:HOH:O      | 2.08                     | 0.54              |
| 1:E:402:GLU:OE1    | 1:E:439:HIS:CE1    | 2.61                     | 0.54              |
| 1:E:493[B]:SER:HB3 | 1:E:495:LYS:HG2    | 1.89                     | 0.54              |
| 1:F:420:THR:OG1    | 1:F:421:LYS:N      | 2.38                     | 0.54              |
| 2:D:7:PRO:O        | 2:D:8:THR:C        | 2.50                     | 0.54              |
| 1:F:399:LEU:HB2    | 1:F:412:ILE:HB     | 1.89                     | 0.54              |
| 1:F:399:LEU:CD1    | 1:F:478:ILE:HD11   | 2.37                     | 0.54              |
| 1:B:546:THR:O      | 1:B:549:GLN:CB     | 2.56                     | 0.53              |
| 1:A:543:LEU:HD22   | 1:A:576:LEU:HD11   | 1.90                     | 0.53              |
| 1:E:391:LEU:O      | 1:E:391:LEU:HD13   | 2.08                     | 0.53              |
| 1:E:412:ILE:HG12   | 1:E:422:HIS:CG     | 2.43                     | 0.53              |
| 1:F:448:ALA:HA     | 1:F:451:ASN:HD22   | 1.73                     | 0.53              |
| 1:A:600:GLU:N      | 4:A:768:HOH:O      | 2.40                     | 0.53              |
| 1:B:547:ARG:HG3    | 1:B:569:LEU:CD2    | 2.39                     | 0.53              |
| 1:E:514:LYS:O      | 1:E:518:ASP:CB     | 2.56                     | 0.53              |
| 1:B:411:LEU:HD11   | 1:B:474:VAL:HG12   | 1.90                     | 0.53              |
| 1:E:391:LEU:HD22   | 1:E:392:LEU:N      | 2.24                     | 0.53              |
| 1:E:417:THR:O      | 1:E:420:THR:HB     | 2.09                     | 0.53              |
| 1:E:442:GLN:HB2    | 1:E:454:LEU:HD21   | 1.90                     | 0.53              |
| 1:F:407:VAL:CG2    | 1:F:533:VAL:HG11   | 2.38                     | 0.53              |
| 1:A:471:GLN:O      | 1:A:491:LYS:HG3    | 2.09                     | 0.53              |
| 1:B:392:LEU:HD13   | 1:B:417:THR:CG2    | 2.39                     | 0.53              |
| 1:B:546:THR:HA     | 1:B:549:GLN:HB2    | 1.91                     | 0.53              |
| 1:E:536:ARG:HA     | 1:E:576:LEU:HD22   | 1.90                     | 0.53              |
| 1:F:580:ASP:CG     | 1:F:583:ALA:HB2    | 2.34                     | 0.53              |
| 1:A:390:LEU:N      | 1:A:390:LEU:HD23   | 2.24                     | 0.53              |
| 1:A:569:LEU:HD23   | 1:A:591:LEU:HD22   | 1.91                     | 0.53              |
| 1:B:404:MET:CE     | 2:C:3:ALC:HD22     | 2.35                     | 0.53              |
| 1:E:497:GLN:NE2    | 1:E:498:LYS:H      | 1.96                     | 0.53              |
| 1:F:546:THR:O      | 1:F:546:THR:HG22   | 2.07                     | 0.53              |
| 1:A:440:VAL:CG1    | 1:A:441:LEU:N      | 2.72                     | 0.53              |
| 1:A:497:GLN:HE21   | 1:A:498:LYS:H      | 1.57                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:B:502[A]:LYS:HB3 | 1:B:502[A]:LYS:HZ3 | 1.74                     | 0.53              |
| 1:E:395:THR:N      | 1:E:418:ILE:HD13   | 2.24                     | 0.53              |
| 1:B:510:ASP:O      | 1:B:514[A]:LYS:HG3 | 2.08                     | 0.53              |
| 1:F:563:THR:OG1    | 1:F:564:ALA:N      | 2.40                     | 0.53              |
| 1:E:541:HIS:O      | 1:E:545:SER:HB2    | 2.09                     | 0.53              |
| 1:E:562:LYS:O      | 1:E:563:THR:C      | 2.51                     | 0.53              |
| 1:F:600:GLU:C      | 1:F:602:ALA:N      | 2.67                     | 0.53              |
| 1:E:513:GLN:HG2    | 1:E:517[A]:ARG:NE  | 2.24                     | 0.52              |
| 1:E:516:VAL:HB     | 1:E:517[B]:ARG:NH1 | 2.24                     | 0.52              |
| 1:F:580:ASP:OD2    | 1:F:583:ALA:HB2    | 2.09                     | 0.52              |
| 1:B:447:ARG:O      | 1:B:448:ALA:C      | 2.52                     | 0.52              |
| 1:B:595:SER:CB     | 1:B:599:MET:CE     | 2.80                     | 0.52              |
| 1:E:434:SER:CA     | 1:E:462:ILE:CG2    | 2.87                     | 0.52              |
| 1:A:434:SER:O      | 1:A:435:ALA:HB2    | 2.09                     | 0.52              |
| 1:E:430:GLU:OE1    | 1:E:433:GLN:OE1    | 2.27                     | 0.52              |
| 1:E:574:THR:O      | 1:E:574:THR:HG22   | 2.09                     | 0.52              |
| 1:F:402:GLU:CG     | 1:F:403:THR:N      | 2.60                     | 0.52              |
| 1:A:593:GLN:C      | 1:A:595:SER:H      | 2.16                     | 0.52              |
| 1:F:575:ALA:CB     | 4:F:925:HOH:O      | 2.57                     | 0.52              |
| 1:A:591:LEU:C      | 1:A:593:GLN:H      | 2.16                     | 0.52              |
| 1:B:476:PHE:CD1    | 1:B:486:VAL:HG13   | 2.44                     | 0.52              |
| 1:E:561:ASP:O      | 1:E:565:ILE:CG1    | 2.51                     | 0.52              |
| 1:B:549:GLN:HA     | 1:B:549:GLN:HE21   | 1.75                     | 0.52              |
| 1:E:434:SER:HA     | 1:E:462:ILE:CG2    | 2.40                     | 0.52              |
| 1:F:549:GLN:HG2    | 1:F:598:LEU:CD2    | 2.40                     | 0.52              |
| 1:E:507:LEU:HD13   | 1:E:511:GLU:C      | 2.34                     | 0.52              |
| 1:E:508:ASN:C      | 1:E:508:ASN:OD1    | 2.53                     | 0.52              |
| 1:F:592:ALA:O      | 1:F:593:GLN:C      | 2.52                     | 0.52              |
| 1:B:439:HIS:HD2    | 1:B:456:GLN:HB3    | 1.75                     | 0.52              |
| 1:E:512:ILE:HG22   | 4:E:1009:HOH:O     | 2.10                     | 0.52              |
| 1:E:523:ALA:O      | 1:E:524:GLU:C      | 2.52                     | 0.52              |
| 1:E:412:ILE:C      | 4:E:1163:HOH:O     | 2.52                     | 0.52              |
| 1:F:431:ASP:N      | 1:F:467:ARG:HB3    | 2.25                     | 0.52              |
| 1:F:477:ASP:HB3    | 1:F:485:HIS:HB2    | 1.92                     | 0.51              |
| 2:D:8:THR:C        | 4:D:27:HOH:O       | 2.53                     | 0.51              |
| 1:A:547:ARG:O      | 1:A:550:VAL:HG12   | 2.11                     | 0.51              |
| 1:E:414:LYS:HD3    | 1:E:444:GLU:CD     | 2.29                     | 0.51              |
| 1:F:438:ILE:HD11   | 2:G:4:LEU:HD13     | 1.92                     | 0.51              |
| 1:F:492:ASN:HB3    | 4:F:769:HOH:O      | 2.10                     | 0.51              |
| 1:F:600:GLU:O      | 1:F:602:ALA:N      | 2.42                     | 0.51              |
| 1:A:486:VAL:HB     | 1:A:499:ILE:HG22   | 1.92                     | 0.51              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:596:GLN:O    | 1:A:599:MET:HB3    | 2.10                     | 0.51              |
| 1:A:591:LEU:C    | 1:A:593:GLN:N      | 2.68                     | 0.51              |
| 1:B:448:ALA:C    | 1:B:450:ASP:N      | 2.69                     | 0.51              |
| 1:B:564:ALA:O    | 1:B:567:SER:OG     | 2.29                     | 0.51              |
