



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:19 PM UTC

PDB ID : 2C5V / pdb\_00002c5v  
Title : Differential Binding Of Inhibitors To Active And Inactive Cdk2 Provides Insights For Drug Design  
Authors : Kontopidis, G.; McInnes, C.; Pandalaneni, S.R.; McNae, I.; Gibson, D.; Mezna, M.; Thomas, M.; Wood, G.; Wang, S.; Walkinshaw, M.D.; Fischer, P.M.  
Deposited on : 2005-11-02  
Resolution : 2.90 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](#) ①) 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                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

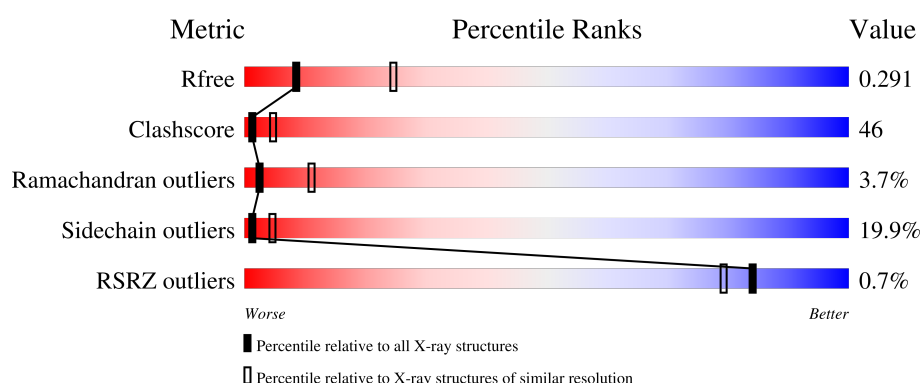
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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                      | 2481 (2.90-2.90)                                      |
| Clashscore            | 190562                      | 2690 (2.90-2.90)                                      |
| Ramachandran outliers | 187476                      | 2623 (2.90-2.90)                                      |
| Sidechain outliers    | 187428                      | 2625 (2.90-2.90)                                      |
| RSRZ outliers         | 180081                      | 2481 (2.90-2.90)                                      |

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     | 298    | <div> <div>%</div> <div> <div></div> <div>37%</div> <div>44%</div> <div>15%</div> <div>••</div> </div> </div> |
| 1   | C     | 298    | <div> <div>%</div> <div> <div></div> <div>38%</div> <div>44%</div> <div>15%</div> <div>••</div> </div> </div> |
| 2   | B     | 259    | <div> <div></div> <div> <div>36%</div> <div>50%</div> <div>13%</div> <div>•</div> </div> </div>               |
| 2   | D     | 259    | <div> <div></div> <div> <div>43%</div> <div>44%</div> <div>11%</div> <div>•</div> </div> </div>               |
| 3   | F     | 9      | <div> <div></div> <div> <div>22%</div> <div>11%</div> <div>44%</div> <div>22%</div> </div> </div>             |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 3   | H     | 9      |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3   | PFF  | F     | 508  | -         | -        | X       | -                |
| 4   | CK4  | A     | 1297 | -         | -        | X       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9289 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 CELL DIVISION PROTEIN KINASE 2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 296      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1547 | 403 | 420 | 8 |         |         |       |
| 1   | C     | 296      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2384  | 1550 | 406 | 420 | 8 |         |         |       |

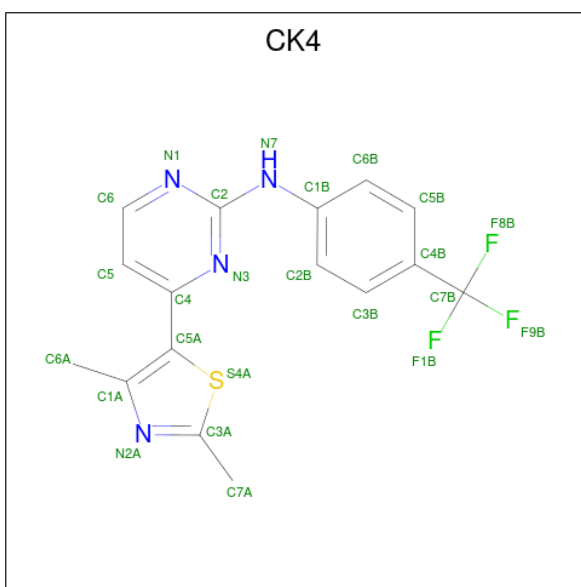
- Molecule 2 is a protein called CYCLIN A2.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 258      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2083  | 1350 | 339 | 383 | 11 |         |         |       |
| 2   | D     | 258      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2084  | 1350 | 339 | 384 | 11 |         |         |       |

- Molecule 3 is a protein called ALA-ALA-ABA-ARG-SER-LEU-ILE-PFF-NH2.

| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---|---------|---------|-------|
| 3   | F     | 9        | Total | C  | F | N  | O | 0       | 0       | 1     |
|     |       |          | 62    | 40 | 1 | 12 | 9 |         |         |       |
| 3   | H     | 9        | Total | C  | F | N  | O | 0       | 0       | 1     |
|     |       |          | 62    | 40 | 1 | 12 | 9 |         |         |       |

- Molecule 4 is 4-(2,4-DIMETHYL-1,3-THIAZOL-5-YL)-N-[4-(TRIFLUOROMETHYL)PHE NYL]PYRIMIDIN-2-AMINE (CCD ID: CK4) (formula: C<sub>16</sub>H<sub>13</sub>F<sub>3</sub>N<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 4   | A     | 1        | Total | C  | F | N | S | 0       | 0       |
|     |       |          | 24    | 16 | 3 | 4 | 1 |         |         |
| 4   | C     | 1        | Total | C  | F | N | S | 0       | 0       |
|     |       |          | 24    | 16 | 3 | 4 | 1 |         |         |

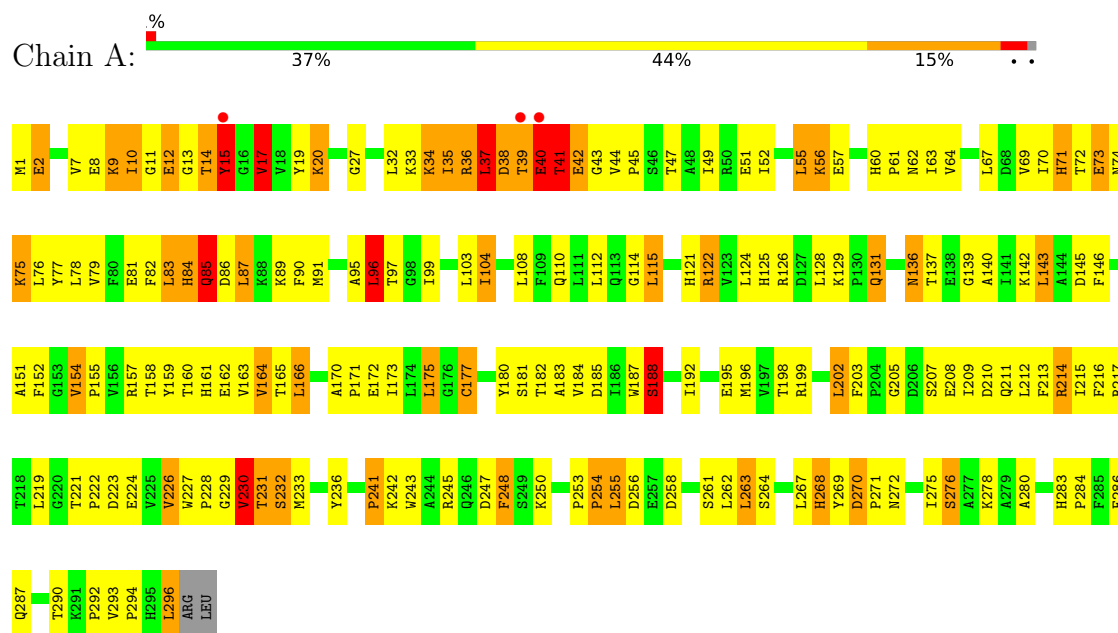
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 48       | Total | O  | 0       | 0       |
|     |       |          | 48    | 48 |         |         |
| 5   | B     | 44       | Total | O  | 0       | 0       |
|     |       |          | 44    | 44 |         |         |
| 5   | C     | 39       | Total | O  | 0       | 0       |
|     |       |          | 39    | 39 |         |         |
| 5   | D     | 52       | Total | O  | 0       | 0       |
|     |       |          | 52    | 52 |         |         |
| 5   | F     | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 5   | H     | 3        | Total | O  | 0       | 0       |
|     |       |          | 3     | 3  |         |         |

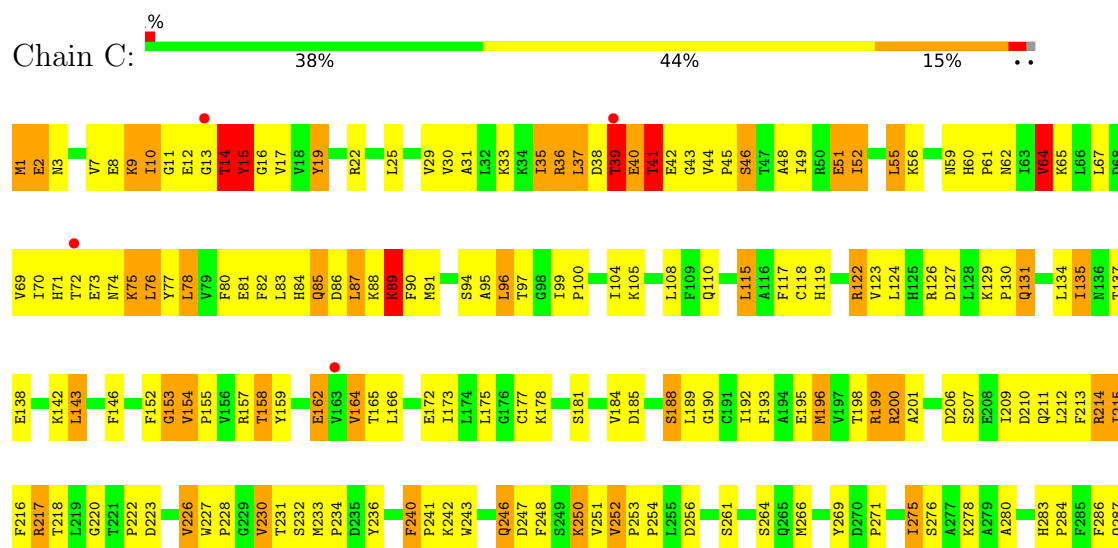
### 3 Residue-property plots

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: CELL DIVISION PROTEIN KINASE 2



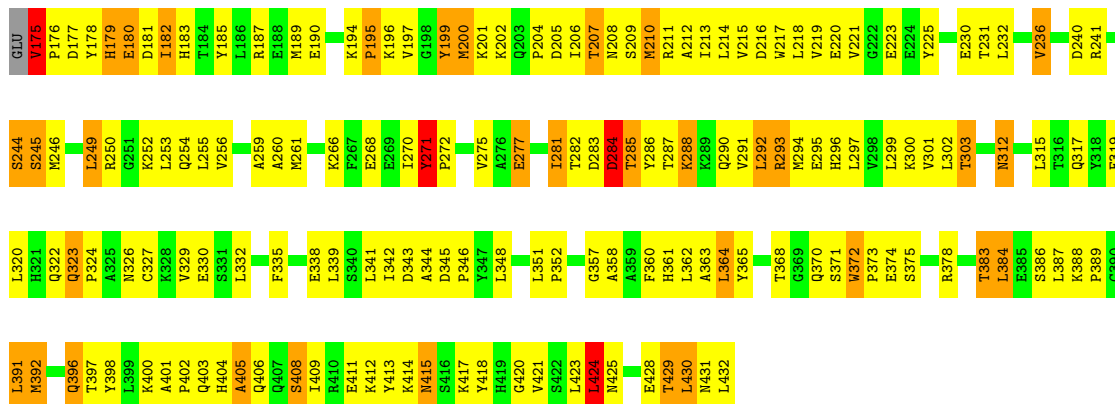
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2





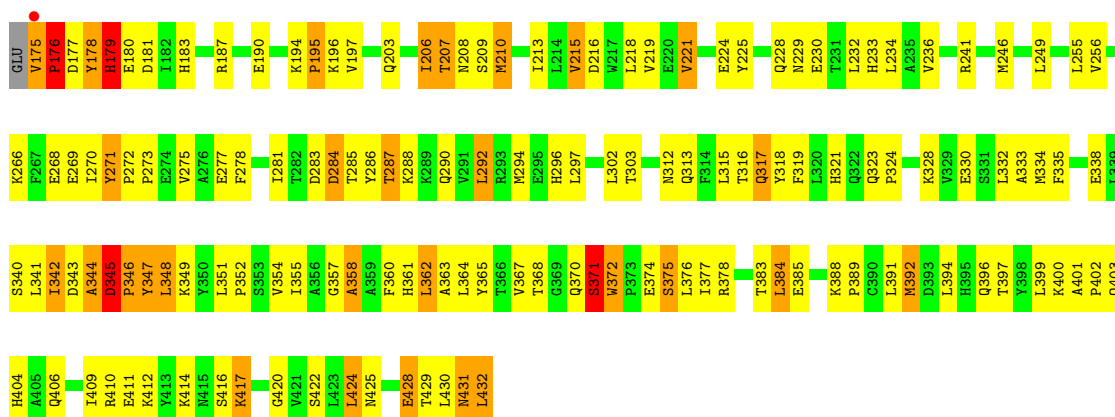
• Molecule 2: CYCLIN A2

Chain B: 36% 50% 13%



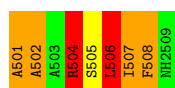
• Molecule 2: CYCLIN A2

Chain D: 43% 44% 11%



• Molecule 3: ALA-ALA-ABA-ARG-SER-LEU-ILE-PFF-NH2

Chain F: 22% 11% 44% 22%



• Molecule 3: ALA-ALA-ABA-ARG-SER-LEU-ILE-PFF-NH2

Chain H: 11% 33% 44% 11%





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 74.50Å 114.55Å 156.99Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 10.00 – 2.90<br>10.00 – 2.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 84.5 (10.00-2.90)<br>82.1 (10.00-2.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.10                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.46 (at 2.92Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0005                                             | Depositor        |
| R, $R_{free}$                                                           | 0.171 , 0.282<br>0.182 , 0.291                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1029 reflections (4.06%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 46.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.049                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 61.7                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 9289                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 38.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ABA, CK4, NH2, PFF

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     | 0.73         | 0/2440        | 1.16        | 7/3313 (0.2%)   |
| 1   | C     | 0.70         | 0/2451        | 1.13        | 13/3327 (0.4%)  |
| 2   | B     | 0.68         | 0/2133        | 1.20        | 14/2897 (0.5%)  |
| 2   | D     | 0.73         | 1/2134 (0.0%) | 1.21        | 15/2897 (0.5%)  |
| 3   | F     | 1.27         | 1/41 (2.4%)   | 1.73        | 0/52            |
| 3   | H     | 1.23         | 1/41 (2.4%)   | 2.16        | 2/52 (3.8%)     |
| All | All   | 0.72         | 3/9240 (0.0%) | 1.18        | 51/12538 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 6                   |
| 1   | C     | 0                   | 2                   |
| 2   | B     | 0                   | 4                   |
| 2   | D     | 0                   | 6                   |
| 3   | F     | 0                   | 1                   |
| 3   | H     | 0                   | 1                   |
| All | All   | 0                   | 20                  |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | F     | 504 | ARG  | CB-CG | -6.19 | 1.33        | 1.52     |
| 3   | H     | 504 | ARG  | CB-CG | -6.16 | 1.33        | 1.52     |
| 2   | D     | 176 | PRO  | N-CA  | -5.80 | 1.39        | 1.47     |