| 1:F:532:LEU:C    | 1:F:534:GLN:N      | 2.68                     | 0.51              |
| 1:F:418:ILE:HD12 | 1:F:480:ALA:HA     | 1.92                     | 0.51              |
| 1:B:539:GLY:HA3  | 1:B:576:LEU:HD21   | 1.91                     | 0.51              |
| 1:F:411:LEU:HA   | 1:F:422:HIS:HD2    | 1.76                     | 0.51              |
| 1:A:394:VAL:C    | 1:A:418:ILE:HD11   | 2.35                     | 0.51              |
| 1:A:563:THR:HA   | 1:A:566:GLU:CD     | 2.36                     | 0.51              |
| 1:B:565:ILE:CD1  | 1:B:598:LEU:HD22   | 2.37                     | 0.51              |
| 1:E:404:MET:HE1  | 1:E:540:ASP:OD2    | 2.10                     | 0.51              |
| 1:F:401:ILE:HD11 | 1:F:426:PHE:CE2    | 2.46                     | 0.51              |
| 1:F:407:VAL:CG1  | 1:F:408:MET:N      | 2.73                     | 0.51              |
| 1:B:398:SER:HB2  | 1:B:443:GLY:O      | 2.11                     | 0.51              |
| 1:B:411:LEU:CD1  | 1:B:474:VAL:HG12   | 2.41                     | 0.51              |
| 1:B:439:HIS:HE2  | 1:B:453:SER:HG     | 1.58                     | 0.51              |
| 1:B:482:GLY:O    | 1:B:503:ALA:CB     | 2.57                     | 0.51              |
| 1:F:591:LEU:O    | 1:F:595:SER:OG     | 2.27                     | 0.51              |
| 1:A:552:GLU:O    | 1:A:552:GLU:CG     | 2.58                     | 0.51              |
| 1:B:528:LYS:HD3  | 1:B:529:PHE:N      | 2.26                     | 0.51              |
| 1:B:534:GLN:O    | 1:B:538:GLN:CG     | 2.59                     | 0.50              |
| 1:B:574:THR:HG22 | 4:B:720:HOH:O      | 2.11                     | 0.50              |
| 1:F:402:GLU:C    | 1:F:403:THR:HG22   | 2.37                     | 0.50              |
| 1:F:529:PHE:HD1  | 1:F:579[A]:GLU:OE1 | 1.95                     | 0.50              |
| 1:A:543:LEU:HD13 | 1:A:572:LEU:CD2    | 2.37                     | 0.50              |
| 1:B:568:ALA:HB3  | 1:B:591:LEU:HD12   | 1.92                     | 0.50              |
| 1:F:585:GLU:HA   | 1:F:588:MET:HE3    | 1.92                     | 0.50              |
| 1:F:590:GLU:O    | 1:F:594:VAL:HG12   | 2.11                     | 0.50              |
| 1:B:412:ILE:CD1  | 1:B:476:PHE:HB3    | 2.42                     | 0.50              |
| 1:B:446:LYS:HE3  | 1:B:446:LYS:N      | 2.25                     | 0.50              |
| 1:B:591:LEU:O    | 1:B:592:ALA:C      | 2.54                     | 0.50              |
| 1:E:543:LEU:O    | 1:E:547:ARG:HD2    | 2.10                     | 0.50              |
| 1:F:438:ILE:CD1  | 2:G:4:LEU:HD13     | 2.41                     | 0.50              |
| 1:B:508:ASN:O    | 1:B:512:ILE:N      | 2.41                     | 0.50              |
| 1:B:558:PRO:C    | 1:B:560:ASP:N      | 2.69                     | 0.50              |
| 1:F:436:VAL:HG13 | 1:F:462:ILE:CD1    | 2.41                     | 0.50              |
| 1:A:433:GLN:HG3  | 2:D:6:ARG:CG       | 2.41                     | 0.50              |
| 1:A:479:ASP:C    | 1:A:479:ASP:OD1    | 2.54                     | 0.50              |
| 1:B:435:ALA:CB   | 1:B:460:ASP:HA     | 2.41                     | 0.50              |
| 1:F:542:LEU:C    | 1:F:544:HIS:H      | 2.20                     | 0.50              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:F:467:ARG:NH2     | 1:F:541:HIS:HA     | 2.27                     | 0.50              |
| 1:A:542:LEU:HD11    | 4:A:932:HOH:O      | 2.11                     | 0.50              |
| 1:A:478:ILE:HG12    | 1:A:484:LEU:HD13   | 1.94                     | 0.50              |
| 1:E:543:LEU:HD13    | 1:E:573[B]:GLU:OE1 | 2.11                     | 0.50              |
| 1:E:561:ASP:OD2     | 1:E:597:LYS:HE2    | 2.12                     | 0.50              |
| 2:G:6[A]:ARG:HH12   | 2:G:9:PRO:CD       | 2.17                     | 0.50              |
| 2:G:7:PRO:O         | 2:G:8:THR:C        | 2.55                     | 0.50              |
| 1:A:470:PRO:HA      | 4:A:751:HOH:O      | 2.12                     | 0.50              |
| 1:A:565:ILE:CD1     | 1:A:595:SER:OG     | 2.60                     | 0.50              |
| 1:A:497:GLN:CG      | 1:A:498:LYS:N      | 2.75                     | 0.49              |
| 1:A:565:ILE:HD12    | 1:A:595:SER:OG     | 2.12                     | 0.49              |
| 1:A:444:GLU:OE1     | 1:A:444:GLU:CA     | 2.59                     | 0.49              |
| 1:B:438[B]:ILE:HG21 | 1:B:457:PHE:CZ     | 2.48                     | 0.49              |
| 1:B:592:ALA:O       | 1:B:593:GLN:C      | 2.54                     | 0.49              |
| 1:A:557:LEU:O       | 1:A:559:ALA:N      | 2.46                     | 0.49              |
| 1:B:575:ALA:C       | 1:B:577:LYS:N      | 2.69                     | 0.49              |
| 1:E:410:THR:HB      | 4:E:1163:HOH:O     | 2.12                     | 0.49              |
| 1:E:432:ASN:HA      | 1:E:465:ALA:H      | 1.78                     | 0.49              |
| 1:F:546:THR:O       | 1:F:546:THR:CG2    | 2.60                     | 0.49              |
| 1:A:463:ASN:O       | 1:A:464:PRO:C      | 2.51                     | 0.49              |
| 1:A:557:LEU:O       | 1:A:558:PRO:C      | 2.55                     | 0.49              |
| 1:B:394:VAL:HA      | 1:B:416:THR:O      | 2.13                     | 0.49              |
| 1:E:514:LYS:O       | 1:E:518:ASP:OD1    | 2.30                     | 0.49              |
| 1:F:509:GLU:HA      | 1:F:512:ILE:HD12   | 1.93                     | 0.49              |
| 1:F:527:ARG:O       | 1:F:530:GLU:HB2    | 2.12                     | 0.49              |
| 1:A:478:ILE:HG12    | 1:A:484:LEU:CD1    | 2.42                     | 0.49              |
| 1:B:529:PHE:O       | 1:B:533:VAL:N      | 2.43                     | 0.49              |
| 1:E:586:ALA:O       | 1:E:589:GLN:HB3    | 2.13                     | 0.49              |
| 1:F:411:LEU:HD12    | 1:F:422:HIS:CD2    | 2.47                     | 0.49              |
| 1:F:512:ILE:O       | 1:F:516:VAL:HG23   | 2.13                     | 0.49              |
| 1:F:531[B]:GLU:CD   | 1:F:534:GLN:NE2    | 2.59                     | 0.49              |
| 1:A:527:ARG:C       | 1:A:529:PHE:H      | 2.20                     | 0.49              |
| 1:E:426:PHE:CE1     | 1:E:474:VAL:HB     | 2.48                     | 0.49              |
| 1:E:444:GLU:N       | 1:E:515:MET:HE3    | 2.27                     | 0.49              |
| 1:E:446[A]:LYS:HZ2  | 1:E:446[A]:LYS:N   | 2.11                     | 0.49              |
| 1:B:445:ARG:HG2     | 1:B:519:ALA:HB2    | 1.94                     | 0.48              |
| 1:A:546:THR:HG23    | 1:A:598:LEU:HD23   | 1.94                     | 0.48              |
| 1:E:444:GLU:H       | 1:E:515:MET:HE3    | 1.78                     | 0.48              |
| 1:B:435:ALA:HB2     | 1:B:460:ASP:HA     | 1.94                     | 0.48              |
| 1:B:442:GLN:OE1     | 1:B:506:GLY:CA     | 2.48                     | 0.48              |
| 1:F:436:VAL:HG13    | 1:F:462:ILE:HD11   | 1.95                     | 0.48              |

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| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 1:B:438[B]:ILE:HG23 | 1:B:457:PHE:O    | 2.14                     | 0.48              |
| 1:B:478:ILE:HA      | 1:B:483:ILE:O    | 2.13                     | 0.48              |
| 1:B:545[B]:SER:O    | 1:B:549:GLN:N    | 2.47                     | 0.48              |
| 1:F:565:ILE:HG22    | 1:F:566:GLU:N    | 2.28                     | 0.48              |
| 1:A:469:MET:HB3     | 1:A:470:PRO:HD3  | 1.95                     | 0.48              |
| 1:A:472[A]:ILE:HD13 | 1:A:490:ASP:CB   | 2.43                     | 0.48              |
| 1:B:394:VAL:HB      | 1:B:415:ASN:CA   | 2.38                     | 0.48              |
| 1:B:441:LEU:HD13    | 1:B:448:ALA:HB1  | 1.96                     | 0.48              |
| 1:B:600:GLU:O       | 1:B:602:ALA:N    | 2.46                     | 0.48              |
| 1:F:401:ILE:CG1     | 1:F:402:GLU:H    | 2.05                     | 0.48              |
| 1:E:442:GLN:N       | 1:E:452:LYS:O    | 2.25                     | 0.48              |
| 1:E:507:LEU:HB3     | 1:E:512:ILE:HG13 | 1.95                     | 0.48              |
| 1:E:426:PHE:HE1     | 1:E:474:VAL:HB   | 1.77                     | 0.48              |
| 2:G:2:TYR:C         | 2:G:3:ALC:HD12   | 2.38                     | 0.48              |
| 1:A:513[A]:GLN:HE21 | 1:A:517:ARG:HH21 | 1.60                     | 0.48              |
| 1:F:563:THR:O       | 1:F:564:ALA:C    | 2.57                     | 0.48              |
| 1:A:496:GLU:HG2     | 1:A:497:GLN:N    | 2.29                     | 0.47              |
| 1:B:554:GLY:C       | 1:B:556:LYS:N    | 2.57                     | 0.47              |
| 1:F:473:GLU:HB3     | 1:F:491:LYS:NZ   | 2.29                     | 0.47              |
| 1:F:477:ASP:O       | 1:F:484:LEU:HA   | 2.14                     | 0.47              |
| 2:H:0:LYS:HG2       | 2:H:1:LEU:N      | 2.28                     | 0.47              |
| 1:A:411:LEU:HD11    | 1:A:424:GLN:HB3  | 1.96                     | 0.47              |
| 1:B:438[B]:ILE:HG21 | 1:B:457:PHE:CE2  | 2.48                     | 0.47              |
| 1:E:426:PHE:CD1     | 1:E:474:VAL:CG2  | 2.97                     | 0.47              |
| 1:A:513[A]:GLN:NE2  | 1:A:517:ARG:NH2  | 2.60                     | 0.47              |
| 1:A:532:LEU:HD21    | 1:A:579:GLU:HG2  | 1.96                     | 0.47              |
| 1:A:569:LEU:O       | 1:A:573:GLU:HB3  | 2.15                     | 0.47              |
| 1:A:390:LEU:N       | 1:A:390:LEU:CD2  | 2.76                     | 0.47              |
| 1:A:424:GLN:HG3     | 1:A:425:VAL:N    | 2.30                     | 0.47              |
| 1:B:399:LEU:O       | 1:B:410:THR:HG23 | 2.15                     | 0.47              |
| 1:B:569:LEU:O       | 1:B:570:THR:C    | 2.57                     | 0.47              |
| 1:B:584:ILE:HG22    | 1:B:588:MET:HE1  | 1.88                     | 0.47              |
| 1:F:599:MET:SD      | 4:F:847:HOH:O    | 2.61                     | 0.47              |
| 1:A:555:ASP:C       | 1:A:557:LEU:H    | 2.21                     | 0.47              |
| 1:A:460:ASP:OD1     | 1:A:460:ASP:O    | 2.32                     | 0.47              |
| 1:E:507:LEU:HB3     | 1:E:512:ILE:CG1  | 2.45                     | 0.47              |
| 1:E:546:THR:C       | 1:E:548:LYS:H    | 2.22                     | 0.47              |
| 1:F:485:HIS:CE1     | 1:F:500:THR:HG23 | 2.49                     | 0.47              |
| 1:A:413:ALA:O       | 1:A:416:THR:OG1  | 2.24                     | 0.47              |
| 1:A:556:LYS:CG      | 1:A:562:LYS:HD3  | 2.44                     | 0.47              |
| 1:E:398:SER:HB2     | 1:E:443:GLY:O    | 2.15                     | 0.47              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:E:403:THR:HG21    | 2:H:2:TYR:HB3      | 1.97                     | 0.47              |
| 1:E:542:LEU:HD12    | 1:E:542:LEU:HA     | 1.52                     | 0.47              |
| 1:F:412:ILE:HD13    | 1:F:478:ILE:CD1    | 2.44                     | 0.47              |
| 1:F:534:GLN:O       | 1:F:537:ASN:HB2    | 2.13                     | 0.47              |
| 1:F:542:LEU:HD21    | 1:F:591:LEU:HG     | 1.95                     | 0.47              |
| 1:F:559:ALA:O       | 1:F:563:THR:HG23   | 2.14                     | 0.47              |
| 1:B:547:ARG:O       | 1:B:551:GLU:HB2    | 2.15                     | 0.47              |
| 1:E:425[B]:VAL:HG13 | 1:E:473:GLU:OE1    | 2.14                     | 0.47              |
| 1:E:546:THR:HG21    | 1:E:569:LEU:HD21   | 1.96                     | 0.47              |
| 1:F:428:THR:HB      | 1:F:433:GLN:HB3    | 1.97                     | 0.47              |
| 1:A:548:LYS:O       | 1:A:549:GLN:C      | 2.56                     | 0.47              |
| 1:B:514[A]:LYS:O    | 1:B:515:MET:C      | 2.57                     | 0.47              |
| 1:B:545[A]:SER:O    | 1:B:549:GLN:N      | 2.48                     | 0.47              |
| 1:B:472:ILE:HA      | 1:B:489:LYS:O      | 2.15                     | 0.47              |
| 1:E:517[B]:ARG:O    | 1:E:521:ALA:HB2    | 2.15                     | 0.47              |
| 1:F:542:LEU:HG      | 1:F:591:LEU:CD2    | 2.44                     | 0.47              |
| 1:A:497:GLN:CG      | 1:A:498:LYS:H      | 2.25                     | 0.46              |
| 1:B:411:LEU:HD11    | 1:B:474:VAL:CG1    | 2.44                     | 0.46              |
| 1:B:586:ALA:C       | 1:B:588:MET:N      | 2.72                     | 0.46              |
| 1:B:589:GLN:O       | 1:B:589:GLN:HG3    | 2.15                     | 0.46              |
| 2:G:9:PRO:CB        | 2:G:10:PRO:HD2     | 2.44                     | 0.46              |
| 1:B:439:HIS:CE1     | 1:B:441:LEU:HD21   | 2.50                     | 0.46              |
| 1:B:549:GLN:CG      | 1:B:598:LEU:HG     | 2.46                     | 0.46              |
| 1:E:517[A]:ARG:HH11 | 1:E:517[A]:ARG:CB  | 2.19                     | 0.46              |
| 1:F:513:GLN:CG      | 1:F:517:ARG:NH2    | 2.71                     | 0.46              |
| 1:B:508:ASN:O       | 1:B:512:ILE:HG13   | 2.15                     | 0.46              |
| 1:B:589:GLN:O       | 1:B:593:GLN:HG3    | 2.16                     | 0.46              |
| 1:B:476:PHE:HE1     | 1:B:486:VAL:HG11   | 1.79                     | 0.46              |
| 1:A:462[B]:ILE:O    | 1:A:462[B]:ILE:CG2 | 2.64                     | 0.46              |
| 1:A:594:VAL:O       | 1:A:594:VAL:HG23   | 2.15                     | 0.46              |
| 1:B:550:VAL:CG1     | 1:B:557:LEU:CD2    | 2.80                     | 0.46              |
| 1:B:559:ALA:O       | 1:B:563:THR:OG1    | 2.34                     | 0.46              |
| 1:E:442:GLN:HB3     | 1:E:452:LYS:HB3    | 1.98                     | 0.46              |