All (51) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 2   | B     | 175 | VAL  | CA-C-N   | -11.67 | 105.25      | 119.84   |
| 2   | B     | 175 | VAL  | C-N-CA   | -11.67 | 105.25      | 119.84   |
| 1   | A     | 270 | ASP  | CA-C-N   | 9.10   | 128.84      | 119.56   |
| 1   | A     | 270 | ASP  | C-N-CA   | 9.10   | 128.84      | 119.56   |
| 1   | A     | 230 | VAL  | CB-CA-C  | -8.60  | 100.88      | 111.88   |
| 2   | B     | 430 | LEU  | N-CA-C   | -7.98  | 104.01      | 114.31   |
| 1   | A     | 17  | VAL  | N-CA-C   | 7.32   | 124.55      | 109.34   |
| 2   | D     | 271 | TYR  | CA-C-N   | 7.25   | 124.88      | 119.66   |
| 2   | D     | 271 | TYR  | C-N-CA   | 7.25   | 124.88      | 119.66   |
| 2   | D     | 372 | TRP  | CA-C-N   | 7.23   | 127.40      | 120.31   |
| 2   | D     | 372 | TRP  | C-N-CA   | 7.23   | 127.40      | 120.31   |
| 2   | D     | 272 | PRO  | CA-C-N   | 7.10   | 127.13      | 119.89   |
| 2   | D     | 272 | PRO  | C-N-CA   | 7.10   | 127.13      | 119.89   |
| 2   | B     | 271 | TYR  | CA-C-N   | 6.96   | 127.55      | 120.38   |
| 2   | B     | 271 | TYR  | C-N-CA   | 6.96   | 127.55      | 120.38   |
| 1   | A     | 188 | SER  | N-CA-C   | -6.91  | 103.77      | 111.71   |
| 2   | D     | 315 | LEU  | N-CA-C   | -6.67  | 104.00      | 111.28   |
| 1   | C     | 64  | VAL  | CB-CA-C  | -6.39  | 100.81      | 111.29   |
| 1   | C     | 94  | SER  | N-CA-C   | -6.32  | 105.50      | 113.72   |
| 2   | D     | 272 | PRO  | O-C-N    | 6.19   | 124.06      | 121.15   |
| 2   | B     | 175 | VAL  | CB-CA-C  | 6.16   | 123.10      | 111.40   |
| 1   | A     | 36  | ARG  | N-CA-C   | 6.03   | 117.93      | 111.36   |
| 2   | D     | 234 | LEU  | N-CA-C   | -5.95  | 104.71      | 111.14   |
| 2   | B     | 215 | VAL  | CB-CA-C  | -5.92  | 104.31      | 111.88   |
| 2   | B     | 205 | ASP  | CA-C-N   | -5.90  | 115.37      | 123.46   |
| 2   | B     | 205 | ASP  | C-N-CA   | -5.90  | 115.37      | 123.46   |
| 1   | C     | 41  | THR  | N-CA-C   | -5.86  | 98.32       | 110.80   |
| 1   | C     | 240 | PHE  | CA-C-N   | 5.78   | 127.06      | 119.84   |
| 1   | C     | 240 | PHE  | C-N-CA   | 5.78   | 127.06      | 119.84   |
| 2   | D     | 215 | VAL  | CB-CA-C  | -5.75  | 104.52      | 111.88   |
| 3   | H     | 504 | ARG  | CA-CB-CG | 5.70   | 125.49      | 114.10   |
| 2   | D     | 236 | VAL  | CB-CA-C  | -5.61  | 104.56      | 112.14   |
| 2   | D     | 241 | ARG  | N-CA-C   | -5.57  | 104.71      | 112.45   |
| 1   | C     | 10  | ILE  | CB-CA-C  | -5.52  | 104.92      | 111.65   |
| 2   | B     | 365 | TYR  | N-CA-C   | -5.42  | 105.27      | 111.07   |
| 2   | D     | 221 | VAL  | CB-CA-C  | -5.39  | 104.87      | 112.14   |
| 2   | B     | 236 | VAL  | CB-CA-C  | -5.36  | 105.02      | 112.04   |
| 1   | C     | 52  | ILE  | N-CA-C   | -5.35  | 105.32      | 110.72   |
| 1   | C     | 35  | ILE  | CB-CA-C  | -5.33  | 103.90      | 111.21   |
| 2   | B     | 372 | TRP  | CA-C-N   | 5.33   | 125.30      | 120.03   |
| 2   | B     | 372 | TRP  | C-N-CA   | 5.33   | 125.30      | 120.03   |
| 1   | A     | 37  | LEU  | N-CA-C   | 5.32   | 122.14      | 110.80   |
| 1   | C     | 252 | VAL  | CA-C-N   | 5.28   | 125.82      | 120.38   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 252 | VAL  | C-N-CA | 5.28  | 125.82      | 120.38   |
| 2   | D     | 371 | SER  | N-CA-C | 5.27  | 116.66      | 109.18   |
| 1   | C     | 89  | LYS  | N-CA-C | -5.21 | 105.50      | 111.07   |
| 1   | C     | 188 | SER  | N-CA-C | -5.10 | 105.81      | 111.36   |
| 2   | B     | 317 | GLN  | N-CA-C | -5.09 | 105.64      | 111.14   |
| 2   | D     | 177 | ASP  | N-CA-C | -5.04 | 106.22      | 112.93   |
| 3   | H     | 506 | LEU  | CA-C-O | -5.04 | 116.14      | 120.88   |
| 1   | C     | 51  | GLU  | N-CA-C | -5.01 | 105.71      | 111.07   |

There are no chirality outliers.

All (20) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 177 | CYS  | Peptide   |
| 1   | A     | 19  | TYR  | Peptide   |
| 1   | A     | 35  | ILE  | Peptide   |
| 1   | A     | 41  | THR  | Peptide   |
| 1   | A     | 83  | LEU  | Peptide   |
| 1   | A     | 85  | GLN  | Mainchain |
| 2   | B     | 175 | VAL  | Mainchain |
| 2   | B     | 270 | ILE  | Peptide   |
| 2   | B     | 424 | LEU  | Mainchain |
| 2   | B     | 429 | THR  | Peptide   |
| 1   | C     | 19  | TYR  | Peptide   |
| 1   | C     | 41  | THR  | Mainchain |
| 2   | D     | 179 | HIS  | Sidechain |
| 2   | D     | 206 | ILE  | Peptide   |
| 2   | D     | 271 | TYR  | Mainchain |
| 2   | D     | 344 | ALA  | Peptide   |
| 2   | D     | 345 | ASP  | Peptide   |
| 2   | D     | 347 | TYR  | Sidechain |
| 3   | F     | 501 | ALA  | Peptide   |
| 3   | H     | 504 | ARG  | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2378  | 0        | 2426     | 267     | 0            |
| 1   | C     | 2384  | 0        | 2435     | 224     | 1            |
| 2   | B     | 2083  | 0        | 2107     | 195     | 1            |
| 2   | D     | 2084  | 0        | 2107     | 169     | 0            |
| 3   | F     | 62    | 0        | 62       | 22      | 0            |
| 3   | H     | 62    | 0        | 63       | 11      | 0            |
| 4   | A     | 24    | 0        | 13       | 9       | 0            |
| 4   | C     | 24    | 0        | 13       | 5       | 0            |
| 5   | A     | 48    | 0        | 0        | 27      | 0            |
| 5   | B     | 44    | 0        | 0        | 15      | 0            |
| 5   | C     | 39    | 0        | 0        | 7       | 0            |
| 5   | D     | 52    | 0        | 0        | 16      | 0            |
| 5   | F     | 2     | 0        | 0        | 0       | 0            |
| 5   | H     | 3     | 0        | 0        | 1       | 0            |
| All | All   | 9289  | 0        | 9226     | 849     | 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 46.

All (849) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:210:MET:HG3  | 3:F:508:PFF:CD2  | 1.58                     | 1.33              |
| 1:A:71:HIS:CE1   | 2:B:296:HIS:CE1  | 2.24                     | 1.26              |
| 1:A:163:VAL:HG12 | 5:A:2026:HOH:O   | 1.29                     | 1.23              |
| 1:A:268:HIS:CG   | 5:A:2044:HOH:O   | 1.86                     | 1.23              |
| 5:B:2015:HOH:O   | 3:F:502:ALA:HB1  | 1.33                     | 1.22              |
| 1:A:40:GLU:O     | 1:A:41:THR:HG23  | 1.41                     | 1.18              |
| 5:D:2018:HOH:O   | 3:H:503:ABA:HG1  | 1.43                     | 1.17              |
| 1:A:164:VAL:HG21 | 5:A:2023:HOH:O   | 1.46                     | 1.16              |
| 1:C:131:GLN:H    | 1:C:131:GLN:NE2  | 1.44                     | 1.15              |
| 1:A:11:GLY:HA3   | 5:A:2005:HOH:O   | 1.45                     | 1.12              |
| 1:C:15:TYR:CE2   | 1:C:33:LYS:HD3   | 1.85                     | 1.11              |
| 1:C:39:THR:HG21  | 1:C:43:GLY:HA2   | 1.21                     | 1.10              |
| 1:A:57:GLU:OE1   | 2:B:185:TYR:OH   | 1.74                     | 1.05              |
| 2:B:210:MET:HG3  | 3:F:508:PFF:HD2  | 1.36                     | 1.05              |
| 1:C:214:ARG:HG2  | 1:C:214:ARG:HH11 | 1.21                     | 1.04              |
| 1:C:39:THR:HG21  | 1:C:43:GLY:CA    | 1.86                     | 1.03              |
| 3:F:501:ALA:CB   | 3:F:502:ALA:HB2  | 1.88                     | 1.03              |
| 3:F:501:ALA:HB1  | 3:F:502:ALA:HB2  | 1.39                     | 1.03              |
| 2:D:178:TYR:O    | 2:D:181:ASP:N    | 1.91                     | 1.03              |
| 1:C:162:GLU:HG3  | 1:C:164:VAL:HG23 | 1.41                     | 1.03              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:388:LYS:O    | 2:D:392:MET:HG2  | 1.60                     | 1.02              |
| 1:A:85:GLN:HA    | 4:A:1297:CK4:C5B | 1.90                     | 1.01              |
| 2:B:282:THR:O    | 2:B:285:THR:HG22 | 1.60                     | 0.99              |
| 1:C:1:MET:HE2    | 1:C:1:MET:HA     | 1.44                     | 0.99              |
| 2:D:404:HIS:CD2  | 2:D:406:GLN:HB2  | 1.97                     | 0.99              |
| 1:C:85:GLN:HE22  | 1:C:89:LYS:HB3   | 1.29                     | 0.98              |
| 1:A:159:TYR:HD2  | 5:A:2022:HOH:O   | 1.48                     | 0.96              |
| 1:A:37:LEU:HA    | 1:A:39:THR:OG1   | 1.65                     | 0.96              |
| 1:A:39:THR:HG21  | 1:A:43:GLY:C     | 1.91                     | 0.96              |
| 1:A:15:TYR:CE2   | 1:A:33:LYS:HD2   | 1.99                     | 0.96              |
| 1:C:286:PHE:O    | 1:C:289:VAL:HG12 | 1.64                     | 0.95              |
| 1:A:95:ALA:O     | 1:A:96:LEU:HB3   | 1.64                     | 0.95              |
| 1:C:162:GLU:CG   | 1:C:164:VAL:HG23 | 1.96                     | 0.95              |
| 5:B:2015:HOH:O   | 3:F:502:ALA:CB   | 1.97                     | 0.95              |
| 1:A:71:HIS:CE1   | 2:B:296:HIS:NE2  | 2.35                     | 0.94              |
| 2:D:190:GLU:HG3  | 2:D:351:LEU:HD22 | 1.50                     | 0.94              |
| 2:B:210:MET:CG   | 3:F:508:PFF:CD2  | 2.46                     | 0.93              |
| 1:C:214:ARG:HH11 | 1:C:214:ARG:CG   | 1.81                     | 0.93              |
| 1:C:38:ASP:O     | 1:C:40:GLU:N     | 2.02                     | 0.93              |
| 1:C:85:GLN:NE2   | 1:C:89:LYS:HB3   | 1.84                     | 0.92              |
| 2:B:412:LYS:HA   | 5:B:2039:HOH:O   | 1.69                     | 0.92              |
| 1:C:115:LEU:HD11 | 1:C:185:ASP:HB3  | 1.52                     | 0.92              |
| 2:D:431:ASN:O    | 2:D:432:LEU:HD22 | 1.70                     | 0.92              |
| 1:A:216:PHE:CE1  | 1:A:222:PRO:HD3  | 2.06                     | 0.91              |
| 2:B:282:THR:O    | 2:B:285:THR:CG2  | 2.18                     | 0.91              |
| 2:D:229:ASN:HB3  | 5:D:2029:HOH:O   | 1.70                     | 0.90              |
| 1:C:131:GLN:HE21 | 1:C:131:GLN:N    | 1.69                     | 0.90              |
| 1:A:227:TRP:HB3  | 1:A:230:VAL:HG22 | 1.53                     | 0.90              |
| 2:B:404:HIS:HA   | 5:B:2036:HOH:O   | 1.72                     | 0.90              |
| 1:C:135:ILE:HD12 | 5:C:2014:HOH:O   | 1.71                     | 0.89              |
| 2:D:374:GLU:HG3  | 5:D:2034:HOH:O   | 1.72                     | 0.89              |
| 1:C:39:THR:CG2   | 1:C:43:GLY:HA2   | 2.03                     | 0.89              |
| 1:C:13:GLY:O     | 1:C:14:THR:O     | 1.90                     | 0.89              |
| 1:C:127:ASP:OD1  | 1:C:164:VAL:HG12 | 1.73                     | 0.88              |
| 3:F:501:ALA:CB   | 3:F:502:ALA:CB   | 2.51                     | 0.88              |
| 1:C:127:ASP:OD1  | 1:C:164:VAL:CG1  | 2.20                     | 0.88              |
| 1:A:15:TYR:HB3   | 1:A:35:ILE:HG23  | 1.55                     | 0.88              |
| 1:C:44:VAL:O     | 2:D:266:LYS:NZ   | 2.06                     | 0.87              |
| 2:B:404:HIS:NE2  | 2:B:406:GLN:HB2  | 1.89                     | 0.87              |
| 1:A:39:THR:HG21  | 1:A:43:GLY:O     | 1.73                     | 0.87              |
| 1:A:242:LYS:HE2  | 5:A:2040:HOH:O   | 1.74                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:190:GLU:HG3  | 2:B:351:LEU:HD22 | 1.56                     | 0.86              |
| 1:C:39:THR:HG22  | 1:C:39:THR:O     | 1.74                     | 0.86              |
| 1:A:37:LEU:HD22  | 1:A:39:THR:OG1   | 1.76                     | 0.86              |
| 1:A:37:LEU:C     | 1:A:39:THR:H     | 1.82                     | 0.86              |
| 1:C:294:PRO:HG2  | 1:C:296:LEU:HD11 | 1.57                     | 0.86              |
| 1:C:131:GLN:H    | 1:C:131:GLN:HE21 | 0.90                     | 0.85              |
| 1:A:60:HIS:HD2   | 1:A:62:ASN:H     | 1.19                     | 0.85              |
| 1:C:253:PRO:HG2  | 1:C:254:PRO:HD3  | 1.54                     | 0.85              |
| 1:A:73:GLU:CD    | 1:C:2:GLU:HG2    | 2.01                     | 0.85              |
| 1:C:76:LEU:HD12  | 1:C:77:TYR:N     | 1.92                     | 0.85              |
| 1:A:214:ARG:HG2  | 1:A:214:ARG:HH11 | 1.41                     | 0.85              |
| 2:D:178:TYR:HE2  | 5:D:2006:HOH:O   | 1.59                     | 0.85              |
| 1:C:39:THR:CG2   | 1:C:43:GLY:CA    | 2.56                     | 0.84              |
| 1:A:60:HIS:CD2   | 1:A:62:ASN:H     | 1.96                     | 0.84              |
| 2:D:404:HIS:HD2  | 2:D:406:GLN:HB2  | 1.41                     | 0.84              |
| 1:A:71:HIS:HE1   | 2:B:296:HIS:CE1  | 1.92                     | 0.83              |
| 2:B:200:MET:HG2  | 2:B:208:ASN:HD22 | 1.42                     | 0.83              |
| 1:A:40:GLU:O     | 1:A:41:THR:CG2   | 2.26                     | 0.83              |
| 2:D:319:PHE:CD2  | 2:D:330:GLU:HG2  | 2.13                     | 0.83              |
| 3:H:501:ALA:N    | 3:H:502:ALA:HB3  | 1.93                     | 0.83              |
| 1:C:39:THR:CG2   | 1:C:39:THR:O     | 2.27                     | 0.83              |
| 1:C:231:THR:HA   | 1:C:236:TYR:CD1  | 2.13                     | 0.82              |
| 1:A:162:GLU:HB2  | 5:A:2024:HOH:O   | 1.78                     | 0.82              |
| 2:B:430:LEU:HB3  | 2:B:432:LEU:HD23 | 1.61                     | 0.82              |
| 1:C:162:GLU:CD   | 1:C:164:VAL:HG23 | 2.05                     | 0.82              |
| 1:A:73:GLU:CG    | 1:C:2:GLU:HG2    | 2.10                     | 0.82              |
| 1:A:15:TYR:CD2   | 1:A:33:LYS:HD2   | 2.15                     | 0.81              |
| 1:A:89:LYS:HE2   | 5:A:2018:HOH:O   | 1.82                     | 0.80              |
| 2:D:210:MET:HG3  | 3:H:508:PFF:HD2  | 1.64                     | 0.80              |
| 2:D:400:LYS:HD2  | 5:D:2041:HOH:O   | 1.80                     | 0.80              |
| 1:C:52:ILE:O     | 1:C:56:LYS:HG3   | 1.81                     | 0.80              |
| 1:A:217:ARG:HD2  | 5:A:2035:HOH:O   | 1.81                     | 0.79              |
| 2:B:332:LEU:HD23 | 2:B:363:ALA:HA   | 1.63                     | 0.79              |
| 1:C:131:GLN:NE2  | 1:C:131:GLN:N    | 2.26                     | 0.79              |
| 1:C:37:LEU:C     | 1:C:39:THR:H     | 1.90                     | 0.79              |
| 1:A:175:LEU:HD21 | 1:A:212:LEU:HD21 | 1.65                     | 0.79              |
| 3:F:501:ALA:HB3  | 3:F:502:ALA:CB   | 2.11                     | 0.79              |
| 2:B:209:SER:HA   | 5:B:2014:HOH:O   | 1.81                     | 0.79              |
| 2:B:404:HIS:CD2  | 2:B:405:ALA:N    | 2.50                     | 0.78              |
| 1:C:35:ILE:HD12  | 1:C:76:LEU:HG    | 1.64                     | 0.78              |
| 1:C:60:HIS:HD2   | 1:C:62:ASN:H     | 1.31                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:20:LYS:HD3   | 1:A:82:PHE:CE2   | 2.18                     | 0.78              |
| 1:A:154:VAL:HG21 | 2:B:312:ASN:HD21 | 1.49                     | 0.78              |
| 2:D:183:HIS:HB2  | 2:D:317:GLN:HE22 | 1.46                     | 0.78              |
| 1:A:13:GLY:O     | 1:A:14:THR:O     | 2.02                     | 0.78              |
| 2:B:319:PHE:CE2  | 2:B:330:GLU:HG2  | 2.20                     | 0.77              |
| 2:D:335:PHE:HE1  | 2:D:409:ILE:HG22 | 1.48                     | 0.77              |
| 1:A:13:GLY:C     | 1:A:14:THR:O     | 2.27                     | 0.77              |
| 2:B:207:THR:HG22 | 2:B:210:MET:H    | 1.50                     | 0.77              |
| 1:A:164:VAL:CG2  | 5:A:2023:HOH:O   | 2.12                     | 0.77              |
| 1:A:51:GLU:HG2   | 1:A:55:LEU:HD22  | 1.66                     | 0.76              |
| 1:A:15:TYR:HE2   | 1:A:33:LYS:HZ2   | 1.30                     | 0.76              |
| 1:A:163:VAL:HG13 | 5:A:2025:HOH:O   | 1.84                     | 0.76              |
| 1:C:1:MET:HA     | 1:C:1:MET:CE     | 2.15                     | 0.76              |
| 2:D:203:GLN:NE2  | 2:D:246:MET:O    | 2.18                     | 0.76              |
| 1:C:212:LEU:HD22 | 1:C:216:PHE:CZ   | 2.21                     | 0.76              |
| 2:D:388:LYS:O    | 2:D:392:MET:CG   | 2.33                     | 0.76              |
| 1:C:60:HIS:CD2   | 1:C:62:ASN:H     | 2.04                     | 0.75              |
| 2:D:210:MET:HG2  | 3:H:508:PFF:CD2  | 2.15                     | 0.75              |
| 1:A:9:LYS:NZ     | 1:A:12:GLU:OE1   | 2.20                     | 0.75              |
| 2:D:175:VAL:HG12 | 2:D:179:HIS:CG   | 2.21                     | 0.75              |
| 1:A:175:LEU:CD2  | 1:A:212:LEU:HD11 | 2.17                     | 0.75              |
| 2:D:178:TYR:CE2  | 5:D:2006:HOH:O   | 2.37                     | 0.75              |
| 2:B:404:HIS:HD2  | 2:B:405:ALA:N    | 1.84                     | 0.75              |
| 2:B:207:THR:HG22 | 2:B:210:MET:HE2  | 1.68                     | 0.75              |
| 2:D:207:THR:HG22 | 2:D:210:MET:CE   | 2.17                     | 0.75              |
| 1:A:39:THR:HG21  | 1:A:43:GLY:CA    | 2.16                     | 0.74              |
| 2:B:220:GLU:OE2  | 3:F:501:ALA:HA   | 1.87                     | 0.74              |
| 2:B:404:HIS:CD2  | 2:B:406:GLN:HB2  | 2.22                     | 0.74              |
| 2:D:335:PHE:CE1  | 2:D:409:ILE:HG22 | 2.21                     | 0.74              |
| 1:C:15:TYR:CD2   | 1:C:33:LYS:HD3   | 2.22                     | 0.74              |
| 1:A:216:PHE:CE1  | 1:A:222:PRO:CD   | 2.71                     | 0.74              |
| 2:B:324:PRO:HA   | 5:B:2030:HOH:O   | 1.86                     | 0.74              |
| 2:D:431:ASN:C    | 2:D:432:LEU:HD22 | 2.12                     | 0.73              |
| 2:B:206:ILE:HA   | 2:B:210:MET:HE3  | 1.69                     | 0.73              |
| 4:C:1297:CK4:N3  | 4:C:1297:CK4:H2B | 2.03                     | 0.73              |
| 1:C:7:VAL:HG12   | 1:C:8:GLU:HG2    | 1.71                     | 0.73              |
| 1:A:104:ILE:HD13 | 1:A:196:MET:HB3  | 1.71                     | 0.72              |
| 2:D:233:HIS:HD2  | 5:D:2026:HOH:O   | 1.71                     | 0.72              |
| 2:D:207:THR:CG2  | 2:D:210:MET:CE   | 2.67                     | 0.72              |
| 2:D:319:PHE:CE2  | 2:D:330:GLU:HG2  | 2.24                     | 0.72              |
| 1:A:13:GLY:O     | 5:A:2007:HOH:O   | 2.07                     | 0.72              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:76:LEU:HD12  | 1:C:76:LEU:C      | 2.15                     | 0.72              |
| 1:C:13:GLY:O     | 1:C:14:THR:C      | 2.32                     | 0.72              |
| 2:D:417:LYS:O    | 2:D:417:LYS:HG2   | 1.90                     | 0.72              |
| 1:A:71:HIS:ND1   | 2:B:296:HIS:CE1   | 2.56                     | 0.71              |
| 2:B:178:TYR:O    | 2:B:181:ASP:N     | 2.23                     | 0.71              |
| 1:A:227:TRP:O    | 1:A:228:PRO:C     | 2.33                     | 0.71              |
| 1:C:217:ARG:HD2  | 5:C:2030:HOH:O    | 1.91                     | 0.71              |
| 2:D:178:TYR:O    | 2:D:179:HIS:C     | 2.33                     | 0.71              |
| 2:B:210:MET:HG3  | 3:F:508:PFF:CE2   | 2.19                     | 0.71              |
| 1:C:78:LEU:HD23  | 1:C:78:LEU:N      | 2.05                     | 0.71              |
| 1:A:145:ASP:OD2  | 4:A:1297:CK4:H7A1 | 1.91                     | 0.71              |
| 1:A:162:GLU:HG3  | 1:A:164:VAL:HG23  | 1.72                     | 0.71              |
| 1:A:121:HIS:O    | 1:A:122:ARG:HD2   | 1.91                     | 0.70              |
| 2:B:217:TRP:HZ2  | 2:B:281:ILE:HG23  | 1.57                     | 0.70              |
| 1:A:42:GLU:HA    | 2:B:275:VAL:CG2   | 2.21                     | 0.70              |
| 1:C:39:THR:CG2   | 1:C:43:GLY:N      | 2.54                     | 0.70              |
| 1:C:253:PRO:CG   | 1:C:254:PRO:HD3   | 2.20                     | 0.70              |
| 2:D:332:LEU:HD23 | 2:D:363:ALA:HA    | 1.72                     | 0.70              |
| 1:C:115:LEU:HD13 | 1:C:119:HIS:CE1   | 2.27                     | 0.70              |
| 1:A:42:GLU:O     | 2:B:266:LYS:NZ    | 2.14                     | 0.70              |
| 2:B:200:MET:HG2  | 2:B:208:ASN:ND2   | 2.06                     | 0.70              |
| 3:F:501:ALA:HB3  | 3:F:502:ALA:HB2   | 1.70                     | 0.70              |
| 2:B:323:GLN:H    | 2:B:323:GLN:NE2   | 1.90                     | 0.70              |
| 2:D:210:MET:CG   | 3:H:508:PFF:CD2   | 2.69                     | 0.70              |
| 1:A:34:LYS:HB2   | 1:A:77:TYR:CE2    | 2.27                     | 0.69              |
| 1:A:162:GLU:OE1  | 1:A:164:VAL:CG2   | 2.40                     | 0.69              |
| 2:B:210:MET:CG   | 3:F:508:PFF:HD2   | 2.16                     | 0.69              |
| 1:C:177:CYS:HB2  | 5:C:2024:HOH:O    | 1.90                     | 0.69              |
| 2:D:287:THR:HG23 | 2:D:290:GLN:HG3   | 1.74                     | 0.69              |
| 2:D:401:ALA:HA   | 5:D:2040:HOH:O    | 1.92                     | 0.69              |
| 2:B:404:HIS:HD2  | 2:B:406:GLN:N     | 1.90                     | 0.69              |
| 1:C:39:THR:O     | 1:C:41:THR:N      | 2.25                     | 0.69              |
| 1:C:15:TYR:CE2   | 1:C:33:LYS:CD     | 2.72                     | 0.69              |
| 2:B:200:MET:CG   | 2:B:208:ASN:HD22  | 2.07                     | 0.68              |
| 2:D:363:ALA:O    | 2:D:367:VAL:HG23  | 1.93                     | 0.68              |
| 1:A:45:PRO:O     | 1:A:49:ILE:HG12   | 1.93                     | 0.68              |
| 1:A:227:TRP:HB3  | 1:A:230:VAL:CG2   | 2.23                     | 0.68              |
| 1:C:2:GLU:OE2    | 1:C:2:GLU:N       | 2.23                     | 0.68              |
| 1:C:64:VAL:HG22  | 1:C:143:LEU:O     | 1.93                     | 0.68              |
| 1:C:175:LEU:HD23 | 1:C:212:LEU:HD11  | 1.76                     | 0.68              |
| 2:B:218:LEU:HD22 | 2:B:261:MET:SD    | 2.33                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:207:THR:HG22 | 2:D:210:MET:HB2  | 1.75                     | 0.68              |
| 1:A:75:LYS:HE3   | 1:A:77:TYR:OH    | 1.94                     | 0.68              |
| 1:C:9:LYS:HE3    | 1:C:9:LYS:C      | 2.19                     | 0.68              |
| 1:A:72:THR:HB    | 5:A:2016:HOH:O   | 1.93                     | 0.68              |
| 2:B:187:ARG:HD2  | 2:B:190:GLU:OE2  | 1.93                     | 0.68              |
| 1:C:15:TYR:OH    | 1:C:51:GLU:OE1   | 2.10                     | 0.68              |
| 1:A:51:GLU:HG3   | 1:A:146:PHE:HB2  | 1.75                     | 0.67              |
| 1:A:37:LEU:C     | 1:A:39:THR:N     | 2.52                     | 0.67              |
| 2:B:271:TYR:N    | 2:B:271:TYR:CD1  | 2.63                     | 0.67              |
| 2:D:345:ASP:OD2  | 2:D:346:PRO:CD   | 2.42                     | 0.67              |
| 2:D:221:VAL:HG22 | 2:D:281:ILE:HD12 | 1.77                     | 0.67              |
| 2:D:225:TYR:CE1  | 2:D:281:ILE:HG21 | 2.29                     | 0.67              |
| 1:C:39:THR:HG23  | 1:C:43:GLY:N     | 2.10                     | 0.67              |
| 1:A:294:PRO:HG2  | 1:A:296:LEU:HD11 | 1.75                     | 0.67              |
| 2:B:430:LEU:CB   | 2:B:432:LEU:HD23 | 2.25                     | 0.67              |
| 2:D:207:THR:CG2  | 2:D:210:MET:HE2  | 2.25                     | 0.66              |
| 1:A:76:LEU:C     | 1:A:76:LEU:HD23  | 2.20                     | 0.66              |
| 1:A:84:HIS:O     | 4:A:1297:CK4:H5B | 1.95                     | 0.66              |
| 2:D:361:HIS:CE1  | 2:D:371:SER:HB3  | 2.31                     | 0.66              |
| 1:C:85:GLN:HA    | 4:C:1297:CK4:C5B | 2.25                     | 0.66              |
| 1:A:143:LEU:N    | 1:A:143:LEU:HD23 | 2.10                     | 0.66              |
| 2:D:207:THR:HG22 | 2:D:210:MET:H    | 1.59                     | 0.66              |
| 2:D:424:LEU:HD13 | 5:D:2048:HOH:O   | 1.96                     | 0.66              |
| 2:B:175:VAL:O    | 2:B:179:HIS:CG   | 2.49                     | 0.66              |
| 1:C:15:TYR:HB3   | 1:C:35:ILE:HG23  | 1.76                     | 0.66              |
| 2:D:221:VAL:HG13 | 2:D:281:ILE:HD13 | 1.78                     | 0.66              |
| 2:D:384:LEU:HD12 | 2:D:384:LEU:O    | 1.96                     | 0.66              |
| 1:C:218:THR:HA   | 1:C:246:GLN:HE21 | 1.61                     | 0.65              |
| 1:C:138:GLU:CD   | 1:C:138:GLU:H    | 2.04                     | 0.65              |
| 1:C:294:PRO:HG2  | 1:C:296:LEU:CD1  | 2.26                     | 0.65              |
| 2:D:207:THR:HG22 | 2:D:210:MET:HE3  | 1.76                     | 0.65              |
| 1:A:42:GLU:HA    | 2:B:275:VAL:HG21 | 1.77                     | 0.65              |
| 1:A:51:GLU:HG2   | 1:A:55:LEU:CD2   | 2.26                     | 0.65              |
| 1:A:91:MET:HE3   | 1:A:196:MET:HA   | 1.78                     | 0.65              |
| 1:A:247:ASP:O    | 1:A:250:LYS:HB2  | 1.96                     | 0.65              |
| 1:A:263:LEU:HD12 | 1:A:263:LEU:O    | 1.97                     | 0.65              |
| 1:C:214:ARG:CG   | 1:C:214:ARG:NH1  | 2.47                     | 0.65              |
| 2:D:207:THR:HB   | 2:D:210:MET:CE   | 2.26                     | 0.65              |
| 1:A:164:VAL:HG12 | 1:A:165:THR:HG22 | 1.79                     | 0.65              |
| 2:B:277:GLU:CD   | 5:B:2023:HOH:O   | 2.39                     | 0.65              |
| 2:D:175:VAL:O    | 2:D:176:PRO:C    | 2.39                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:501:ALA:HB3  | 3:F:502:ALA:HB3  | 1.79                     | 0.65              |
| 1:C:152:PHE:C    | 1:C:154:VAL:H    | 2.05                     | 0.65              |
| 2:D:392:MET:HE3  | 2:D:392:MET:HA   | 1.79                     | 0.65              |
| 1:A:38:ASP:O     | 1:A:40:GLU:N     | 2.24                     | 0.65              |
| 1:A:175:LEU:HD21 | 1:A:212:LEU:HD11 | 1.78                     | 0.65              |
| 2:B:207:THR:CG2  | 2:B:209:SER:HB3  | 2.27                     | 0.65              |
| 2:B:404:HIS:CD2  | 2:B:406:GLN:N    | 2.66                     | 0.64              |
| 2:B:430:LEU:HB3  | 2:B:432:LEU:CD2  | 2.27                     | 0.64              |
| 1:C:77:TYR:C     | 1:C:78:LEU:HD23  | 2.23                     | 0.64              |
| 1:A:211:GLN:O    | 1:A:212:LEU:C    | 2.41                     | 0.64              |
| 1:C:3:ASN:HB2    | 5:C:2001:HOH:O   | 1.96                     | 0.64              |
| 2:B:254:GLN:HG2  | 2:B:286:TYR:HE2  | 1.62                     | 0.64              |
| 1:C:177:CYS:HB3  | 1:C:233:MET:HE1  | 1.78                     | 0.64              |
| 1:A:2:GLU:H      | 1:A:2:GLU:CD     | 2.06                     | 0.64              |
| 1:C:143:LEU:N    | 1:C:143:LEU:HD23 | 2.11                     | 0.64              |
| 1:A:39:THR:HG22  | 1:A:43:GLY:H     | 1.63                     | 0.64              |
| 1:A:161:HIS:O    | 5:A:2022:HOH:O   | 2.15                     | 0.64              |
| 2:B:319:PHE:CD2  | 2:B:330:GLU:HG2  | 2.32                     | 0.64              |
| 1:C:95:ALA:O     | 1:C:96:LEU:HB3   | 1.98                     | 0.64              |
| 1:C:115:LEU:HD11 | 1:C:185:ASP:CB   | 2.26                     | 0.64              |
| 1:A:85:GLN:OE1   | 1:A:296:LEU:HD23 | 1.98                     | 0.63              |
| 1:A:85:GLN:HA    | 4:A:1297:CK4:H5B | 1.79                     | 0.63              |
| 2:D:361:HIS:HE1  | 2:D:371:SER:HB3  | 1.63                     | 0.63              |
| 2:B:283:ASP:O    | 2:B:285:THR:N    | 2.31                     | 0.63              |
| 1:C:85:GLN:NE2   | 1:C:89:LYS:CB    | 2.58                     | 0.63              |
| 2:B:414:LYS:O    | 2:B:415:ASN:C    | 2.41                     | 0.63              |
| 2:D:221:VAL:CG2  | 2:D:281:ILE:CD1  | 2.76                     | 0.63              |
| 1:A:253:PRO:O    | 1:A:255:LEU:N    | 2.31                     | 0.63              |
| 1:C:39:THR:HA    | 1:C:41:THR:OG1   | 1.99                     | 0.63              |
| 1:C:42:GLU:OE2   | 2:D:275:VAL:HG23 | 1.99                     | 0.63              |
| 1:C:91:MET:HE3   | 1:C:196:MET:HG3  | 1.80                     | 0.63              |
| 2:D:397:THR:HG23 | 5:D:2039:HOH:O   | 1.99                     | 0.63              |
| 1:C:216:PHE:O    | 1:C:220:GLY:N    | 2.32                     | 0.63              |
| 2:D:345:ASP:OD2  | 2:D:346:PRO:HD3  | 1.99                     | 0.63              |
| 2:B:266:LYS:NZ   | 2:B:295:GLU:OE1  | 2.32                     | 0.62              |
| 1:A:67:LEU:HB2   | 1:A:79:VAL:HG12  | 1.82                     | 0.62              |
| 2:B:178:TYR:O    | 2:B:179:HIS:C    | 2.43                     | 0.62              |
| 2:B:335:PHE:CZ   | 2:B:339:LEU:HD11 | 2.34                     | 0.62              |
| 2:B:200:MET:CG   | 2:B:208:ASN:ND2  | 2.63                     | 0.62              |
| 1:C:214:ARG:HG2  | 1:C:214:ARG:NH1  | 2.02                     | 0.62              |
| 1:A:231:THR:HA   | 1:A:236:TYR:CD1  | 2.35                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:288:LYS:HE2  | 5:B:2026:HOH:O   | 1.98                     | 0.62              |
| 1:C:152:PHE:C    | 1:C:154:VAL:N    | 2.56                     | 0.62              |
| 2:D:210:MET:CG   | 3:H:508:PFF:HD2  | 2.27                     | 0.62              |
| 1:A:27:GLY:HA3   | 2:D:249:LEU:HD22 | 1.81                     | 0.62              |
| 2:D:338:GLU:O    | 2:D:341:LEU:HB2  | 1.98                     | 0.62              |
| 1:A:7:VAL:HG12   | 1:A:8:GLU:HG2    | 1.82                     | 0.61              |
| 1:A:162:GLU:HA   | 5:A:2022:HOH:O   | 1.99                     | 0.61              |
| 2:B:401:ALA:N    | 2:B:402:PRO:CD   | 2.63                     | 0.61              |
| 1:A:268:HIS:ND1  | 5:A:2044:HOH:O   | 2.10                     | 0.61              |
| 2:B:207:THR:HG23 | 2:B:209:SER:N    | 2.15                     | 0.61              |
| 2:B:396:GLN:OE1  | 2:B:396:GLN:HA   | 1.95                     | 0.61              |
| 1:A:270:ASP:OD1  | 1:A:270:ASP:C    | 2.44                     | 0.61              |
| 2:D:207:THR:CG2  | 2:D:210:MET:H    | 2.14                     | 0.61              |
| 1:A:71:HIS:ND1   | 2:B:296:HIS:NE2  | 2.49                     | 0.61              |
| 1:A:121:HIS:HD2  | 2:B:185:TYR:CE1  | 2.19                     | 0.61              |
| 4:A:1297:CK4:N3  | 4:A:1297:CK4:H2B | 2.16                     | 0.61              |
| 2:B:312:ASN:C    | 2:B:312:ASN:ND2  | 2.59                     | 0.61              |