| 1:E:514:LYS:O       | 1:E:518:ASP:HB2    | 2.15                     | 0.46              |
| 1:F:475:THR:N       | 1:F:487:SER:O      | 2.40                     | 0.46              |
| 1:F:504:SER:O       | 1:F:505:SER:C      | 2.59                     | 0.46              |
| 1:A:446:LYS:HG3     | 1:A:526:ASP:HB3    | 1.97                     | 0.46              |
| 1:A:596:GLN:O       | 1:A:599:MET:CB     | 2.63                     | 0.46              |
| 1:E:412:ILE:HD11    | 1:E:476:PHE:HB3    | 1.98                     | 0.46              |
| 1:E:570:THR:O       | 1:E:570:THR:CG2    | 2.64                     | 0.46              |
| 1:E:597:LYS:O       | 1:E:597:LYS:HG2    | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:558:PRO:HG2   | 1:F:561:ASP:CG    | 2.40                     | 0.46              |
| 1:F:585:GLU:HA    | 1:F:588:MET:CE    | 2.46                     | 0.46              |
| 1:E:421:LYS:HD2   | 1:E:477:ASP:OD1   | 2.16                     | 0.46              |
| 1:E:508:ASN:O     | 1:E:509:GLU:C     | 2.58                     | 0.46              |
| 1:F:473:GLU:O     | 1:F:488:ALA:HA    | 2.15                     | 0.46              |
| 1:A:496:GLU:HG2   | 1:A:497:GLN:H     | 1.81                     | 0.46              |
| 1:B:469:MET:HB3   | 1:F:469:MET:HE3   | 1.97                     | 0.46              |
| 1:B:446:LYS:HE3   | 1:B:446:LYS:CA    | 2.45                     | 0.46              |
| 1:E:402:GLU:CD    | 1:E:439:HIS:CE1   | 2.94                     | 0.46              |
| 1:A:517:ARG:C     | 1:A:519:ALA:H     | 2.24                     | 0.46              |
| 1:A:524:GLU:HA    | 1:A:524:GLU:OE1   | 2.16                     | 0.46              |
| 1:B:446:LYS:HE3   | 1:B:446:LYS:HA    | 1.97                     | 0.46              |
| 1:E:446[A]:LYS:HA | 1:E:446[A]:LYS:CE | 2.46                     | 0.46              |
| 1:F:466:PRO:O     | 1:F:469:MET:HB2   | 2.15                     | 0.46              |
| 1:A:527:ARG:O     | 1:A:530:GLU:N     | 2.49                     | 0.45              |
| 1:A:535:THR:OG1   | 1:A:581:LYS:HE2   | 2.16                     | 0.45              |
| 1:B:472:ILE:N     | 1:B:472:ILE:HD13  | 2.31                     | 0.45              |
| 1:E:437:THR:O     | 1:E:437:THR:HG23  | 2.16                     | 0.45              |
| 1:F:478:ILE:HG12  | 1:F:484:LEU:CD1   | 2.46                     | 0.45              |
| 1:F:530:GLU:C     | 1:F:532:LEU:N     | 2.73                     | 0.45              |
| 1:A:411:LEU:HD13  | 1:A:411:LEU:HA    | 1.86                     | 0.45              |
| 1:A:543:LEU:CD2   | 1:A:576:LEU:CD1   | 2.94                     | 0.45              |
| 1:A:561:ASP:C     | 1:A:561:ASP:OD1   | 2.59                     | 0.45              |
| 1:B:447:ARG:NH2   | 1:B:529:PHE:HD1   | 2.13                     | 0.45              |
| 1:B:454:LEU:CB    | 1:B:501:ILE:HD13  | 2.47                     | 0.45              |
| 1:F:412:ILE:HD13  | 1:F:478:ILE:HD12  | 1.98                     | 0.45              |
| 1:F:592:ALA:C     | 1:F:594:VAL:N     | 2.74                     | 0.45              |
| 1:B:447:ARG:O     | 1:B:450:ASP:N     | 2.48                     | 0.45              |
| 1:B:509:GLU:O     | 1:B:512:ILE:HB    | 2.16                     | 0.45              |
| 1:B:569:LEU:C     | 1:B:571:ALA:N     | 2.72                     | 0.45              |
| 1:F:552:GLU:OE1   | 1:F:602:ALA:HB1   | 2.17                     | 0.45              |
| 1:B:532:LEU:HD21  | 1:B:579:GLU:HA    | 1.98                     | 0.45              |
| 1:B:543:LEU:HD23  | 1:B:543:LEU:O     | 2.17                     | 0.45              |
| 1:E:467:ARG:HD3   | 4:E:1172:HOH:O    | 2.17                     | 0.45              |
| 1:F:479:ASP:C     | 1:F:481:ASP:N     | 2.73                     | 0.45              |
| 1:A:507:LEU:HD22  | 1:A:511:GLU:CB    | 2.45                     | 0.45              |
| 1:B:580:ASP:OD2   | 1:B:583:ALA:HB2   | 2.16                     | 0.45              |
| 1:B:440:VAL:HG21  | 1:B:486:VAL:HG21  | 1.97                     | 0.45              |
| 1:B:442:GLN:HB3   | 1:B:454:LEU:HD21  | 1.99                     | 0.45              |
| 1:B:542:LEU:HD13  | 4:B:716:HOH:O     | 2.16                     | 0.45              |
| 1:B:434:SER:C     | 1:B:462:ILE:HB    | 2.41                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:B:471:GLN:O       | 1:B:491:LYS:HB2     | 2.17                     | 0.45              |
| 1:B:493:SER:HB2     | 4:B:795:HOH:O       | 2.17                     | 0.45              |
| 1:F:470:PRO:C       | 1:F:471[B]:GLN:HE21 | 2.25                     | 0.45              |
| 1:A:557:LEU:HD12    | 1:A:557:LEU:HA      | 1.78                     | 0.45              |
| 1:B:452:LYS:CB      | 1:B:507:LEU:HG      | 2.44                     | 0.45              |
| 1:B:502[C]:LYS:H    | 1:B:502[C]:LYS:HG2  | 1.56                     | 0.45              |
| 1:B:572:LEU:HA      | 1:B:587:LYS:HB3     | 1.99                     | 0.45              |
| 1:E:507:LEU:O       | 1:E:512:ILE:HD11    | 2.17                     | 0.45              |
| 1:A:418:ILE:HG22    | 1:A:419:PRO:HA      | 1.97                     | 0.45              |
| 1:F:538:GLN:C       | 1:F:541:HIS:HB2     | 2.42                     | 0.45              |
| 2:G:4:LEU:HD23      | 2:G:4:LEU:HA        | 1.67                     | 0.45              |
| 1:E:390:LEU:HD23    | 1:E:390:LEU:HA      | 1.65                     | 0.44              |
| 1:E:396:PRO:HB2     | 1:E:512:ILE:HD13    | 1.99                     | 0.44              |
| 1:F:430:GLU:CD      | 1:F:544:HIS:NE2     | 2.75                     | 0.44              |
| 1:B:587:LYS:HA      | 1:B:587:LYS:HD3     | 1.63                     | 0.44              |
| 1:F:532:LEU:C       | 1:F:534:GLN:H       | 2.25                     | 0.44              |
| 1:A:487:SER:HB3     | 1:A:498:LYS:HG3     | 2.00                     | 0.44              |
| 1:B:514[B]:LYS:O    | 1:B:515:MET:C       | 2.60                     | 0.44              |
| 1:E:419:PRO:HA      | 1:E:478:ILE:O       | 2.18                     | 0.44              |
| 1:E:517[A]:ARG:O    | 2:G:8:THR:HG21      | 2.18                     | 0.44              |
| 1:F:437:THR:C       | 1:F:438:ILE:HD13    | 2.42                     | 0.44              |
| 1:F:437:THR:O       | 1:F:438:ILE:HD13    | 2.17                     | 0.44              |
| 1:A:562:LYS:O       | 1:A:566:GLU:HG3     | 2.17                     | 0.44              |
| 1:B:571:ALA:C       | 1:B:573:GLU:N       | 2.72                     | 0.44              |
| 1:E:425[A]:VAL:CG2  | 1:E:473:GLU:OE1     | 2.64                     | 0.44              |
| 1:E:561:ASP:CG      | 1:E:597:LYS:HE2     | 2.42                     | 0.44              |
| 1:E:573[A]:GLU:O    | 1:E:573[A]:GLU:HG2  | 2.18                     | 0.44              |
| 1:F:532:LEU:HA      | 1:F:532:LEU:HD12    | 1.79                     | 0.44              |