| 1:A:108:LEU:HD11 | 1:A:112:LEU:HD11 | 1.82                     | 0.61              |
| 2:B:194:LYS:O    | 2:B:195:PRO:O    | 2.19                     | 0.61              |
| 1:C:39:THR:CG2   | 1:C:43:GLY:H     | 2.14                     | 0.61              |
| 1:C:154:VAL:O    | 1:C:155:PRO:C    | 2.43                     | 0.61              |
| 1:A:162:GLU:OE2  | 5:A:2024:HOH:O   | 2.16                     | 0.61              |
| 2:D:256:VAL:HG22 | 2:D:294:MET:HE3  | 1.83                     | 0.60              |
| 2:D:344:ALA:HB1  | 2:D:348:LEU:HD22 | 1.82                     | 0.60              |
| 2:D:221:VAL:CG2  | 2:D:281:ILE:HD12 | 2.31                     | 0.60              |
| 1:A:162:GLU:OE1  | 1:A:164:VAL:HG21 | 2.02                     | 0.60              |
| 1:A:44:VAL:HG11  | 1:A:49:ILE:CD1   | 2.31                     | 0.60              |
| 1:A:70:ILE:HB    | 1:A:77:TYR:HB2   | 1.82                     | 0.60              |
| 2:D:388:LYS:N    | 2:D:389:PRO:HD2  | 2.16                     | 0.60              |
| 1:A:207:SER:O    | 1:A:208:GLU:C    | 2.43                     | 0.60              |
| 1:A:96:LEU:HG    | 1:A:97:THR:HG23  | 1.84                     | 0.60              |
| 1:A:154:VAL:O    | 1:A:155:PRO:C    | 2.45                     | 0.60              |
| 2:B:175:VAL:O    | 2:B:179:HIS:ND1  | 2.35                     | 0.60              |
| 2:B:401:ALA:N    | 2:B:402:PRO:HD3  | 2.17                     | 0.60              |
| 1:A:39:THR:CG2   | 1:A:43:GLY:CA    | 2.80                     | 0.59              |
| 1:A:294:PRO:HG2  | 1:A:296:LEU:CD1  | 2.32                     | 0.59              |
| 2:B:404:HIS:CD2  | 2:B:404:HIS:C    | 2.79                     | 0.59              |
| 1:A:202:LEU:HD22 | 1:A:203:PHE:CE1  | 2.37                     | 0.59              |
| 2:D:178:TYR:O    | 2:D:180:GLU:N    | 2.35                     | 0.59              |
| 1:A:89:LYS:CE    | 5:A:2018:HOH:O   | 2.47                     | 0.59              |
| 1:C:15:TYR:HE2   | 1:C:33:LYS:HD3   | 1.60                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:346:PRO:O    | 2:D:349:LYS:HG3  | 2.03                     | 0.59              |
| 2:D:221:VAL:HG22 | 2:D:281:ILE:CD1  | 2.31                     | 0.59              |
| 2:B:175:VAL:HG13 | 2:B:176:PRO:HD3  | 1.84                     | 0.59              |
| 2:B:207:THR:CG2  | 2:B:210:MET:HE2  | 2.33                     | 0.59              |
| 2:D:342:ILE:O    | 2:D:342:ILE:HG22 | 2.01                     | 0.59              |
| 1:A:177:CYS:HB3  | 1:A:233:MET:HE2  | 1.85                     | 0.59              |
| 2:B:207:THR:CG2  | 2:B:210:MET:H    | 2.16                     | 0.59              |
| 2:D:400:LYS:C    | 2:D:402:PRO:CD   | 2.76                     | 0.59              |
| 1:A:256:ASP:OD1  | 1:A:256:ASP:C    | 2.45                     | 0.59              |
| 2:B:268:GLU:HG3  | 2:B:268:GLU:O    | 2.00                     | 0.59              |
| 1:C:175:LEU:CD2  | 1:C:212:LEU:HD11 | 2.33                     | 0.59              |
| 1:A:34:LYS:HB2   | 1:A:77:TYR:CD2   | 2.38                     | 0.58              |
| 1:C:38:ASP:C     | 1:C:40:GLU:H     | 2.06                     | 0.58              |
| 1:A:39:THR:HG22  | 1:A:43:GLY:N     | 2.17                     | 0.58              |
| 1:A:60:HIS:CG    | 1:A:61:PRO:HD2   | 2.38                     | 0.58              |
| 2:B:297:LEU:O    | 2:B:301:VAL:HG23 | 2.03                     | 0.58              |
| 1:C:36:ARG:HA    | 5:C:2008:HOH:O   | 2.03                     | 0.58              |
| 1:A:13:GLY:O     | 1:A:14:THR:C     | 2.47                     | 0.58              |
| 2:B:256:VAL:HG22 | 2:B:294:MET:HE3  | 1.85                     | 0.58              |
| 2:D:207:THR:HG22 | 2:D:210:MET:HE2  | 1.84                     | 0.58              |
| 1:A:83:LEU:O     | 4:A:1297:CK4:H6B | 2.03                     | 0.58              |
| 1:A:214:ARG:HG2  | 1:A:214:ARG:NH1  | 2.13                     | 0.58              |
| 2:B:415:ASN:HB2  | 5:B:2040:HOH:O   | 2.02                     | 0.58              |
| 2:B:383:THR:O    | 2:B:386:SER:OG   | 2.21                     | 0.58              |
| 1:A:188:SER:O    | 1:A:192:ILE:HG13 | 2.04                     | 0.58              |
| 1:C:162:GLU:CD   | 1:C:164:VAL:CG2  | 2.77                     | 0.58              |
| 2:B:277:GLU:HG3  | 5:B:2023:HOH:O   | 2.04                     | 0.58              |
| 2:B:400:LYS:C    | 2:B:402:PRO:CD   | 2.76                     | 0.58              |
| 1:C:105:LYS:NZ   | 1:C:288:ASP:OD1  | 2.37                     | 0.58              |
| 1:C:177:CYS:HB3  | 1:C:233:MET:CE   | 2.33                     | 0.58              |
| 2:D:190:GLU:HG3  | 2:D:351:LEU:CD2  | 2.30                     | 0.58              |
| 1:A:81:GLU:HG3   | 1:A:83:LEU:HD11  | 1.84                     | 0.58              |
| 1:A:86:ASP:C     | 1:A:86:ASP:OD1   | 2.47                     | 0.58              |
| 1:C:104:ILE:HD13 | 1:C:196:MET:HB3  | 1.86                     | 0.58              |
| 2:B:256:VAL:CG2  | 2:B:294:MET:HE3  | 2.33                     | 0.58              |
| 2:B:303:THR:O    | 2:B:303:THR:OG1  | 2.21                     | 0.58              |
| 1:A:40:GLU:O     | 1:A:40:GLU:HG3   | 2.03                     | 0.57              |
| 2:B:252:LYS:O    | 2:B:255:LEU:HB3  | 2.04                     | 0.57              |
| 2:B:338:GLU:OE1  | 2:B:412:LYS:NZ   | 2.30                     | 0.57              |
| 1:A:216:PHE:CD1  | 1:A:222:PRO:HD3  | 2.38                     | 0.57              |
| 1:A:15:TYR:CB    | 1:A:35:ILE:HG23  | 2.32                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:415:ASN:ND2  | 5:B:2041:HOH:O   | 2.37                     | 0.57              |
| 2:D:357:GLY:O    | 2:D:358:ALA:C    | 2.48                     | 0.57              |
| 1:A:85:GLN:NE2   | 1:A:89:LYS:HB3   | 2.20                     | 0.57              |
| 1:A:76:LEU:HD21  | 1:A:78:LEU:HD21  | 1.86                     | 0.57              |
| 2:B:418:TYR:O    | 2:B:421:VAL:HG22 | 2.05                     | 0.57              |
| 2:D:357:GLY:O    | 2:D:360:PHE:N    | 2.33                     | 0.57              |
| 1:C:40:GLU:O     | 1:C:40:GLU:HG3   | 2.05                     | 0.57              |
| 1:C:231:THR:HA   | 1:C:236:TYR:CE1  | 2.39                     | 0.57              |
| 2:D:246:MET:HE2  | 2:D:297:LEU:HD21 | 1.87                     | 0.57              |
| 1:A:14:THR:OG1   | 1:A:15:TYR:CE2   | 2.56                     | 0.57              |
| 1:A:241:PRO:HB2  | 1:A:243:TRP:CZ3  | 2.40                     | 0.57              |
| 1:C:223:ASP:OD1  | 1:C:226:VAL:HG23 | 2.05                     | 0.57              |
| 2:B:420:GLY:O    | 2:B:423:LEU:HB2  | 2.05                     | 0.56              |
| 3:F:501:ALA:HB1  | 3:F:502:ALA:CB   | 2.21                     | 0.56              |
| 1:A:95:ALA:O     | 1:A:96:LEU:CB    | 2.43                     | 0.56              |
| 2:B:207:THR:HG22 | 2:B:210:MET:HB2  | 1.86                     | 0.56              |
| 1:C:36:ARG:NH1   | 1:C:36:ARG:HG3   | 2.20                     | 0.56              |
| 1:A:87:LEU:HD22  | 1:A:87:LEU:O     | 2.06                     | 0.56              |
| 1:A:177:CYS:HB3  | 1:A:233:MET:CE   | 2.35                     | 0.56              |
| 2:B:220:GLU:OE1  | 3:F:504:ARG:NH2  | 2.39                     | 0.56              |
| 1:C:123:VAL:HG12 | 1:C:124:LEU:N    | 2.20                     | 0.56              |
| 1:C:256:ASP:OD1  | 1:C:256:ASP:C    | 2.45                     | 0.56              |
| 2:D:388:LYS:N    | 2:D:389:PRO:CD   | 2.67                     | 0.56              |
| 2:D:431:ASN:HB2  | 5:D:2052:HOH:O   | 2.05                     | 0.56              |
| 2:D:225:TYR:HE1  | 2:D:281:ILE:HG21 | 1.67                     | 0.56              |
| 1:C:90:PHE:CZ    | 1:C:294:PRO:CB   | 2.88                     | 0.56              |
| 1:C:37:LEU:HD22  | 1:C:39:THR:OG1   | 2.05                     | 0.56              |
| 2:D:321:HIS:HD1  | 2:D:375:SER:HB2  | 1.71                     | 0.56              |
| 1:C:223:ASP:OD1  | 1:C:223:ASP:C    | 2.48                     | 0.56              |
| 1:A:175:LEU:HD22 | 1:A:212:LEU:HD11 | 1.86                     | 0.56              |
| 2:D:221:VAL:CG1  | 2:D:281:ILE:HD13 | 2.35                     | 0.55              |
| 1:C:86:ASP:OD1   | 1:C:88:LYS:HB3   | 2.06                     | 0.55              |
| 2:B:220:GLU:OE2  | 3:F:501:ALA:CA   | 2.55                     | 0.55              |
| 2:D:195:PRO:HG2  | 5:D:2015:HOH:O   | 2.05                     | 0.55              |
| 2:D:207:THR:CB   | 2:D:210:MET:CE   | 2.85                     | 0.55              |
| 2:D:431:ASN:C    | 2:D:432:LEU:CD2  | 2.79                     | 0.55              |
| 1:A:115:LEU:HD11 | 1:A:185:ASP:HB3  | 1.88                     | 0.55              |
| 2:B:404:HIS:CD2  | 2:B:406:GLN:H    | 2.23                     | 0.55              |
| 1:A:202:LEU:HD13 | 1:A:203:PHE:CE2  | 2.42                     | 0.55              |
| 2:B:396:GLN:O    | 2:B:400:LYS:HG3  | 2.07                     | 0.55              |
| 1:C:70:ILE:HB    | 1:C:77:TYR:HB2   | 1.89                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:218:THR:O    | 1:C:218:THR:HG22 | 2.06                     | 0.55              |
| 2:D:175:VAL:O    | 2:D:176:PRO:O    | 2.24                     | 0.55              |
| 1:A:10:ILE:O     | 1:A:10:ILE:HG13  | 2.07                     | 0.54              |
| 1:A:212:LEU:HD22 | 1:A:216:PHE:CZ   | 2.42                     | 0.54              |
| 2:B:254:GLN:OE1  | 3:F:506:LEU:HG   | 2.07                     | 0.54              |
| 2:B:323:GLN:NE2  | 2:B:323:GLN:N    | 2.55                     | 0.54              |
| 2:B:431:ASN:C    | 2:B:432:LEU:HD22 | 2.32                     | 0.54              |
| 1:C:75:LYS:NZ    | 1:C:77:TYR:OH    | 2.41                     | 0.54              |
| 2:D:216:ASP:O    | 2:D:219:VAL:HB   | 2.07                     | 0.54              |
| 2:B:241:ARG:HA   | 2:B:244:SER:OG   | 2.07                     | 0.54              |
| 3:H:501:ALA:CA   | 3:H:502:ALA:HB3  | 2.37                     | 0.54              |
| 1:A:108:LEU:CD1  | 1:A:112:LEU:HD11 | 2.37                     | 0.54              |
| 1:A:122:ARG:HA   | 1:A:152:PHE:CE1  | 2.41                     | 0.54              |
| 2:B:266:LYS:HZ2  | 2:B:295:GLU:CD   | 2.14                     | 0.54              |
| 1:A:162:GLU:OE1  | 1:A:164:VAL:HG23 | 2.07                     | 0.54              |
| 1:A:268:HIS:CE1  | 5:A:2044:HOH:O   | 2.57                     | 0.54              |
| 2:D:400:LYS:C    | 2:D:402:PRO:HD2  | 2.33                     | 0.54              |
| 1:A:15:TYR:CE2   | 1:A:33:LYS:CD    | 2.86                     | 0.54              |
| 1:A:275:ILE:HA   | 5:A:2046:HOH:O   | 2.07                     | 0.54              |
| 2:D:255:LEU:HD23 | 2:D:294:MET:HE2  | 1.89                     | 0.54              |
| 2:D:347:TYR:OH   | 2:D:394:LEU:HA   | 2.08                     | 0.54              |
| 2:D:411:GLU:HG3  | 5:D:2044:HOH:O   | 2.06                     | 0.54              |
| 1:A:203:PHE:O    | 1:A:211:GLN:NE2  | 2.26                     | 0.54              |
| 1:A:283:HIS:ND1  | 1:A:284:PRO:HD2  | 2.23                     | 0.54              |
| 1:C:40:GLU:O     | 1:C:40:GLU:CG    | 2.55                     | 0.54              |
| 1:C:158:THR:HB   | 1:C:178:LYS:O    | 2.08                     | 0.54              |
| 1:C:207:SER:OG   | 1:C:209:ILE:HG22 | 2.07                     | 0.53              |
| 1:A:44:VAL:HG11  | 1:A:49:ILE:HD13  | 1.89                     | 0.53              |
| 1:A:96:LEU:HG    | 1:A:97:THR:CG2   | 2.38                     | 0.53              |
| 1:A:232:SER:O    | 1:A:232:SER:OG   | 2.12                     | 0.53              |
| 2:B:283:ASP:C    | 2:B:285:THR:N    | 2.66                     | 0.53              |
| 2:B:320:LEU:N    | 2:B:320:LEU:HD23 | 2.23                     | 0.53              |
| 2:B:335:PHE:CE1  | 2:B:409:ILE:HG22 | 2.43                     | 0.53              |
| 1:C:55:LEU:HD11  | 1:C:146:PHE:CD1  | 2.43                     | 0.53              |
| 1:A:9:LYS:CE     | 1:A:12:GLU:OE1   | 2.56                     | 0.53              |
| 1:C:37:LEU:C     | 1:C:39:THR:N     | 2.58                     | 0.53              |
| 1:A:71:HIS:CE1   | 2:B:296:HIS:CD2  | 2.95                     | 0.53              |
| 2:B:217:TRP:O    | 2:B:221:VAL:HG23 | 2.09                     | 0.53              |
| 2:B:220:GLU:HG3  | 2:B:408:SER:HB3  | 1.89                     | 0.53              |
| 1:A:37:LEU:HB2   | 1:A:75:LYS:HA    | 1.90                     | 0.53              |
| 1:A:87:LEU:HD22  | 1:A:91:MET:HG3   | 1.89                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:326:ASN:CG   | 2:B:329:VAL:HG23 | 2.34                     | 0.53              |
| 1:A:163:VAL:CG1  | 5:A:2025:HOH:O   | 2.48                     | 0.53              |
| 1:A:248:PHE:CE2  | 1:A:264:SER:HB3  | 2.43                     | 0.53              |
| 2:B:335:PHE:HB2  | 2:B:413:TYR:CD2  | 2.44                     | 0.53              |
| 1:C:124:LEU:HD12 | 1:C:126:ARG:HG3  | 1.89                     | 0.53              |
| 1:A:205:GLY:HA3  | 1:A:211:GLN:OE1  | 2.09                     | 0.53              |
| 2:B:199:TYR:CD1  | 2:B:199:TYR:C    | 2.86                     | 0.53              |
| 2:B:225:TYR:HE2  | 2:B:277:GLU:OE1  | 1.91                     | 0.53              |
| 1:C:117:PHE:O    | 1:C:118:CYS:C    | 2.51                     | 0.53              |
| 4:C:1297:CK4:H5  | 4:C:1297:CK4:C6A | 2.39                     | 0.53              |
| 1:A:112:LEU:HD22 | 1:A:280:ALA:HB3  | 1.92                     | 0.52              |
| 1:A:253:PRO:HG2  | 1:A:254:PRO:HD3  | 1.91                     | 0.52              |
| 2:B:230:GLU:OE1  | 2:B:312:ASN:ND2  | 2.43                     | 0.52              |
| 1:C:222:PRO:HG3  | 1:C:269:TYR:CZ   | 2.44                     | 0.52              |
| 2:D:256:VAL:CG2  | 2:D:294:MET:HE3  | 2.38                     | 0.52              |
| 2:D:404:HIS:HD2  | 2:D:406:GLN:CB   | 2.16                     | 0.52              |
| 2:D:343:ASP:C    | 2:D:345:ASP:H    | 2.17                     | 0.52              |
| 1:A:40:GLU:O     | 1:A:40:GLU:CG    | 2.57                     | 0.52              |
| 1:A:89:LYS:NZ    | 5:A:2018:HOH:O   | 2.43                     | 0.52              |
| 1:A:170:ALA:O    | 1:A:171:PRO:C    | 2.52                     | 0.52              |
| 2:B:207:THR:HG23 | 2:B:209:SER:H    | 1.74                     | 0.52              |
| 2:D:342:ILE:O    | 2:D:342:ILE:CG2  | 2.57                     | 0.52              |
| 2:B:195:PRO:HG3  | 2:B:240:ASP:HB3  | 1.92                     | 0.52              |
| 2:B:283:ASP:O    | 2:B:284:ASP:C    | 2.52                     | 0.52              |
| 2:B:388:LYS:HE2  | 2:B:392:MET:SD   | 2.49                     | 0.52              |
| 2:B:409:ILE:O    | 2:B:412:LYS:HB3  | 2.10                     | 0.52              |
| 1:A:63:ILE:O     | 1:A:64:VAL:C     | 2.53                     | 0.52              |
| 1:A:224:GLU:CD   | 1:A:229:GLY:H    | 2.18                     | 0.52              |
| 2:D:207:THR:CG2  | 2:D:210:MET:HE3  | 2.37                     | 0.52              |
| 3:F:505:SER:O    | 3:F:506:LEU:C    | 2.53                     | 0.52              |
| 1:A:73:GLU:HG3   | 1:C:2:GLU:HG2    | 1.89                     | 0.51              |
| 1:C:39:THR:C     | 1:C:41:THR:OG1   | 2.53                     | 0.51              |
| 1:C:159:TYR:CE1  | 2:D:270:ILE:HG23 | 2.45                     | 0.51              |
| 2:D:343:ASP:HB3  | 2:D:345:ASP:OD2  | 2.10                     | 0.51              |
| 1:C:211:GLN:O    | 1:C:212:LEU:C    | 2.52                     | 0.51              |
| 2:D:230:GLU:OE2  | 2:D:313:GLN:NE2  | 2.35                     | 0.51              |
| 2:B:182:ILE:HG22 | 2:B:183:HIS:N    | 2.26                     | 0.51              |
| 1:A:15:TYR:CE1   | 1:A:47:THR:OG1   | 2.63                     | 0.51              |
| 1:A:173:ILE:HD11 | 1:A:184:VAL:HG11 | 1.91                     | 0.51              |
| 1:A:275:ILE:HG12 | 1:A:276:SER:O    | 2.11                     | 0.51              |
| 1:C:39:THR:HG23  | 1:C:43:GLY:H     | 1.73                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:216:ASP:CG   | 2:B:408:SER:OG   | 2.54                     | 0.51              |
| 2:B:312:ASN:C    | 2:B:312:ASN:HD22 | 2.18                     | 0.51              |
| 1:C:31:ALA:HB3   | 1:C:80:PHE:HB2   | 1.91                     | 0.51              |
| 1:A:51:GLU:O     | 1:A:55:LEU:HB2   | 2.11                     | 0.51              |
| 1:A:268:HIS:CD2  | 5:A:2044:HOH:O   | 2.34                     | 0.51              |
| 2:B:400:LYS:C    | 2:B:402:PRO:HD2  | 2.35                     | 0.51              |
| 2:B:404:HIS:C    | 2:B:406:GLN:H    | 2.18                     | 0.51              |
| 1:C:39:THR:C     | 1:C:41:THR:N     | 2.69                     | 0.51              |
| 2:D:268:GLU:HG3  | 2:D:268:GLU:O    | 2.11                     | 0.51              |
| 1:A:125:HIS:CG   | 1:A:128:LEU:HD21 | 2.46                     | 0.51              |
| 2:D:183:HIS:HB2  | 2:D:317:GLN:NE2  | 2.20                     | 0.51              |
| 2:D:255:LEU:HB2  | 2:D:286:TYR:CZ   | 2.46                     | 0.51              |
| 2:D:345:ASP:OD2  | 2:D:346:PRO:HD2  | 2.10                     | 0.51              |
| 1:A:122:ARG:O    | 1:A:122:ARG:CD   | 2.59                     | 0.51              |
| 2:B:236:VAL:HG21 | 2:B:341:LEU:HD13 | 1.93                     | 0.51              |
| 1:C:76:LEU:C     | 1:C:76:LEU:CD1   | 2.84                     | 0.51              |
| 1:C:253:PRO:N    | 1:C:254:PRO:CD   | 2.73                     | 0.51              |
| 2:D:332:LEU:HB3  | 2:D:363:ALA:HB1  | 1.92                     | 0.51              |
| 2:D:374:GLU:O    | 2:D:375:SER:C    | 2.54                     | 0.51              |
| 1:A:99:ILE:HG23  | 1:A:103:LEU:HD23 | 1.93                     | 0.50              |
| 1:C:7:VAL:HG12   | 1:C:8:GLU:N      | 2.26                     | 0.50              |
| 1:C:227:TRP:O    | 1:C:230:VAL:HG12 | 2.10                     | 0.50              |
| 2:D:400:LYS:O    | 2:D:402:PRO:HD2  | 2.10                     | 0.50              |
| 3:H:503:ABA:O    | 3:H:503:ABA:HG2  | 2.10                     | 0.50              |
| 1:A:108:LEU:O    | 1:A:112:LEU:HD12 | 2.11                     | 0.50              |
| 1:C:162:GLU:OE2  | 1:C:162:GLU:HA   | 2.11                     | 0.50              |
| 2:D:430:LEU:HB3  | 2:D:432:LEU:HD23 | 1.92                     | 0.50              |
| 1:C:172:GLU:OE1  | 1:C:184:VAL:HG12 | 2.12                     | 0.50              |
| 3:F:506:LEU:HD12 | 3:F:508:PFF:F    | 2.01                     | 0.50              |
| 1:A:39:THR:CG2   | 1:A:43:GLY:N     | 2.74                     | 0.50              |
| 2:D:224:GLU:O    | 2:D:224:GLU:HG3  | 2.11                     | 0.50              |
| 2:B:363:ALA:O    | 2:B:364:LEU:C    | 2.54                     | 0.50              |
| 2:D:277:GLU:O    | 2:D:281:ILE:HG23 | 2.11                     | 0.50              |
| 1:A:157:ARG:HD3  | 5:B:2016:HOH:O   | 2.12                     | 0.50              |
| 1:C:71:HIS:CG    | 2:D:296:HIS:NE2  | 2.80                     | 0.50              |
| 2:D:323:GLN:O    | 2:D:323:GLN:HG2  | 2.10                     | 0.50              |
| 1:C:42:GLU:O     | 2:D:266:LYS:NZ   | 2.41                     | 0.50              |
| 2:D:190:GLU:CG   | 2:D:351:LEU:HD22 | 2.33                     | 0.50              |
| 2:D:207:THR:CB   | 2:D:210:MET:HE3  | 2.42                     | 0.50              |
| 1:A:14:THR:C     | 1:A:15:TYR:CD2   | 2.90                     | 0.50              |
| 2:B:216:ASP:OD1  | 2:B:408:SER:OG   | 2.29                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:335:PHE:HE1  | 2:B:409:ILE:HG22  | 1.77                     | 0.50              |
| 1:A:9:LYS:HE3    | 1:A:12:GLU:OE1    | 2.11                     | 0.50              |
| 4:C:1297:CK4:H5  | 4:C:1297:CK4:H6A2 | 1.93                     | 0.50              |
| 1:A:40:GLU:CA    | 1:A:40:GLU:OE1    | 2.60                     | 0.49              |
| 1:C:123:VAL:CG1  | 1:C:124:LEU:N     | 2.75                     | 0.49              |
| 1:C:90:PHE:CZ    | 1:C:294:PRO:HB3   | 2.47                     | 0.49              |
| 1:A:64:VAL:HG12  | 1:A:143:LEU:O     | 2.13                     | 0.49              |
| 2:B:402:PRO:HB2  | 2:B:403:GLN:HE22  | 1.78                     | 0.49              |
| 1:A:39:THR:CG2   | 1:A:43:GLY:O      | 2.53                     | 0.49              |
| 2:D:410:ARG:O    | 2:D:414:LYS:HG3   | 2.12                     | 0.49              |
| 1:A:253:PRO:C    | 1:A:255:LEU:H     | 2.19                     | 0.49              |
| 1:C:71:HIS:CG    | 2:D:296:HIS:HE2   | 2.31                     | 0.49              |
| 2:B:391:LEU:O    | 2:B:391:LEU:HD12  | 2.13                     | 0.49              |
| 1:C:85:GLN:OE1   | 1:C:296:LEU:HD23  | 2.13                     | 0.49              |
| 1:C:275:ILE:HD11 | 1:C:280:ALA:HA    | 1.95                     | 0.49              |
| 1:A:227:TRP:CB   | 1:A:230:VAL:HG22  | 2.35                     | 0.49              |
| 2:B:338:GLU:O    | 2:B:341:LEU:HB2   | 2.13                     | 0.49              |
| 1:A:44:VAL:CG1   | 1:A:49:ILE:HD11   | 2.43                     | 0.49              |
| 2:B:404:HIS:HD2  | 2:B:406:GLN:H     | 1.56                     | 0.49              |
| 1:C:84:HIS:ND1   | 1:C:137:THR:HG23  | 2.28                     | 0.49              |
| 1:A:122:ARG:HA   | 1:A:152:PHE:CZ    | 2.48                     | 0.48              |
| 1:A:209:ILE:HG23 | 1:A:210:ASP:N     | 2.26                     | 0.48              |
| 1:A:262:LEU:O    | 1:A:263:LEU:C     | 2.56                     | 0.48              |
| 4:A:1297:CK4:C6A | 4:A:1297:CK4:H5   | 2.43                     | 0.48              |
| 2:B:210:MET:HA   | 2:B:213:ILE:HD13  | 1.95                     | 0.48              |
| 2:B:302:LEU:N    | 2:B:302:LEU:HD23  | 2.26                     | 0.48              |
| 1:C:122:ARG:HA   | 1:C:152:PHE:CE1   | 2.47                     | 0.48              |
| 2:B:223:GLU:CD   | 2:B:412:LYS:HG3   | 2.37                     | 0.48              |
| 1:C:233:MET:O    | 1:C:234:PRO:C     | 2.54                     | 0.48              |
| 2:B:212:ALA:O    | 2:B:213:ILE:C     | 2.55                     | 0.48              |
| 1:C:83:LEU:O     | 4:C:1297:CK4:H6B  | 2.12                     | 0.48              |
| 1:C:157:ARG:HD3  | 5:D:2012:HOH:O    | 2.13                     | 0.48              |
| 1:C:247:ASP:O    | 1:C:250:LYS:HB2   | 2.13                     | 0.48              |
| 2:D:428:GLU:C    | 2:D:429:THR:CG2   | 2.86                     | 0.48              |
| 1:A:129:LYS:HA   | 1:A:192:ILE:HD11  | 1.96                     | 0.48              |
| 1:C:230:VAL:O    | 1:C:233:MET:HG3   | 2.13                     | 0.48              |
| 2:D:246:MET:CE   | 2:D:297:LEU:HD21  | 2.44                     | 0.48              |
| 1:A:207:SER:OG   | 1:A:209:ILE:HG22  | 2.13                     | 0.48              |
| 1:A:223:ASP:OD1  | 1:A:226:VAL:HG23  | 2.14                     | 0.48              |
| 2:B:207:THR:O    | 2:B:208:ASN:C     | 2.56                     | 0.48              |
| 2:B:412:LYS:CA   | 5:B:2039:HOH:O    | 2.44                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:287:THR:HG23 | 2:D:290:GLN:CG   | 2.42                     | 0.48              |
| 3:H:505:SER:O    | 3:H:506:LEU:C    | 2.55                     | 0.48              |
| 2:B:277:GLU:CG   | 5:B:2023:HOH:O   | 2.59                     | 0.48              |
| 1:C:9:LYS:HE3    | 1:C:9:LYS:O      | 2.13                     | 0.48              |
| 1:A:198:THR:O    | 1:A:199:ARG:HB2  | 2.13                     | 0.48              |
| 1:A:81:GLU:OE1   | 1:A:142:LYS:NZ   | 2.45                     | 0.48              |
| 1:A:222:PRO:HG3  | 1:A:269:TYR:CE1  | 2.49                     | 0.48              |
| 2:B:178:TYR:O    | 2:B:180:GLU:N    | 2.47                     | 0.48              |
| 2:B:213:ILE:HD12 | 2:B:213:ILE:H    | 1.78                     | 0.48              |
| 1:C:83:LEU:HD21  | 1:C:142:LYS:HE3  | 1.96                     | 0.48              |
| 1:C:198:THR:C    | 1:C:199:ARG:HG3  | 2.39                     | 0.48              |
| 1:A:136:ASN:C    | 1:A:136:ASN:OD1  | 2.56                     | 0.47              |
| 1:A:181:SER:C    | 1:A:183:ALA:N    | 2.71                     | 0.47              |
| 2:B:361:HIS:CD2  | 2:B:361:HIS:C    | 2.92                     | 0.47              |
| 1:C:59:ASN:HB2   | 5:C:2010:HOH:O   | 2.14                     | 0.47              |
| 2:B:194:LYS:C    | 2:B:195:PRO:O    | 2.57                     | 0.47              |
| 2:B:339:LEU:HD23 | 2:B:409:ILE:HD12 | 1.96                     | 0.47              |
| 2:D:349:LYS:NZ   | 5:D:2031:HOH:O   | 2.30                     | 0.47              |
| 2:B:217:TRP:CZ2  | 2:B:281:ILE:HG23 | 2.45                     | 0.47              |
| 1:C:78:LEU:N     | 1:C:78:LEU:CD2   | 2.76                     | 0.47              |
| 1:C:15:TYR:HE2   | 1:C:33:LYS:CD    | 2.22                     | 0.47              |
| 1:C:230:VAL:HA   | 1:C:233:MET:HG3  | 1.97                     | 0.47              |
| 2:D:332:LEU:O    | 2:D:333:ALA:C    | 2.55                     | 0.47              |
| 1:A:253:PRO:CG   | 1:A:254:PRO:HD3  | 2.45                     | 0.47              |
| 2:B:371:SER:OG   | 2:B:372:TRP:N    | 2.48                     | 0.47              |
| 1:C:115:LEU:HD13 | 1:C:119:HIS:HE1  | 1.78                     | 0.47              |
| 2:D:207:THR:HB   | 2:D:210:MET:HE1  | 1.97                     | 0.47              |
| 1:A:20:LYS:CD    | 1:A:82:PHE:CE2   | 2.95                     | 0.47              |
| 2:B:343:ASP:C    | 2:B:345:ASP:N    | 2.71                     | 0.47              |
| 2:B:411:GLU:O    | 2:B:412:LYS:C    | 2.55                     | 0.47              |
| 1:C:188:SER:O    | 1:C:192:ILE:HG13 | 2.14                     | 0.47              |
| 1:A:83:LEU:HD12  | 1:A:83:LEU:N     | 2.30                     | 0.47              |
| 1:A:108:LEU:CD1  | 1:A:112:LEU:CD1  | 2.92                     | 0.47              |
| 2:B:387:LEU:O    | 2:B:388:LYS:C    | 2.58                     | 0.47              |
| 1:C:9:LYS:HE2    | 1:C:9:LYS:HB3    | 1.75                     | 0.47              |
| 1:C:122:ARG:HA   | 1:C:152:PHE:CZ   | 2.50                     | 0.47              |
| 1:A:40:GLU:OE1   | 1:A:40:GLU:C     | 2.57                     | 0.46              |
| 1:A:125:HIS:CE1  | 1:A:128:LEU:HD23 | 2.50                     | 0.46              |
| 1:A:223:ASP:OD1  | 1:A:223:ASP:C    | 2.59                     | 0.46              |
| 1:C:15:TYR:HE1   | 1:C:48:ALA:N     | 2.14                     | 0.46              |
| 1:A:253:PRO:CB   | 1:A:254:PRO:HD3  | 2.46                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:153:GLY:HA3  | 2:D:313:GLN:HG2  | 1.96                     | 0.46              |
| 2:D:221:VAL:HG21 | 2:D:281:ILE:CD1  | 2.44                     | 0.46              |
| 1:A:44:VAL:CG1   | 1:A:49:ILE:CD1   | 2.94                     | 0.46              |
| 1:C:71:HIS:CE1   | 2:D:296:HIS:CD2  | 3.04                     | 0.46              |
| 1:C:135:ILE:HB   | 5:C:2015:HOH:O   | 2.15                     | 0.46              |
| 2:D:229:ASN:ND2  | 2:D:334:MET:HE3  | 2.31                     | 0.46              |
| 1:C:90:PHE:CZ    | 1:C:294:PRO:HB2  | 2.51                     | 0.46              |
| 2:D:401:ALA:N    | 2:D:402:PRO:CD   | 2.79                     | 0.46              |
| 1:A:248:PHE:C    | 1:A:250:LYS:N    | 2.72                     | 0.46              |
| 1:A:41:THR:C     | 1:A:42:GLU:HG2   | 2.41                     | 0.46              |
| 1:C:30:VAL:C     | 1:C:82:PHE:HB2   | 2.40                     | 0.46              |
| 2:D:318:TYR:O    | 2:D:319:PHE:C    | 2.57                     | 0.46              |
| 1:A:38:ASP:C     | 1:A:38:ASP:OD1   | 2.58                     | 0.46              |
| 1:A:231:THR:HG22 | 1:A:236:TYR:CE1  | 2.51                     | 0.46              |
| 2:D:273:PRO:HB2  | 2:D:278:PHE:CE2  | 2.50                     | 0.46              |
| 1:A:69:VAL:HG13  | 1:A:78:LEU:CD2   | 2.45                     | 0.46              |
| 1:A:166:LEU:HD13 | 1:A:166:LEU:HA   | 1.79                     | 0.46              |
| 2:B:432:LEU:HD13 | 2:B:432:LEU:HA   | 1.76                     | 0.46              |
| 1:C:90:PHE:CE1   | 1:C:294:PRO:HB2  | 2.50                     | 0.46              |
| 2:D:287:THR:O    | 2:D:288:LYS:C    | 2.59                     | 0.46              |
| 2:D:340:SER:HB2  | 2:D:347:TYR:CG   | 2.51                     | 0.46              |
| 1:A:9:LYS:HE2    | 5:A:2004:HOH:O   | 2.17                     | 0.45              |
| 1:A:212:LEU:HD23 | 1:A:212:LEU:HA   | 1.84                     | 0.45              |
| 2:B:208:ASN:O    | 2:B:209:SER:C    | 2.57                     | 0.45              |
| 2:B:230:GLU:O    | 2:B:231:THR:C    | 2.59                     | 0.45              |
| 2:B:254:GLN:O    | 2:B:254:GLN:HG3  | 2.15                     | 0.45              |
| 3:F:507:ILE:O    | 3:F:507:ILE:HG13 | 2.14                     | 0.45              |
| 1:A:37:LEU:HA    | 1:A:39:THR:HG1   | 1.77                     | 0.45              |
| 1:A:125:HIS:ND1  | 1:A:128:LEU:HD23 | 2.31                     | 0.45              |
| 2:B:361:HIS:HB2  | 2:B:372:TRP:HB2  | 1.97                     | 0.45              |
| 1:A:81:GLU:HG3   | 1:A:83:LEU:CD1   | 2.47                     | 0.45              |
| 1:A:87:LEU:O     | 1:A:87:LEU:CD2   | 2.65                     | 0.45              |
| 1:C:67:LEU:HD11  | 1:C:81:GLU:HA    | 1.98                     | 0.45              |
| 1:A:44:VAL:HG11  | 1:A:49:ILE:HD11  | 1.99                     | 0.45              |
| 1:C:9:LYS:HA     | 1:C:19:TYR:CD2   | 2.51                     | 0.45              |
| 1:C:162:GLU:HG3  | 1:C:164:VAL:CG2  | 2.28                     | 0.45              |
| 1:C:192:ILE:O    | 1:C:196:MET:HE2  | 2.16                     | 0.45              |
| 1:C:200:ARG:HG3  | 1:C:201:ALA:N    | 2.32                     | 0.45              |
| 2:D:207:THR:HG23 | 2:D:209:SER:N    | 2.31                     | 0.45              |
| 2:B:271:TYR:HA   | 2:B:272:PRO:HD3  | 1.79                     | 0.45              |
| 2:B:424:LEU:HD12 | 2:B:424:LEU:HA   | 1.63                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:37:LEU:HB2   | 1:C:75:LYS:HA    | 1.98                     | 0.45              |
| 3:H:502:ALA:O    | 3:H:503:ABA:C    | 2.63                     | 0.45              |
| 2:D:365:TYR:CD2  | 2:D:365:TYR:C    | 2.94                     | 0.45              |
| 3:F:506:LEU:H    | 3:F:506:LEU:HD23 | 1.81                     | 0.45              |
| 1:A:137:THR:C    | 1:A:139:GLY:N    | 2.75                     | 0.45              |
| 1:A:171:PRO:HD3  | 1:A:187:TRP:CZ2  | 2.52                     | 0.45              |
| 1:C:14:THR:O     | 1:C:15:TYR:C     | 2.60                     | 0.45              |
| 2:D:190:GLU:OE1  | 2:D:352:PRO:HD2  | 2.17                     | 0.45              |
| 2:D:221:VAL:O    | 2:D:221:VAL:HG12 | 2.16                     | 0.45              |
| 2:D:372:TRP:CD1  | 2:D:377:ILE:CG1  | 3.00                     | 0.45              |
| 1:A:40:GLU:O     | 1:A:41:THR:CB    | 2.63                     | 0.45              |
| 2:B:190:GLU:OE1  | 2:B:352:PRO:HD2  | 2.17                     | 0.45              |
| 2:B:223:GLU:OE1  | 2:B:412:LYS:HG3  | 2.17                     | 0.44              |
| 1:C:71:HIS:CE1   | 2:D:296:HIS:NE2  | 2.85                     | 0.44              |
| 1:C:173:ILE:HD11 | 1:C:184:VAL:HG11 | 1.99                     | 0.44              |
| 1:C:189:LEU:HD12 | 1:C:189:LEU:HA   | 1.81                     | 0.44              |
| 1:C:190:GLY:N    | 1:C:266:MET:HE2  | 2.31                     | 0.44              |
| 1:C:60:HIS:CG    | 1:C:61:PRO:HD2   | 2.51                     | 0.44              |
| 1:A:86:ASP:OD1   | 1:A:86:ASP:O     | 2.34                     | 0.44              |
| 1:C:172:GLU:HG2  | 1:C:173:ILE:N    | 2.32                     | 0.44              |
| 1:C:218:THR:O    | 1:C:218:THR:CG2  | 2.65                     | 0.44              |
| 1:A:91:MET:HE3   | 1:A:196:MET:CA   | 2.46                     | 0.44              |
| 2:B:206:ILE:CA   | 2:B:210:MET:HE3  | 2.42                     | 0.44              |
| 1:C:1:MET:N      | 1:C:2:GLU:OE2    | 2.44                     | 0.44              |
| 1:C:15:TYR:HB2   | 1:C:16:GLY:H     | 1.60                     | 0.44              |
| 1:C:122:ARG:C    | 1:C:152:PHE:CE1  | 2.96                     | 0.44              |
| 1:C:211:GLN:C    | 1:C:213:PHE:N    | 2.74                     | 0.44              |
| 2:D:225:TYR:CE2  | 2:D:277:GLU:HB3  | 2.53                     | 0.44              |
| 2:D:283:ASP:C    | 2:D:285:THR:N    | 2.75                     | 0.44              |
| 1:A:2:GLU:HG2    | 1:C:73:GLU:HG3   | 1.99                     | 0.44              |
| 1:A:42:GLU:HA    | 2:B:275:VAL:HG23 | 1.95                     | 0.44              |
| 1:A:62:ASN:HD22  | 1:A:110:GLN:HB3  | 1.82                     | 0.44              |
| 1:A:114:GLY:O    | 1:A:115:LEU:C    | 2.59                     | 0.44              |
| 2:B:293:ARG:HH11 | 2:B:293:ARG:CG   | 2.30                     | 0.44              |
| 1:C:25:LEU:HD23  | 1:C:25:LEU:HA    | 1.58                     | 0.44              |
| 1:C:95:ALA:O     | 1:C:96:LEU:CB    | 2.63                     | 0.44              |
| 1:C:195:GLU:HG3  | 1:C:200:ARG:C    | 2.42                     | 0.44              |
| 1:A:73:GLU:OE1   | 1:C:2:GLU:HG2    | 2.16                     | 0.44              |
| 1:A:211:GLN:C    | 1:A:213:PHE:N    | 2.71                     | 0.44              |
| 2:B:175:VAL:O    | 2:B:179:HIS:CE1  | 2.70                     | 0.44              |
| 2:D:225:TYR:CE1  | 2:D:281:ILE:CG2  | 2.98                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:283:ASP:C    | 2:D:285:THR:H    | 2.26                     | 0.44              |
| 1:A:263:LEU:HD12 | 1:A:263:LEU:C    | 2.41                     | 0.44              |
| 2:B:196:LYS:NZ   | 5:B:2010:HOH:O   | 2.50                     | 0.44              |
| 1:C:152:PHE:O    | 1:C:154:VAL:N    | 2.51                     | 0.44              |
| 2:D:207:THR:HG23 | 2:D:209:SER:H    | 1.83                     | 0.44              |
| 2:D:430:LEU:CB   | 2:D:432:LEU:HD23 | 2.48                     | 0.44              |
| 2:B:275:VAL:HG11 | 2:B:292:LEU:HD13 | 2.00                     | 0.44              |
| 1:A:84:HIS:O     | 4:A:1297:CK4:C5B | 2.64                     | 0.43              |
| 1:A:89:LYS:O     | 1:A:90:PHE:C     | 2.58                     | 0.43              |
| 2:B:209:SER:O    | 2:B:212:ALA:HB3  | 2.17                     | 0.43              |
| 1:C:9:LYS:HD2    | 1:C:11:GLY:H     | 1.83                     | 0.43              |
| 1:C:42:GLU:OE2   | 1:C:42:GLU:HA    | 2.18                     | 0.43              |
| 1:C:88:LYS:HA    | 1:C:88:LYS:HD3   | 1.82                     | 0.43              |
| 1:A:9:LYS:HD2    | 1:A:11:GLY:H     | 1.83                     | 0.43              |
| 1:A:81:GLU:CD    | 1:A:142:LYS:NZ   | 2.76                     | 0.43              |
| 2:B:323:GLN:HA   | 2:B:324:PRO:HA   | 1.65                     | 0.43              |
| 2:B:430:LEU:O    | 2:B:431:ASN:HB2  | 2.16                     | 0.43              |
| 1:C:29:VAL:HG12  | 1:C:82:PHE:HB3   | 2.00                     | 0.43              |
| 1:A:270:ASP:OD1  | 1:A:272:ASN:N    | 2.41                     | 0.43              |
| 2:B:218:LEU:O    | 2:B:219:VAL:C    | 2.61                     | 0.43              |
| 2:B:253:LEU:C    | 2:B:255:LEU:H    | 2.26                     | 0.43              |
| 1:C:1:MET:CE     | 1:C:1:MET:CA     | 2.89                     | 0.43              |
| 1:C:3:ASN:HD21   | 1:C:25:LEU:HD12  | 1.83                     | 0.43              |
| 1:C:55:LEU:HD12  | 1:C:55:LEU:HA    | 1.70                     | 0.43              |
| 1:A:181:SER:C    | 1:A:183:ALA:H    | 2.25                     | 0.43              |
| 2:B:372:TRP:HA   | 2:B:373:PRO:HD3  | 1.72                     | 0.43              |
| 1:C:17:VAL:HG13  | 1:C:19:TYR:CE1   | 2.54                     | 0.43              |
| 1:C:39:THR:HG21  | 1:C:43:GLY:C     | 2.41                     | 0.43              |
| 1:C:72:THR:OG1   | 1:C:75:LYS:HG3   | 2.18                     | 0.43              |
| 1:C:214:ARG:NH1  | 1:C:214:ARG:HG3  | 2.32                     | 0.43              |
| 1:A:195:GLU:O    | 1:A:196:MET:C    | 2.62                     | 0.43              |
| 1:A:256:ASP:OD1  | 1:A:258:ASP:N    | 2.51                     | 0.43              |
| 2:B:281:ILE:HD12 | 2:B:281:ILE:HA   | 1.83                     | 0.43              |
| 2:B:287:THR:O    | 2:B:288:LYS:C    | 2.61                     | 0.43              |
| 1:C:87:LEU:O     | 1:C:88:LYS:C     | 2.61                     | 0.43              |
| 1:C:283:HIS:HA   | 1:C:284:PRO:HD3  | 1.84                     | 0.43              |
| 2:B:253:LEU:C    | 2:B:255:LEU:N    | 2.73                     | 0.43              |
| 2:D:176:PRO:HG2  | 2:D:179:HIS:CD2  | 2.53                     | 0.43              |
| 2:D:284:ASP:CG   | 5:D:2020:HOH:O   | 2.61                     | 0.43              |
| 2:D:420:GLY:O    | 2:D:422:SER:N    | 2.52                     | 0.43              |
| 2:B:211:ARG:O    | 2:B:214:LEU:HB3  | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:39:THR:CA    | 1:C:41:THR:OG1   | 2.66                     | 0.43              |
| 1:C:138:GLU:CD   | 1:C:138:GLU:N    | 2.74                     | 0.43              |
| 1:A:122:ARG:O    | 1:A:151:ALA:HA   | 2.18                     | 0.43              |
| 2:B:315:LEU:O    | 2:B:319:PHE:CD1  | 2.71                     | 0.43              |
| 1:C:99:ILE:O     | 1:C:100:PRO:C    | 2.60                     | 0.43              |
| 1:C:165:THR:O    | 1:C:165:THR:HG23 | 2.19                     | 0.43              |
| 2:D:283:ASP:O    | 2:D:285:THR:N    | 2.51                     | 0.43              |
| 2:B:384:LEU:HD12 | 2:B:384:LEU:O    | 2.19                     | 0.43              |
| 1:C:62:ASN:ND2   | 1:C:110:GLN:HB3  | 2.34                     | 0.43              |
| 1:C:96:LEU:O     | 1:C:199:ARG:NH1  | 2.52                     | 0.43              |
| 1:C:214:ARG:O    | 1:C:215:ILE:C    | 2.61                     | 0.43              |
| 2:D:225:TYR:HE1  | 2:D:281:ILE:CG2  | 2.32                     | 0.43              |
| 2:D:361:HIS:CD2  | 2:D:361:HIS:C    | 2.96                     | 0.43              |
| 1:A:110:GLN:OE1  | 1:A:140:ALA:HA   | 2.19                     | 0.42              |
| 2:B:213:ILE:HD12 | 2:B:213:ILE:N    | 2.34                     | 0.42              |
| 1:C:196:MET:HB2  | 1:C:196:MET:HE3  | 1.61                     | 0.42              |
| 2:D:302:LEU:O    | 2:D:303:THR:C    | 2.62                     | 0.42              |
| 1:A:121:HIS:HD2  | 2:B:185:TYR:CZ   | 2.36                     | 0.42              |
| 2:B:404:HIS:HD2  | 2:B:404:HIS:C    | 2.25                     | 0.42              |
| 1:C:74:ASN:OD1   | 1:C:74:ASN:N     | 2.52                     | 0.42              |
| 1:C:162:GLU:CG   | 1:C:164:VAL:CG2  | 2.82                     | 0.42              |
| 1:A:71:HIS:CE1   | 2:B:296:HIS:ND1  | 2.79                     | 0.42              |
| 1:A:270:ASP:HA   | 1:A:271:PRO:HD3  | 1.69                     | 0.42              |
| 2:B:368:THR:OG1  | 2:B:370:GLN:HG3  | 2.19                     | 0.42              |
| 2:B:432:LEU:HD22 | 2:B:432:LEU:N    | 2.34                     | 0.42              |
| 1:C:36:ARG:HG3   | 1:C:36:ARG:HH11  | 1.82                     | 0.42              |
| 1:C:65:LYS:H     | 1:C:81:GLU:HG2   | 1.82                     | 0.42              |
| 2:D:368:THR:OG1  | 2:D:370:GLN:HG3  | 2.19                     | 0.42              |
| 2:D:404:HIS:C    | 2:D:406:GLN:H    | 2.26                     | 0.42              |
| 2:D:409:ILE:O    | 2:D:410:ARG:C    | 2.62                     | 0.42              |
| 1:A:41:THR:C     | 1:A:42:GLU:CG    | 2.92                     | 0.42              |
| 2:B:299:LEU:O    | 2:B:300:LYS:C    | 2.62                     | 0.42              |
| 2:B:357:GLY:O    | 2:B:360:PHE:N    | 2.52                     | 0.42              |
| 1:C:15:TYR:HE2   | 1:C:33:LYS:CE    | 2.33                     | 0.42              |
| 2:D:207:THR:O    | 2:D:208:ASN:C    | 2.63                     | 0.42              |
| 1:A:121:HIS:O    | 1:A:122:ARG:C    | 2.62                     | 0.42              |
| 2:B:207:THR:HG21 | 2:B:209:SER:HB3  | 2.01                     | 0.42              |
| 2:B:259:ALA:O    | 2:B:260:ALA:C    | 2.60                     | 0.42              |
| 1:C:108:LEU:HD22 | 1:C:193:PHE:CG   | 2.55                     | 0.42              |
| 1:C:195:GLU:O    | 1:C:196:MET:C    | 2.62                     | 0.42              |
| 1:A:125:HIS:CG   | 1:A:128:LEU:CD2  | 3.03                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:159:TYR:CD2  | 5:A:2022:HOH:O   | 2.38                     | 0.42              |
| 1:A:284:PRO:C    | 1:A:286:PHE:N    | 2.76                     | 0.42              |
| 1:A:290:THR:OG1  | 1:A:292:PRO:HD3  | 2.19                     | 0.42              |
| 2:B:387:LEU:C    | 2:B:389:PRO:HD2  | 2.44                     | 0.42              |
| 2:D:209:SER:O    | 2:D:210:MET:C    | 2.62                     | 0.42              |
| 1:A:128:LEU:HB2  | 1:A:188:SER:HB2  | 2.02                     | 0.42              |
| 1:A:181:SER:O    | 1:A:182:THR:C    | 2.62                     | 0.42              |
| 1:C:46:SER:O     | 1:C:49:ILE:HB    | 2.20                     | 0.42              |
| 1:C:124:LEU:HD12 | 1:C:126:ARG:CG   | 2.49                     | 0.42              |
| 1:A:37:LEU:HA    | 1:A:37:LEU:HD22  | 1.85                     | 0.42              |
| 1:A:64:VAL:O     | 1:A:64:VAL:HG13  | 2.19                     | 0.42              |
| 1:A:231:THR:HA   | 1:A:236:TYR:CE1  | 2.55                     | 0.42              |
| 1:C:17:VAL:HG13  | 1:C:19:TYR:HE1   | 1.85                     | 0.42              |
| 2:D:210:MET:HB2  | 2:D:210:MET:HE3  | 1.68                     | 0.42              |
| 2:D:376:LEU:HD23 | 2:D:376:LEU:HA   | 1.80                     | 0.42              |
| 2:D:399:LEU:O    | 2:D:402:PRO:HD3  | 2.19                     | 0.42              |
| 1:A:122:ARG:O    | 1:A:122:ARG:HD3  | 2.20                     | 0.42              |
| 1:A:126:ARG:NH1  | 5:A:2023:HOH:O   | 2.53                     | 0.42              |
| 2:B:209:SER:O    | 2:B:213:ILE:CD1  | 2.68                     | 0.42              |
| 2:B:397:THR:O    | 2:B:398:TYR:C    | 2.63                     | 0.42              |
| 2:B:202:LYS:O    | 2:B:204:PRO:HD3  | 2.20                     | 0.41              |
| 1:C:45:PRO:HD2   | 1:C:48:ALA:HB3   | 2.02                     | 0.41              |
| 2:B:315:LEU:O    | 2:B:319:PHE:CG   | 2.73                     | 0.41              |
| 1:A:181:SER:O    | 1:A:183:ALA:N    | 2.53                     | 0.41              |
| 1:A:196:MET:HE3  | 1:A:196:MET:HB2  | 1.86                     | 0.41              |
| 1:A:211:GLN:O    | 1:A:213:PHE:N    | 2.53                     | 0.41              |
| 4:A:1297:CK4:N3  | 4:A:1297:CK4:C2B | 2.81                     | 0.41              |
| 1:C:3:ASN:ND2    | 1:C:25:LEU:HD12  | 2.35                     | 0.41              |
| 1:C:74:ASN:C     | 1:C:75:LYS:HG2   | 2.45                     | 0.41              |
| 1:A:32:LEU:HA    | 1:A:32:LEU:HD23  | 1.71                     | 0.41              |
| 1:A:253:PRO:C    | 1:A:255:LEU:N    | 2.78                     | 0.41              |
| 2:B:207:THR:O    | 2:B:210:MET:N    | 2.53                     | 0.41              |
| 1:C:275:ILE:CD1  | 1:C:280:ALA:HA   | 2.49                     | 0.41              |
| 1:A:91:MET:HE1   | 1:A:195:GLU:HG2  | 2.01                     | 0.41              |
| 1:A:215:ILE:HG23 | 1:A:219:LEU:HD12 | 2.03                     | 0.41              |
| 2:D:215:VAL:O    | 2:D:218:LEU:HB2  | 2.21                     | 0.41              |
| 1:A:162:GLU:HG3  | 1:A:164:VAL:CG2  | 2.44                     | 0.41              |
| 2:B:287:THR:H    | 2:B:290:GLN:HB2  | 1.86                     | 0.41              |
| 1:A:72:THR:O     | 1:A:73:GLU:C     | 2.63                     | 0.41              |
| 2:D:207:THR:HB   | 2:D:210:MET:HE3  | 2.02                     | 0.41              |
| 1:A:267:LEU:HD23 | 1:A:267:LEU:HA   | 1.82                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:129:LYS:HB2  | 1:C:130:PRO:HD2  | 2.03                     | 0.41              |
| 1:A:72:THR:CB    | 5:A:2016:HOH:O   | 2.60                     | 0.41              |
| 1:A:108:LEU:HG   | 1:A:286:PHE:HZ   | 1.86                     | 0.41              |
| 1:A:162:GLU:CG   | 1:A:164:VAL:HG23 | 2.47                     | 0.41              |
| 1:A:275:ILE:HD11 | 1:A:280:ALA:HA   | 2.02                     | 0.41              |
| 2:B:249:LEU:HA   | 2:B:249:LEU:HD12 | 1.72                     | 0.41              |
| 2:B:315:LEU:HD23 | 2:B:315:LEU:HA   | 1.83                     | 0.41              |
| 2:B:423:LEU:O    | 2:B:424:LEU:C    | 2.64                     | 0.41              |
| 1:C:71:HIS:CE1   | 1:C:76:LEU:HD22  | 2.56                     | 0.41              |
| 1:C:251:VAL:O    | 1:C:251:VAL:HG12 | 2.21                     | 0.41              |
| 2:D:287:THR:O    | 2:D:290:GLN:HB2  | 2.20                     | 0.41              |
| 1:A:108:LEU:O    | 1:A:108:LEU:HD12 | 2.20                     | 0.41              |
| 1:A:209:ILE:CG2  | 1:A:210:ASP:N    | 2.84                     | 0.41              |
| 2:B:207:THR:HG23 | 2:B:209:SER:HB3  | 2.03                     | 0.41              |
| 2:B:245:SER:C    | 2:B:246:MET:HG2  | 2.46                     | 0.41              |
| 2:B:404:HIS:HD2  | 2:B:405:ALA:CA   | 2.34                     | 0.41              |
| 1:C:71:HIS:ND1   | 2:D:296:HIS:NE2  | 2.67                     | 0.41              |
| 2:D:215:VAL:O    | 2:D:218:LEU:N    | 2.54                     | 0.41              |
| 2:D:401:ALA:N    | 2:D:402:PRO:HD3  | 2.36                     | 0.41              |
| 1:A:52:ILE:O     | 1:A:56:LYS:HG3   | 2.21                     | 0.40              |
| 1:A:71:HIS:HE1   | 2:B:296:HIS:ND1  | 2.17                     | 0.40              |
| 1:A:115:LEU:HD23 | 1:A:115:LEU:HA   | 1.76                     | 0.40              |
| 2:D:228:GLN:N    | 2:D:269:GLU:OE2  | 2.48                     | 0.40              |
| 2:D:230:GLU:OE1  | 2:D:312:ASN:ND2  | 2.50                     | 0.40              |
| 2:D:292:LEU:HD12 | 2:D:292:LEU:HA   | 1.57                     | 0.40              |
| 2:D:323:GLN:HA   | 2:D:324:PRO:HA   | 1.74                     | 0.40              |
| 1:A:62:ASN:ND2   | 1:A:110:GLN:HB3  | 2.35                     | 0.40              |
| 2:B:214:LEU:O    | 2:B:217:TRP:HB3  | 2.20                     | 0.40              |
| 1:C:240:PHE:HA   | 1:C:241:PRO:HD2  | 1.77                     | 0.40              |
| 2:D:283:ASP:O    | 2:D:284:ASP:C    | 2.65                     | 0.40              |
| 2:D:409:ILE:O    | 2:D:412:LYS:HB3  | 2.21                     | 0.40              |
| 2:B:338:GLU:CD   | 2:B:412:LYS:NZ   | 2.80                     | 0.40              |
| 2:B:388:LYS:O    | 2:B:389:PRO:C    | 2.63                     | 0.40              |
| 1:C:198:THR:C    | 1:C:199:ARG:CG   | 2.94                     | 0.40              |
| 1:C:269:TYR:O    | 1:C:271:PRO:HD3  | 2.22                     | 0.40              |
| 2:D:362:LEU:HD13 | 2:D:362:LEU:HA   | 1.87                     | 0.40              |
| 2:D:420:GLY:C    | 2:D:422:SER:N    | 2.80                     | 0.40              |
| 1:A:162:GLU:OE2  | 1:A:180:TYR:OH   | 2.39                     | 0.40              |
| 2:B:345:ASP:HA   | 2:B:346:PRO:HA   | 1.74                     | 0.40              |
| 1:C:69:VAL:HG12  | 1:C:70:ILE:N     | 2.37                     | 0.40              |
| 1:C:87:LEU:HD23  | 1:C:87:LEU:HA    | 1.79                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:C:166:LEU:HB3  | 1:C:211:GLN:OE1 | 2.22                     | 0.40              |
| 1:C:217:ARG:HB3  | 1:C:243:TRP:CZ3 | 2.56                     | 0.40              |
| 2:D:392:MET:HA   | 2:D:392:MET:CE  | 2.49                     | 0.40              |
| 1:A:131:GLN:H    | 1:A:131:GLN:HG2 | 1.43                     | 0.40              |
| 1:A:172:GLU:CD   | 1:A:271:PRO:HG3 | 2.47                     | 0.40              |
| 2:D:176:PRO:HG2  | 2:D:179:HIS:NE2 | 2.36                     | 0.40              |
| 2:D:178:TYR:O    | 2:D:180:GLU:C   | 2.60                     | 0.40              |
| 2:D:354:VAL:HG12 | 2:D:355:ILE:N   | 2.36                     | 0.40              |
| 3:H:507:ILE:O    | 5:H:2003:HOH:O  | 2.22                     | 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) |
|-----------------|------------------------|--------------------------|-------------------|
| 2:B:431:ASN:ND2 | 1:C:210:ASP:OD1[2_664] | 2.06                     | 0.14              |