| 1:F:574:THR:CG2     | 1:F:575:ALA:H       | 2.23                     | 0.44              |
| 1:B:404:MET:HE3     | 1:B:537:ASN:ND2     | 2.33                     | 0.44              |
| 1:E:438[B]:ILE:HG22 | 1:E:457:PHE:CG      | 2.52                     | 0.44              |
| 1:E:543:LEU:HD21    | 1:E:547:ARG:CZ      | 2.47                     | 0.44              |
| 1:F:527:ARG:C       | 1:F:530:GLU:HB2     | 2.43                     | 0.44              |
| 1:B:433:GLN:O       | 1:B:462:ILE:CG2     | 2.66                     | 0.44              |
| 1:B:595:SER:O       | 1:B:598:LEU:N       | 2.51                     | 0.44              |
| 1:E:426:PHE:HD1     | 1:E:474:VAL:CG2     | 2.31                     | 0.44              |
| 1:E:437:THR:HG23    | 1:E:439:HIS:NE2     | 2.29                     | 0.44              |
| 1:E:492:ASN:HB3     | 4:E:1030:HOH:O      | 2.18                     | 0.44              |
| 1:E:546:THR:CG2     | 1:E:569:LEU:HD21    | 2.48                     | 0.44              |
| 1:E:508:ASN:O       | 1:E:512:ILE:HG13    | 2.17                     | 0.44              |
| 1:E:541:HIS:O       | 1:E:545:SER:N       | 2.51                     | 0.44              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:E:543:LEU:HD11    | 1:E:573[B]:GLU:CD   | 2.42                     | 0.44              |
| 1:F:549:GLN:CG      | 1:F:598:LEU:HD21    | 2.48                     | 0.44              |
| 1:A:443:GLY:HA3     | 1:A:451:ASN:OD1     | 2.18                     | 0.44              |
| 1:A:587:LYS:HA      | 1:A:587:LYS:HD3     | 1.74                     | 0.43              |
| 1:E:535:THR:CG2     | 1:E:585:GLU:HG3     | 2.48                     | 0.43              |
| 1:E:550:VAL:HG11    | 1:E:565:ILE:CD1     | 2.48                     | 0.43              |
| 1:E:560:ASP:N       | 1:E:563:THR:HG22    | 2.33                     | 0.43              |
| 2:G:11:ARG:HG2      | 2:G:11:ARG:O        | 2.18                     | 0.43              |
| 1:B:602:ALA:HB3     | 4:B:807:HOH:O       | 2.17                     | 0.43              |
| 1:E:407:VAL:HG11    | 4:E:1103:HOH:O      | 2.17                     | 0.43              |
| 1:E:589:GLN:O       | 1:E:593:GLN:HG2     | 2.18                     | 0.43              |
| 1:F:549:GLN:CD      | 1:F:598:LEU:CD2     | 2.91                     | 0.43              |
| 1:B:448:ALA:O       | 1:B:450:ASP:N       | 2.51                     | 0.43              |
| 1:E:514:LYS:NZ      | 4:E:1022:HOH:O      | 2.39                     | 0.43              |
| 1:A:462[A]:ILE:HD13 | 1:A:472[A]:ILE:HD11 | 2.00                     | 0.43              |
| 1:B:397:LEU:HD12    | 4:B:705:HOH:O       | 2.18                     | 0.43              |
| 1:B:546:THR:C       | 1:B:549:GLN:H       | 2.23                     | 0.43              |
| 1:B:595:SER:O       | 1:B:598:LEU:CB      | 2.66                     | 0.43              |
| 1:B:404:MET:HG2     | 1:B:537:ASN:ND2     | 2.33                     | 0.43              |
| 1:B:434:SER:O       | 1:B:462:ILE:HB      | 2.19                     | 0.43              |
| 1:B:508:ASN:O       | 1:B:509:GLU:C       | 2.62                     | 0.43              |
| 1:E:408:MET:SD      | 1:E:451:ASN:CG      | 2.99                     | 0.43              |
| 1:E:425[B]:VAL:CG1  | 1:E:473:GLU:OE1     | 2.67                     | 0.43              |
| 1:B:427:SER:OG      | 1:B:468:GLY:C       | 2.61                     | 0.43              |
| 1:B:585:GLU:O       | 1:B:588:MET:HB2     | 2.18                     | 0.43              |
| 1:E:522:ASN:C       | 1:E:525:ALA:HB3     | 2.44                     | 0.43              |
| 1:A:446:LYS:CG      | 1:A:526:ASP:HB3     | 2.48                     | 0.43              |
| 1:A:546:THR:HG23    | 1:A:598:LEU:CD2     | 2.49                     | 0.43              |
| 1:B:563:THR:O       | 1:B:566:GLU:HB2     | 2.18                     | 0.43              |
| 1:B:572:LEU:HD11    | 1:B:588:MET:HG3     | 2.00                     | 0.43              |
| 1:F:402:GLU:HA      | 1:F:407:VAL:O       | 2.18                     | 0.43              |
| 1:F:546:THR:HG21    | 1:F:591:LEU:HD11    | 2.01                     | 0.43              |
| 1:F:550:VAL:C       | 1:F:552:GLU:N       | 2.75                     | 0.43              |
| 1:B:447:ARG:CZ      | 1:B:529:PHE:CD1     | 3.01                     | 0.43              |
| 1:E:391:LEU:HD13    | 1:E:391:LEU:C       | 2.43                     | 0.43              |
| 1:E:398:SER:H       | 1:E:414:LYS:HB3     | 1.82                     | 0.43              |
| 1:E:462:ILE:HD11    | 1:E:470:PRO:HG2     | 2.00                     | 0.43              |
| 1:E:550:VAL:HG11    | 1:E:565:ILE:HD13    | 2.01                     | 0.43              |
| 1:A:565:ILE:CD1     | 1:A:595:SER:HA      | 2.41                     | 0.42              |
| 1:F:490:ASP:OD1     | 1:F:490:ASP:C       | 2.62                     | 0.42              |
| 2:H:0:LYS:CG        | 2:H:1:LEU:N         | 2.82                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:B:413:ALA:O      | 1:B:414:LYS:C     | 2.62                     | 0.42              |
| 1:B:450:ASP:O      | 1:B:515:MET:HE1   | 2.19                     | 0.42              |
| 1:B:534:GLN:O      | 1:B:538:GLN:OE1   | 2.37                     | 0.42              |
| 1:E:395:THR:HA     | 4:E:1019:HOH:O    | 2.19                     | 0.42              |
| 1:B:394:VAL:HG11   | 1:B:415:ASN:HB3   | 2.01                     | 0.42              |
| 1:E:513:GLN:HG2    | 1:E:517[A]:ARG:CD | 2.48                     | 0.42              |
| 1:F:411:LEU:CA     | 1:F:422:HIS:HD2   | 2.32                     | 0.42              |
| 1:F:446[B]:LYS:NZ  | 1:F:530:GLU:CD    | 2.77                     | 0.42              |
| 1:F:553:ALA:O      | 1:F:554:GLY:C     | 2.63                     | 0.42              |
| 1:A:532:LEU:HB2    | 4:A:675:HOH:O     | 2.20                     | 0.42              |
| 1:B:403:THR:O      | 1:B:404:MET:C     | 2.62                     | 0.42              |
| 1:F:481:ASP:HB2    | 1:F:483:ILE:HG13  | 2.01                     | 0.42              |
| 1:A:576:LEU:HA     | 1:A:576:LEU:HD23  | 1.79                     | 0.42              |
| 1:E:596:GLN:C      | 1:E:598:LEU:H     | 2.26                     | 0.42              |
| 1:B:543:LEU:HD21   | 4:B:909:HOH:O     | 2.20                     | 0.42              |
| 1:B:543:LEU:CD2    | 1:B:547:ARG:NH1   | 2.80                     | 0.42              |
| 1:B:568:ALA:O      | 1:B:571:ALA:HB3   | 2.19                     | 0.42              |
| 1:B:590:GLU:O      | 1:B:593:GLN:HB2   | 2.20                     | 0.42              |
| 1:F:573:GLU:O      | 1:F:576:LEU:CB    | 2.68                     | 0.42              |
| 1:A:570:THR:O      | 1:A:571:ALA:C     | 2.62                     | 0.42              |
| 1:E:583:ALA:O      | 1:E:584:ILE:C     | 2.62                     | 0.42              |