## 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     | 294/298 (99%)   | 254 (86%) | 27 (9%)   | 13 (4%)  | 2           | 8  |
| 1   | C     | 295/298 (99%)   | 259 (88%) | 26 (9%)   | 10 (3%)  | 3           | 12 |
| 2   | B     | 256/259 (99%)   | 217 (85%) | 31 (12%)  | 8 (3%)   | 3           | 14 |
| 2   | D     | 256/259 (99%)   | 228 (89%) | 21 (8%)   | 7 (3%)   | 4           | 16 |
| 3   | F     | 5/9 (56%)       | 2 (40%)   | 1 (20%)   | 2 (40%)  | 0           | 0  |
| 3   | H     | 5/9 (56%)       | 3 (60%)   | 1 (20%)   | 1 (20%)  | 0           | 0  |
| All | All   | 1111/1132 (98%) | 963 (87%) | 107 (10%) | 41 (4%)  | 2           | 11 |

All (41) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | THR  |
| 1   | A     | 17  | VAL  |
| 1   | A     | 39  | THR  |
| 1   | A     | 41  | THR  |
| 2   | B     | 179 | HIS  |
| 2   | B     | 195 | PRO  |
| 2   | B     | 284 | ASP  |
| 2   | B     | 344 | ALA  |
| 2   | B     | 424 | LEU  |
| 1   | C     | 14  | THR  |
| 1   | C     | 15  | TYR  |
| 1   | C     | 39  | THR  |
| 1   | C     | 164 | VAL  |
| 2   | D     | 176 | PRO  |
| 2   | D     | 179 | HIS  |
| 2   | D     | 424 | LEU  |
| 1   | A     | 38  | ASP  |
| 1   | A     | 164 | VAL  |
| 1   | C     | 40  | GLU  |
| 2   | D     | 346 | PRO  |
| 3   | F     | 502 | ALA  |
| 3   | H     | 502 | ALA  |
| 1   | A     | 15  | TYR  |
| 1   | A     | 96  | LEU  |
| 2   | B     | 358 | ALA  |
| 2   | B     | 405 | ALA  |
| 1   | C     | 122 | ARG  |
| 2   | D     | 195 | PRO  |
| 2   | D     | 358 | ALA  |
| 3   | F     | 506 | LEU  |
| 1   | A     | 42  | GLU  |
| 1   | A     | 73  | GLU  |
| 2   | B     | 415 | ASN  |
| 2   | D     | 284 | ASP  |
| 1   | A     | 40  | GLU  |
| 1   | A     | 241 | PRO  |
| 1   | C     | 41  | THR  |
| 1   | C     | 153 | GLY  |
| 1   | C     | 228 | PRO  |
| 1   | C     | 215 | ILE  |
| 1   | A     | 254 | PRO  |