| 1:F:537:ASN:O      | 1:F:538:GLN:C     | 2.63                     | 0.42              |
| 1:B:392:LEU:HD13   | 1:B:417:THR:HG22  | 2.02                     | 0.42              |
| 1:B:412:ILE:HD12   | 1:B:476:PHE:HB3   | 2.00                     | 0.42              |
| 1:B:424:GLN:HE21   | 1:B:424:GLN:HB2   | 1.72                     | 0.42              |
| 1:B:516:VAL:O      | 1:B:517:ARG:C     | 2.61                     | 0.42              |
| 1:B:457:PHE:CD1    | 1:B:499:ILE:HG22  | 2.55                     | 0.42              |
| 1:E:426:PHE:HD1    | 1:E:474:VAL:HG23  | 1.84                     | 0.42              |
| 1:A:575:ALA:O      | 1:A:584:ILE:HG12  | 2.19                     | 0.42              |
| 1:E:391:LEU:HD22   | 1:E:391:LEU:C     | 2.45                     | 0.42              |
| 1:E:546:THR:C      | 1:E:548:LYS:N     | 2.76                     | 0.42              |
| 1:F:445:ARG:NH1    | 1:F:522:ASN:HB3   | 2.34                     | 0.42              |
| 1:F:454:LEU:HD23   | 1:F:454:LEU:HA    | 1.86                     | 0.42              |
| 1:A:508:ASN:OD1    | 1:A:511:GLU:OE1   | 2.38                     | 0.41              |
| 1:E:590:GLU:C      | 1:E:592:ALA:N     | 2.73                     | 0.41              |
| 1:F:391:LEU:HD23   | 1:F:391:LEU:O     | 2.20                     | 0.41              |
| 1:A:442:GLN:O      | 1:A:451:ASN:HB3   | 2.20                     | 0.41              |
| 1:A:508:ASN:HB2    | 1:A:509:GLU:H     | 1.68                     | 0.41              |
| 1:B:470:PRO:HB2    | 4:B:784:HOH:O     | 2.19                     | 0.41              |
| 1:E:446[A]:LYS:HG2 | 1:E:526:ASP:HB3   | 1.94                     | 0.41              |
| 1:A:595:SER:O      | 1:A:598:LEU:N     | 2.47                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:599:MET:HE3    | 4:A:690:HOH:O      | 2.20                     | 0.41              |
| 1:B:595:SER:CB     | 1:B:599:MET:HE3    | 2.50                     | 0.41              |
| 1:E:517[A]:ARG:O   | 1:E:521:ALA:HB2    | 2.20                     | 0.41              |
| 1:E:533:VAL:HG12   | 1:E:537:ASN:ND2    | 2.34                     | 0.41              |
| 1:F:397:LEU:HD23   | 1:F:397:LEU:HA     | 1.88                     | 0.41              |
| 1:F:466:PRO:O      | 1:F:467:ARG:C      | 2.63                     | 0.41              |
| 1:F:522:ASN:OD1    | 4:F:798:HOH:O      | 2.21                     | 0.41              |
| 1:F:565:ILE:HD13   | 1:F:598:LEU:HD12   | 2.02                     | 0.41              |
| 1:E:527:ARG:NH1    | 1:E:531:GLU:CD     | 2.79                     | 0.41              |
| 1:B:493:SER:C      | 1:B:495:LYS:N      | 2.78                     | 0.41              |
| 1:F:488:ALA:O      | 1:F:496:GLU:HG3    | 2.20                     | 0.41              |
| 1:A:546:THR:O      | 1:A:546:THR:HG22   | 2.21                     | 0.41              |
| 1:B:394:VAL:HG21   | 1:B:415:ASN:HD22   | 1.86                     | 0.41              |
| 1:B:478:ILE:HG23   | 1:B:483:ILE:C      | 2.46                     | 0.41              |
| 1:B:598:LEU:C      | 1:B:600:GLU:N      | 2.78                     | 0.41              |
| 1:E:417:THR:HG22   | 1:E:418:ILE:N      | 2.35                     | 0.41              |
| 1:F:531[B]:GLU:HA  | 1:F:534:GLN:HE21   | 1.86                     | 0.41              |
| 1:B:394:VAL:HG21   | 1:B:415:ASN:HA     | 2.01                     | 0.41              |
| 1:B:502[A]:LYS:NZ  | 1:B:502[A]:LYS:HB3 | 2.35                     | 0.41              |
| 1:E:484:LEU:CD2    | 1:E:501:ILE:HD12   | 2.50                     | 0.41              |
| 1:F:552:GLU:C      | 1:F:554:GLY:H      | 2.28                     | 0.41              |
| 1:B:445:ARG:C      | 1:B:447:ARG:H      | 2.28                     | 0.41              |
| 1:B:519:ALA:O      | 1:B:520:GLU:C      | 2.64                     | 0.41              |
| 1:E:449:ALA:O      | 1:F:452:LYS:NZ     | 2.44                     | 0.41              |
| 1:E:454:LEU:HB2    | 1:E:501:ILE:HD13   | 2.01                     | 0.41              |
| 1:E:517[A]:ARG:HB2 | 1:E:517[A]:ARG:NH1 | 2.19                     | 0.41              |
| 1:A:446:LYS:HD2    | 1:A:530:GLU:OE2    | 2.21                     | 0.41              |
| 1:A:558:PRO:O      | 1:A:559:ALA:HB3    | 2.20                     | 0.41              |
| 1:B:441:LEU:HD22   | 4:B:701:HOH:O      | 2.21                     | 0.41              |
| 1:B:478:ILE:HD11   | 1:B:484:LEU:HD13   | 2.02                     | 0.41              |
| 1:B:518:ASP:O      | 1:B:522:ASN:ND2    | 2.39                     | 0.41              |
| 1:B:530:GLU:O      | 1:B:531:GLU:C      | 2.64                     | 0.41              |
| 1:B:539:GLY:HA2    | 1:B:588:MET:CE     | 2.51                     | 0.41              |
| 1:B:572:LEU:CD1    | 1:B:588:MET:CE     | 2.87                     | 0.41              |
| 1:E:412:ILE:HD11   | 1:E:476:PHE:CB     | 2.51                     | 0.41              |
| 1:F:401:ILE:HD11   | 1:F:426:PHE:CZ     | 2.55                     | 0.41              |
| 1:F:478:ILE:CG1    | 1:F:484:LEU:HD13   | 2.50                     | 0.41              |
| 1:F:531[A]:GLU:HA  | 1:F:534:GLN:HE21   | 1.86                     | 0.41              |
| 1:F:543:LEU:CD2    | 1:F:547:ARG:NH1    | 2.84                     | 0.41              |
| 1:F:565:ILE:O      | 1:F:569:LEU:HG     | 2.20                     | 0.41              |
| 1:A:517:ARG:C      | 1:A:519:ALA:N      | 2.79                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:B:515:MET:O       | 1:B:516:VAL:C      | 2.64                     | 0.41              |
| 1:E:542:LEU:HD23    | 1:E:591:LEU:HD23   | 2.03                     | 0.41              |
| 1:F:407:VAL:HG13    | 1:F:446[B]:LYS:HD2 | 2.02                     | 0.41              |
| 1:F:469:MET:CB      | 1:F:470:PRO:HD3    | 2.51                     | 0.41              |
| 1:F:553:ALA:CB      | 1:F:601:ILE:CG2    | 2.65                     | 0.41              |
| 1:A:433:GLN:O       | 1:A:462[B]:ILE:CG2 | 2.69                     | 0.40              |
| 1:B:461:GLY:HA3     | 1:B:495:LYS:HE3    | 2.03                     | 0.40              |
| 1:B:499:ILE:HG12    | 1:B:500:THR:N      | 2.29                     | 0.40              |
| 1:F:535:THR:HA      | 1:F:538:GLN:OE1    | 2.21                     | 0.40              |
| 1:A:472[A]:ILE:HD13 | 1:A:490:ASP:CA     | 2.51                     | 0.40              |
| 1:B:391:LEU:HD23    | 1:B:391:LEU:O      | 2.20                     | 0.40              |
| 1:F:402:GLU:CG      | 1:F:403:THR:H      | 2.32                     | 0.40              |
| 1:F:550:VAL:O       | 1:F:552:GLU:N      | 2.54                     | 0.40              |
| 1:B:490:ASP:OD2     | 1:B:493:SER:OG     | 2.33                     | 0.40              |
| 1:F:487:SER:CB      | 1:F:498:LYS:CG     | 2.97                     | 0.40              |