### 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     | 261/263 (99%)   | 209 (80%) | 52 (20%)  | 1           | 4 |
| 1   | C     | 262/263 (100%)  | 205 (78%) | 57 (22%)  | 1           | 3 |
| 2   | B     | 232/233 (100%)  | 184 (79%) | 48 (21%)  | 1           | 4 |
| 2   | D     | 232/233 (100%)  | 195 (84%) | 37 (16%)  | 2           | 8 |
| 3   | F     | 4/4 (100%)      | 1 (25%)   | 3 (75%)   | 0           | 0 |
| 3   | H     | 4/4 (100%)      | 2 (50%)   | 2 (50%)   | 0           | 0 |
| All | All   | 995/1000 (100%) | 796 (80%) | 199 (20%) | 1           | 4 |

All (199) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | MET  |
| 1   | A     | 2   | GLU  |
| 1   | A     | 9   | LYS  |
| 1   | A     | 10  | ILE  |
| 1   | A     | 12  | GLU  |
| 1   | A     | 15  | TYR  |
| 1   | A     | 17  | VAL  |
| 1   | A     | 20  | LYS  |
| 1   | A     | 34  | LYS  |
| 1   | A     | 36  | ARG  |
| 1   | A     | 37  | LEU  |
| 1   | A     | 40  | GLU  |
| 1   | A     | 55  | LEU  |
| 1   | A     | 56  | LYS  |
| 1   | A     | 71  | HIS  |
| 1   | A     | 74  | ASN  |
| 1   | A     | 75  | LYS  |
| 1   | A     | 84  | HIS  |
| 1   | A     | 85  | GLN  |
| 1   | A     | 87  | LEU  |
| 1   | A     | 96  | LEU  |
| 1   | A     | 104 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 115 | LEU  |
| 1   | A     | 122 | ARG  |
| 1   | A     | 124 | LEU  |
| 1   | A     | 131 | GLN  |
| 1   | A     | 136 | ASN  |
| 1   | A     | 143 | LEU  |
| 1   | A     | 154 | VAL  |
| 1   | A     | 158 | THR  |
| 1   | A     | 160 | THR  |
| 1   | A     | 166 | LEU  |
| 1   | A     | 175 | LEU  |
| 1   | A     | 188 | SER  |
| 1   | A     | 202 | LEU  |
| 1   | A     | 214 | ARG  |
| 1   | A     | 221 | THR  |
| 1   | A     | 226 | VAL  |
| 1   | A     | 230 | VAL  |
| 1   | A     | 231 | THR  |
| 1   | A     | 232 | SER  |
| 1   | A     | 245 | ARG  |
| 1   | A     | 248 | PHE  |
| 1   | A     | 255 | LEU  |
| 1   | A     | 261 | SER  |
| 1   | A     | 263 | LEU  |
| 1   | A     | 268 | HIS  |
| 1   | A     | 276 | SER  |
| 1   | A     | 278 | LYS  |
| 1   | A     | 287 | GLN  |
| 1   | A     | 293 | VAL  |
| 1   | A     | 296 | LEU  |
| 2   | B     | 175 | VAL  |
| 2   | B     | 177 | ASP  |
| 2   | B     | 180 | GLU  |
| 2   | B     | 182 | ILE  |
| 2   | B     | 189 | MET  |
| 2   | B     | 197 | VAL  |
| 2   | B     | 199 | TYR  |
| 2   | B     | 200 | MET  |
| 2   | B     | 201 | LYS  |
| 2   | B     | 207 | THR  |
| 2   | B     | 210 | MET  |
| 2   | B     | 232 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 244 | SER  |
| 2   | B     | 245 | SER  |
| 2   | B     | 249 | LEU  |
| 2   | B     | 250 | ARG  |
| 2   | B     | 271 | TYR  |
| 2   | B     | 277 | GLU  |
| 2   | B     | 281 | ILE  |
| 2   | B     | 284 | ASP  |
| 2   | B     | 285 | THR  |
| 2   | B     | 288 | LYS  |
| 2   | B     | 291 | VAL  |
| 2   | B     | 292 | LEU  |
| 2   | B     | 293 | ARG  |
| 2   | B     | 303 | THR  |
| 2   | B     | 312 | ASN  |
| 2   | B     | 322 | GLN  |
| 2   | B     | 323 | GLN  |
| 2   | B     | 327 | CYS  |
| 2   | B     | 342 | ILE  |
| 2   | B     | 348 | LEU  |
| 2   | B     | 362 | LEU  |
| 2   | B     | 364 | LEU  |
| 2   | B     | 374 | GLU  |
| 2   | B     | 375 | SER  |
| 2   | B     | 378 | ARG  |
| 2   | B     | 383 | THR  |
| 2   | B     | 384 | LEU  |
| 2   | B     | 391 | LEU  |
| 2   | B     | 392 | MET  |
| 2   | B     | 396 | GLN  |
| 2   | B     | 408 | SER  |
| 2   | B     | 417 | LYS  |
| 2   | B     | 424 | LEU  |
| 2   | B     | 425 | ASN  |
| 2   | B     | 428 | GLU  |
| 2   | B     | 429 | THR  |
| 1   | C     | 1   | MET  |
| 1   | C     | 2   | GLU  |
| 1   | C     | 9   | LYS  |
| 1   | C     | 10  | ILE  |
| 1   | C     | 12  | GLU  |
| 1   | C     | 14  | THR  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | C     | 15    | TYR  |
| 1   | C     | 22[A] | ARG  |
| 1   | C     | 22[B] | ARG  |
| 1   | C     | 36    | ARG  |
| 1   | C     | 37    | LEU  |
| 1   | C     | 39    | THR  |
| 1   | C     | 41    | THR  |
| 1   | C     | 46    | SER  |
| 1   | C     | 55    | LEU  |
| 1   | C     | 64    | VAL  |
| 1   | C     | 75    | LYS  |
| 1   | C     | 76    | LEU  |
| 1   | C     | 78    | LEU  |
| 1   | C     | 85    | GLN  |
| 1   | C     | 87    | LEU  |
| 1   | C     | 89    | LYS  |
| 1   | C     | 96    | LEU  |
| 1   | C     | 97    | THR  |
| 1   | C     | 115   | LEU  |
| 1   | C     | 131   | GLN  |
| 1   | C     | 134   | LEU  |
| 1   | C     | 135   | ILE  |
| 1   | C     | 143   | LEU  |
| 1   | C     | 154   | VAL  |
| 1   | C     | 158   | THR  |
| 1   | C     | 162   | GLU  |
| 1   | C     | 181   | SER  |
| 1   | C     | 196   | MET  |
| 1   | C     | 199   | ARG  |
| 1   | C     | 200   | ARG  |
| 1   | C     | 206   | ASP  |
| 1   | C     | 214   | ARG  |
| 1   | C     | 217   | ARG  |
| 1   | C     | 226   | VAL  |
| 1   | C     | 230   | VAL  |
| 1   | C     | 232   | SER  |
| 1   | C     | 242   | LYS  |
| 1   | C     | 246   | GLN  |
| 1   | C     | 248   | PHE  |
| 1   | C     | 250   | LYS  |
| 1   | C     | 252   | VAL  |
| 1   | C     | 261   | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 264 | SER  |
| 1   | C     | 275 | ILE  |
| 1   | C     | 276 | SER  |
| 1   | C     | 278 | LYS  |
| 1   | C     | 287 | GLN  |
| 1   | C     | 289 | VAL  |
| 1   | C     | 291 | LYS  |
| 1   | C     | 293 | VAL  |
| 1   | C     | 296 | LEU  |
| 2   | D     | 175 | VAL  |
| 2   | D     | 178 | TYR  |
| 2   | D     | 187 | ARG  |
| 2   | D     | 194 | LYS  |
| 2   | D     | 196 | LYS  |
| 2   | D     | 197 | VAL  |
| 2   | D     | 206 | ILE  |
| 2   | D     | 207 | THR  |
| 2   | D     | 210 | MET  |
| 2   | D     | 213 | ILE  |
| 2   | D     | 232 | LEU  |
| 2   | D     | 287 | THR  |
| 2   | D     | 292 | LEU  |
| 2   | D     | 316 | THR  |
| 2   | D     | 317 | GLN  |
| 2   | D     | 328 | LYS  |
| 2   | D     | 342 | ILE  |
| 2   | D     | 345 | ASP  |
| 2   | D     | 348 | LEU  |
| 2   | D     | 362 | LEU  |
| 2   | D     | 364 | LEU  |
| 2   | D     | 371 | SER  |
| 2   | D     | 375 | SER  |
| 2   | D     | 378 | ARG  |
| 2   | D     | 383 | THR  |
| 2   | D     | 384 | LEU  |
| 2   | D     | 385 | GLU  |
| 2   | D     | 391 | LEU  |
| 2   | D     | 392 | MET  |
| 2   | D     | 396 | GLN  |
| 2   | D     | 403 | GLN  |
| 2   | D     | 416 | SER  |
| 2   | D     | 417 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 425 | ASN  |
| 2   | D     | 428 | GLU  |
| 2   | D     | 431 | ASN  |
| 2   | D     | 432 | LEU  |
| 3   | F     | 504 | ARG  |
| 3   | F     | 506 | LEU  |
| 3   | F     | 507 | ILE  |
| 3   | H     | 504 | ARG  |
| 3   | H     | 507 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 59  | ASN  |
| 1   | A     | 60  | HIS  |
| 1   | A     | 71  | HIS  |
| 1   | A     | 74  | ASN  |
| 1   | A     | 113 | GLN  |
| 1   | A     | 121 | HIS  |
| 1   | A     | 268 | HIS  |
| 2   | B     | 183 | HIS  |
| 2   | B     | 208 | ASN  |
| 2   | B     | 296 | HIS  |
| 2   | B     | 312 | ASN  |
| 2   | B     | 317 | GLN  |
| 2   | B     | 323 | GLN  |
| 2   | B     | 403 | GLN  |
| 2   | B     | 404 | HIS  |
| 2   | B     | 419 | HIS  |
| 1   | C     | 5   | GLN  |
| 1   | C     | 59  | ASN  |
| 1   | C     | 60  | HIS  |
| 1   | C     | 85  | GLN  |
| 1   | C     | 131 | GLN  |
| 1   | C     | 246 | GLN  |
| 2   | D     | 208 | ASN  |
| 2   | D     | 228 | GLN  |
| 2   | D     | 233 | HIS  |
| 2   | D     | 317 | GLN  |
| 2   | D     | 322 | GLN  |
| 2   | D     | 404 | HIS  |