| 1:F:575:ALA:HB3     | 4:F:925:HOH:O      | 2.20                     | 0.40              |
| 1:A:431:ASP:O       | 1:A:432:ASN:HB2    | 2.21                     | 0.40              |
| 1:B:452:LYS:HB2     | 1:B:507:LEU:CG     | 2.48                     | 0.40              |
| 1:B:532:LEU:CD1     | 1:B:581:LYS:HG3    | 2.49                     | 0.40              |
| 1:E:391:LEU:O       | 1:E:392:LEU:CG     | 2.66                     | 0.40              |
| 1:E:513:GLN:O       | 1:E:517[B]:ARG:CD  | 2.38                     | 0.40              |
| 1:A:559:ALA:C       | 1:A:561:ASP:H      | 2.23                     | 0.40              |
| 1:B:441:LEU:CD1     | 1:B:448:ALA:HB1    | 2.51                     | 0.40              |
| 1:B:543:LEU:HD23    | 1:B:547:ARG:HD3    | 2.02                     | 0.40              |
| 1:E:392:LEU:HD23    | 1:E:392:LEU:HA     | 1.87                     | 0.40              |
| 1:E:497:GLN:HG3     | 1:E:498:LYS:N      | 2.37                     | 0.40              |
| 1:E:526:ASP:C       | 1:E:528:LYS:H      | 2.29                     | 0.40              |
| 1:F:532:LEU:HA      | 1:F:581:LYS:HD3    | 2.03                     | 0.40              |
| 1:F:544:HIS:O       | 1:F:546:THR:N      | 2.54                     | 0.40              |

All (1) 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:B:503:ALA:CB | 1:E:390:LEU:CD1[3_545] | 2.14                     | 0.06              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 215/219 (98%) | 183 (85%) | 23 (11%) | 9 (4%)   | 2           | 3   |
| 1   | B     | 216/219 (99%) | 177 (82%) | 29 (13%) | 10 (5%)  | 2           | 2   |
| 1   | E     | 208/219 (95%) | 186 (89%) | 18 (9%)  | 4 (2%)   | 6           | 13  |
| 1   | F     | 216/219 (99%) | 173 (80%) | 23 (11%) | 20 (9%)  | 0           | 0   |
| 2   | C     | 9/20 (45%)    | 7 (78%)   | 1 (11%)  | 1 (11%)  | 0           | 0   |
| 2   | D     | 6/20 (30%)    | 6 (100%)  | 0        | 0        | 100         | 100 |
| 2   | G     | 10/20 (50%)   | 7 (70%)   | 3 (30%)  | 0        | 100         | 100 |
| 2   | H     | 7/20 (35%)    | 5 (71%)   | 1 (14%)  | 1 (14%)  | 0           | 0   |
| All | All   | 887/956 (93%) | 744 (84%) | 98 (11%) | 45 (5%)  | 1           | 2   |

All (45) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 548 | LYS  |
| 1   | A     | 549 | GLN  |
| 1   | A     | 596 | GLN  |
| 1   | B     | 600 | GLU  |
| 1   | B     | 601 | ILE  |
| 1   | E     | 561 | ASP  |
| 1   | F     | 448 | ALA  |
| 1   | F     | 530 | GLU  |
| 1   | F     | 532 | LEU  |
| 1   | F     | 533 | VAL  |
| 1   | F     | 538 | GLN  |
| 1   | F     | 574 | THR  |
| 1   | F     | 575 | ALA  |
| 1   | F     | 593 | GLN  |
| 1   | A     | 544 | HIS  |
| 1   | A     | 557 | LEU  |
| 1   | A     | 559 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 509 | GLU  |
| 1   | B     | 516 | VAL  |
| 1   | B     | 559 | ALA  |
| 1   | E     | 523 | ALA  |
| 1   | E     | 543 | LEU  |
| 1   | F     | 505 | SER  |
| 1   | F     | 543 | LEU  |
| 1   | F     | 554 | GLY  |
| 1   | F     | 559 | ALA  |
| 1   | F     | 571 | ALA  |
| 2   | C     | 10  | PRO  |
| 1   | A     | 558 | PRO  |
| 1   | B     | 414 | LYS  |
| 1   | B     | 495 | LYS  |
| 1   | F     | 523 | ALA  |
| 1   | F     | 529 | PHE  |
| 1   | F     | 541 | HIS  |
| 1   | F     | 592 | ALA  |
| 2   | H     | 5   | PRO  |
| 1   | A     | 564 | ALA  |
| 1   | B     | 431 | ASP  |
| 1   | B     | 563 | THR  |
| 1   | B     | 581 | LYS  |
| 1   | F     | 551 | GLU  |
| 1   | A     | 543 | LEU  |
| 1   | F     | 401 | ILE  |
| 1   | E     | 584 | ILE  |
| 1   | F     | 601 | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 179/181 (99%) | 160 (89%) | 19 (11%) | 6           | 14 |
| 1   | B     | 180/181 (99%) | 160 (89%) | 20 (11%) | 6           | 12 |
| 1   | E     | 179/181 (99%) | 153 (86%) | 26 (14%) | 3           | 6  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 1   | F     | 181/181 (100%) | 161 (89%) | 20 (11%) | 6           | 13  |
| 2   | C     | 11/19 (58%)    | 10 (91%)  | 1 (9%)   | 9           | 19  |
| 2   | D     | 8/19 (42%)     | 8 (100%)  | 0        | 100         | 100 |
| 2   | G     | 11/19 (58%)    | 11 (100%) | 0        | 100         | 100 |
| 2   | H     | 9/19 (47%)     | 8 (89%)   | 1 (11%)  | 6           | 12  |
| All | All   | 758/800 (95%)  | 671 (88%) | 87 (12%) | 6           | 11  |

All (87) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 390    | LEU  |
| 1   | A     | 391    | LEU  |
| 1   | A     | 395    | THR  |
| 1   | A     | 401    | ILE  |
| 1   | A     | 411    | LEU  |
| 1   | A     | 418    | ILE  |
| 1   | A     | 424    | GLN  |
| 1   | A     | 462[A] | ILE  |
| 1   | A     | 462[B] | ILE  |
| 1   | A     | 473    | GLU  |
| 1   | A     | 498    | LYS  |
| 1   | A     | 520    | GLU  |
| 1   | A     | 526    | ASP  |
| 1   | A     | 528    | LYS  |
| 1   | A     | 550    | VAL  |
| 1   | A     | 556    | LYS  |
| 1   | A     | 557    | LEU  |
| 1   | A     | 567    | SER  |
| 1   | A     | 600    | GLU  |
| 1   | B     | 411    | LEU  |
| 1   | B     | 418    | ILE  |
| 1   | B     | 420    | THR  |
| 1   | B     | 421[A] | LYS  |
| 1   | B     | 421[B] | LYS  |
| 1   | B     | 423    | SER  |
| 1   | B     | 427    | SER  |
| 1   | B     | 446    | LYS  |
| 1   | B     | 460    | ASP  |
| 1   | B     | 497    | GLN  |
| 1   | B     | 499    | ILE  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | B     | 504    | SER  |
| 1   | B     | 505    | SER  |
| 1   | B     | 509    | GLU  |
| 1   | B     | 518    | ASP  |
| 1   | B     | 530    | GLU  |
| 1   | B     | 533    | VAL  |
| 1   | B     | 535    | THR  |
| 1   | B     | 549    | GLN  |
| 1   | B     | 566    | GLU  |
| 1   | E     | 391    | LEU  |
| 1   | E     | 407    | VAL  |
| 1   | E     | 411[A] | LEU  |
| 1   | E     | 411[B] | LEU  |
| 1   | E     | 418    | ILE  |
| 1   | E     | 424    | GLN  |
| 1   | E     | 439    | HIS  |
| 1   | E     | 440    | VAL  |
| 1   | E     | 446[A] | LYS  |
| 1   | E     | 446[B] | LYS  |
| 1   | E     | 462    | ILE  |
| 1   | E     | 471    | GLN  |
| 1   | E     | 505    | SER  |
| 1   | E     | 507    | LEU  |
| 1   | E     | 515    | MET  |
| 1   | E     | 517[A] | ARG  |
| 1   | E     | 517[B] | ARG  |
| 1   | E     | 534    | GLN  |
| 1   | E     | 546    | THR  |
| 1   | E     | 548    | LYS  |
| 1   | E     | 550    | VAL  |
| 1   | E     | 560    | ASP  |
| 1   | E     | 573[A] | GLU  |
| 1   | E     | 573[B] | GLU  |
| 1   | E     | 577    | LYS  |
| 1   | E     | 588    | MET  |
| 1   | F     | 402    | GLU  |
| 1   | F     | 403    | THR  |
| 1   | F     | 411    | LEU  |
| 1   | F     | 420    | THR  |
| 1   | F     | 423    | SER  |
| 1   | F     | 460    | ASP  |
| 1   | F     | 469    | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 479 | ASP  |
| 1   | F     | 483 | ILE  |
| 1   | F     | 486 | VAL  |
| 1   | F     | 499 | ILE  |
| 1   | F     | 510 | ASP  |
| 1   | F     | 518 | ASP  |
| 1   | F     | 520 | GLU  |
| 1   | F     | 544 | HIS  |
| 1   | F     | 555 | ASP  |
| 1   | F     | 567 | SER  |
| 1   | F     | 572 | LEU  |
| 1   | F     | 576 | LEU  |
| 1   | F     | 595 | SER  |
| 2   | C     | 6   | ARG  |
| 2   | H     | 8   | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 415 | ASN  |
| 1   | A     | 422 | HIS  |
| 1   | A     | 424 | GLN  |
| 1   | A     | 497 | GLN  |
| 1   | A     | 593 | GLN  |
| 1   | A     | 596 | GLN  |
| 1   | B     | 415 | ASN  |
| 1   | B     | 424 | GLN  |
| 1   | B     | 458 | ASN  |
| 1   | B     | 513 | GLN  |
| 1   | B     | 534 | GLN  |
| 1   | B     | 537 | ASN  |
| 1   | B     | 541 | HIS  |
| 1   | B     | 549 | GLN  |
| 1   | B     | 593 | GLN  |
| 1   | E     | 439 | HIS  |
| 1   | E     | 458 | ASN  |
| 1   | E     | 463 | ASN  |
| 1   | E     | 497 | GLN  |
| 1   | E     | 513 | GLN  |
| 1   | E     | 538 | GLN  |
| 1   | E     | 544 | HIS  |
| 1   | F     | 422 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 424 | GLN  |
| 1   | F     | 439 | HIS  |
| 1   | F     | 456 | GLN  |
| 1   | F     | 463 | ASN  |
| 1   | F     | 492 | ASN  |
| 1   | F     | 534 | GLN  |
| 1   | F     | 544 | HIS  |
| 1   | F     | 596 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 2   | ALC  | H     | 3   | 2    | 9,11,12      | 0.54 | 0           | 11,13,15    | 1.35 | 1 (9%)      |
| 2   | ALC  | C     | 3   | 2    | 9,11,12      | 0.58 | 0           | 11,13,15    | 1.27 | 1 (9%)      |
| 2   | ALC  | G     | 3   | 2    | 9,11,12      | 0.56 | 0           | 11,13,15    | 1.32 | 1 (9%)      |
| 2   | ALC  | D     | 3   | 2    | 9,11,12      | 0.75 | 0           | 11,13,15    | 0.96 | 1 (9%)      |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | ALC  | H     | 3   | 2    | -       | 0/5/14/16 | 0/1/1/1 |
| 2   | ALC  | C     | 3   | 2    | -       | 0/5/14/16 | 0/1/1/1 |
| 2   | ALC  | G     | 3   | 2    | -       | 1/5/14/16 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | ALC  | D     | 3   | 2    | -       | 0/5/14/16 | 0/1/1/1 |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | H     | 3   | ALC  | CG-CB-CA   | -3.38 | 109.98      | 114.52   |
| 2   | C     | 3   | ALC  | CE2-CD2-CG | -2.47 | 106.89      | 112.08   |
| 2   | G     | 3   | ALC  | CB-CA-C    | -2.41 | 107.28      | 110.99   |
| 2   | D     | 3   | ALC  | CB-CG-CD2  | -2.21 | 106.57      | 111.71   |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 2   | G     | 3   | ALC  | CA-CB-CG-CD1 |

There are no ring outliers.

3 monomers are involved in 6 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | H     | 3   | ALC  | 1       | 0            |
| 2   | C     | 3   | ALC  | 3       | 0            |
| 2   | G     | 3   | ALC  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | SO4  | E     | 1001 | -    | 4,4,4        | 0.31 | 0           | 6,6,6       | 0.32 | 0           |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 2   | G     | 1                |
| 2   | H     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | G     | 3:ALC     | C      | 4:LEU     | N      | 1.63         |
| 1     | H     | 3:ALC     | C      | 4:LEU     | N      | 1.13         |

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|---------------|--------|---------------|-----------------------|---------|
| 1   | A     | 211/219 (96%) | 0.32   | 7 (3%) 49 43  | 2, 16, 38, 53         | 10 (4%) |
| 1   | B     | 211/219 (96%) | 0.65   | 15 (7%) 22 17 | 6, 27, 44, 52         | 10 (4%) |
| 1   | E     | 203/219 (92%) | 0.50   | 11 (5%) 31 26 | 6, 22, 40, 62         | 16 (7%) |
| 1   | F     | 214/219 (97%) | 0.61   | 18 (8%) 17 13 | 6, 25, 44, 51         | 9 (4%)  |
| 2   | C     | 11/20 (55%)   | 0.91   | 1 (9%) 15 11  | 18, 37, 47, 54        | 0       |
| 2   | D     | 8/20 (40%)    | 0.44   | 0 100 100     | 8, 16, 22, 24         | 1 (12%) |
| 2   | G     | 11/20 (55%)   | 1.25   | 3 (27%) 1 1   | 16, 25, 54, 61        | 1 (9%)  |
| 2   | H     | 7/20 (35%)    | 0.50   | 1 (14%) 6 5   | 17, 21, 35, 38        | 0       |
| All | All   | 876/956 (91%) | 0.53   | 56 (6%) 25 20 | 2, 23, 43, 62         | 47 (5%) |

All (56) RSRZ outliers are listed below:

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 2   | C     | 10     | PRO  | 5.1  |
| 1   | E     | 427    | SER  | 4.6  |
| 1   | A     | 548    | LYS  | 4.5  |
| 1   | F     | 531[A] | GLU  | 4.4  |
| 1   | A     | 559    | ALA  | 3.9  |
| 1   | F     | 425    | VAL  | 3.8  |
| 1   | B     | 494    | GLY  | 3.5  |
| 1   | F     | 599    | MET  | 3.4  |
| 1   | B     | 455    | GLY  | 3.2  |
| 1   | B     | 600    | GLU  | 3.1  |
| 1   | E     | 595    | SER  | 3.0  |
| 1   | F     | 545    | SER  | 3.0  |
| 1   | E     | 406    | GLY  | 2.9  |
| 1   | E     | 564    | ALA  | 2.9  |
| 2   | G     | 0      | LYS  | 2.9  |
| 1   | A     | 592    | ALA  | 2.8  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | B     | 533    | VAL  | 2.8  |
| 1   | F     | 486    | VAL  | 2.7  |
| 1   | E     | 599    | MET  | 2.7  |
| 1   | F     | 504    | SER  | 2.7  |
| 1   | F     | 553    | ALA  | 2.7  |
| 1   | B     | 435    | ALA  | 2.7  |
| 1   | A     | 567    | SER  | 2.6  |
| 1   | F     | 416    | THR  | 2.6  |
| 1   | F     | 565    | ILE  | 2.6  |
| 2   | G     | 11     | ARG  | 2.5  |
| 1   | F     | 522    | ASN  | 2.5  |
| 1   | A     | 597    | LYS  | 2.5  |
| 1   | F     | 550    | VAL  | 2.5  |
| 2   | H     | 8      | THR  | 2.5  |
| 1   | B     | 518    | ASP  | 2.5  |
| 1   | E     | 510    | ASP  | 2.5  |
| 1   | B     | 458    | ASN  | 2.4  |
| 1   | E     | 545    | SER  | 2.4  |
| 1   | F     | 479    | ASP  | 2.4  |
| 1   | F     | 469    | MET  | 2.3  |
| 1   | F     | 567    | SER  | 2.3  |
| 1   | A     | 599    | MET  | 2.3  |
| 1   | B     | 394    | VAL  | 2.3  |
| 1   | E     | 580    | ASP  | 2.3  |
| 1   | B     | 419    | PRO  | 2.2  |
| 1   | F     | 552    | GLU  | 2.2  |
| 1   | B     | 482    | GLY  | 2.2  |
| 1   | B     | 512    | ILE  | 2.2  |
| 1   | F     | 575    | ALA  | 2.2  |
| 1   | B     | 545[A] | SER  | 2.2  |
| 1   | F     | 439    | HIS  | 2.2  |
| 1   | B     | 502[A] | LYS  | 2.1  |
| 1   | F     | 482    | GLY  | 2.1  |
| 1   | E     | 527    | ARG  | 2.1  |
| 1   | E     | 577    | LYS  | 2.1  |
| 1   | A     | 449    | ALA  | 2.1  |
| 1   | B     | 505    | SER  | 2.1  |
| 1   | B     | 546    | THR  | 2.1  |
| 2   | G     | 10     | PRO  | 2.0  |
| 1   | E     | 517[A] | ARG  | 2.0  |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | ALC  | C     | 3   | 11/12 | 0.70 | 0.15 | 20,25,29,30                 | 0     |
| 2   | ALC  | G     | 3   | 11/12 | 0.79 | 0.13 | 26,28,35,36                 | 0     |
| 2   | ALC  | D     | 3   | 11/12 | 0.84 | 0.13 | 2,3,9,12                    | 0     |
| 2   | ALC  | H     | 3   | 11/12 | 0.86 | 0.12 | 19,27,31,32                 | 0     |

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | SO4  | E     | 1001 | 5/5   | 0.90 | 0.09 | 51,53,54,55                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.