### 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 |
| 3   | ABA  | H     | 503 | 3    | 4,5,6        | 0.57 | 0        | 1,5,7       | 0.52 | 0        |
| 3   | PFF  | F     | 508 | 3    | 11,12,13     | 0.82 | 0        | 10,15,17    | 1.90 | 5 (50%)  |
| 3   | ABA  | F     | 503 | 3    | 4,5,6        | 0.42 | 0        | 1,5,7       | 0.53 | 0        |
| 3   | PFF  | H     | 508 | 3    | 11,12,13     | 0.92 | 0        | 10,15,17    | 1.32 | 2 (20%)  |

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   |
|-----|------|-------|-----|------|---------|----------|---------|
| 3   | ABA  | H     | 503 | 3    | -       | 1/3/4/6  | -       |
| 3   | PFF  | F     | 508 | 3    | -       | 2/5/6/8  | 0/1/1/1 |
| 3   | ABA  | F     | 503 | 3    | -       | 2/3/4/6  | -       |
| 3   | PFF  | H     | 508 | 3    | -       | 2/5/6/8  | 0/1/1/1 |

There are no bond length outliers.

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | F     | 508 | PFF  | CE2-CZ-CE1 | -3.11 | 118.72      | 122.80   |
| 3   | F     | 508 | PFF  | CB-CG-CD1  | -2.82 | 115.66      | 120.90   |
| 3   | F     | 508 | PFF  | CB-CG-CD2  | -2.42 | 116.40      | 120.90   |
| 3   | F     | 508 | PFF  | CD1-CE1-CZ | 2.21  | 120.65      | 118.38   |
| 3   | H     | 508 | PFF  | CE1-CD1-CG | -2.13 | 118.20      | 121.00   |

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| Mol | Chain | Res | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3   | H     | 508 | PFF  | CD1-CE1-CZ | 2.04 | 120.47      | 118.38   |
| 3   | F     | 508 | PFF  | CD2-CE2-CZ | 2.02 | 120.45      | 118.38   |

There are no chirality outliers.

All (7) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms      |
|-----|-------|-----|------|------------|
| 3   | F     | 503 | ABA  | C-CA-CB-CG |
| 3   | F     | 508 | PFF  | C-CA-CB-CG |
| 3   | F     | 503 | ABA  | N-CA-CB-CG |
| 3   | F     | 508 | PFF  | N-CA-CB-CG |
| 3   | H     | 508 | PFF  | N-CA-CB-CG |
| 3   | H     | 508 | PFF  | C-CA-CB-CG |
| 3   | H     | 503 | ABA  | C-CA-CB-CG |

There are no ring outliers.

3 monomers are involved in 13 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | H     | 503 | ABA  | 3       | 0            |
| 3   | F     | 508 | PFF  | 6       | 0            |
| 3   | H     | 508 | PFF  | 4       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands 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 |
| 4   | CK4  | A     | 1297 | -    | 25,26,26     | 1.39 | 3 (12%)  | 36,38,38    | 2.74 | 13 (36%) |
| 4   | CK4  | C     | 1297 | -    | 25,26,26     | 1.23 | 2 (8%)   | 36,38,38    | 3.01 | 13 (36%) |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 4   | CK4  | A     | 1297 | -    | -       | 0/14/14/14 | 0/3/3/3 |
| 4   | CK4  | C     | 1297 | -    | -       | 0/14/14/14 | 0/3/3/3 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | A     | 1297 | CK4  | C4-C5A  | -5.09 | 1.40        | 1.47     |
| 4   | C     | 1297 | CK4  | C4-C5A  | -4.50 | 1.41        | 1.47     |
| 4   | A     | 1297 | CK4  | C5A-S4A | -2.57 | 1.68        | 1.74     |
| 4   | A     | 1297 | CK4  | C1B-N7  | -2.32 | 1.35        | 1.40     |
| 4   | C     | 1297 | CK4  | C1B-N7  | -2.29 | 1.35        | 1.40     |

All (26) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | C     | 1297 | CK4  | C6-N1-C2    | 6.16  | 120.57      | 115.42   |
| 4   | A     | 1297 | CK4  | C4-N3-C2    | 6.16  | 121.54      | 116.87   |
| 4   | C     | 1297 | CK4  | S4A-C3A-N2A | 6.03  | 118.79      | 114.64   |
| 4   | C     | 1297 | CK4  | C4-N3-C2    | 5.94  | 121.37      | 116.87   |
| 4   | A     | 1297 | CK4  | C6-N1-C2    | 5.58  | 120.08      | 115.42   |
| 4   | A     | 1297 | CK4  | C5A-C1A-N2A | -5.52 | 111.15      | 115.01   |
| 4   | C     | 1297 | CK4  | N1-C2-N3    | -5.48 | 121.12      | 126.42   |
| 4   | A     | 1297 | CK4  | N1-C2-N3    | -5.41 | 121.19      | 126.42   |
| 4   | C     | 1297 | CK4  | C5A-C1A-N2A | -5.35 | 111.28      | 115.01   |
| 4   | C     | 1297 | CK4  | C6-C5-C4    | 5.34  | 120.31      | 117.02   |
| 4   | A     | 1297 | CK4  | C5A-C4-N3   | 4.88  | 121.70      | 115.20   |
| 4   | C     | 1297 | CK4  | C5-C4-N3    | -4.74 | 117.39      | 122.92   |
| 4   | A     | 1297 | CK4  | C5-C4-N3    | -4.67 | 117.47      | 122.92   |
| 4   | C     | 1297 | CK4  | C4-C5A-C1A  | -4.53 | 125.01      | 132.10   |
| 4   | A     | 1297 | CK4  | S4A-C3A-N2A | 4.52  | 117.75      | 114.64   |
| 4   | C     | 1297 | CK4  | C5A-C4-N3   | 4.31  | 120.94      | 115.20   |
| 4   | C     | 1297 | CK4  | C5-C6-N1    | -3.96 | 119.12      | 123.97   |
| 4   | A     | 1297 | CK4  | C6-C5-C4    | 3.78  | 119.34      | 117.02   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | C     | 1297 | CK4  | F1B-C7B-C4B | -3.07 | 106.32      | 112.90   |
| 4   | A     | 1297 | CK4  | C5-C6-N1    | -2.97 | 120.33      | 123.97   |
| 4   | A     | 1297 | CK4  | C4-C5A-C1A  | -2.88 | 127.58      | 132.10   |
| 4   | C     | 1297 | CK4  | C6A-C1A-N2A | -2.82 | 113.65      | 119.32   |
| 4   | C     | 1297 | CK4  | C3A-S4A-C5A | -2.36 | 88.23       | 89.64    |
| 4   | A     | 1297 | CK4  | C3B-C4B-C7B | 2.36  | 123.75      | 119.96   |
| 4   | A     | 1297 | CK4  | C6A-C1A-N2A | -2.35 | 114.60      | 119.32   |
| 4   | A     | 1297 | CK4  | C1A-C5A-S4A | 2.24  | 111.27      | 109.91   |

There are no chirality outliers.

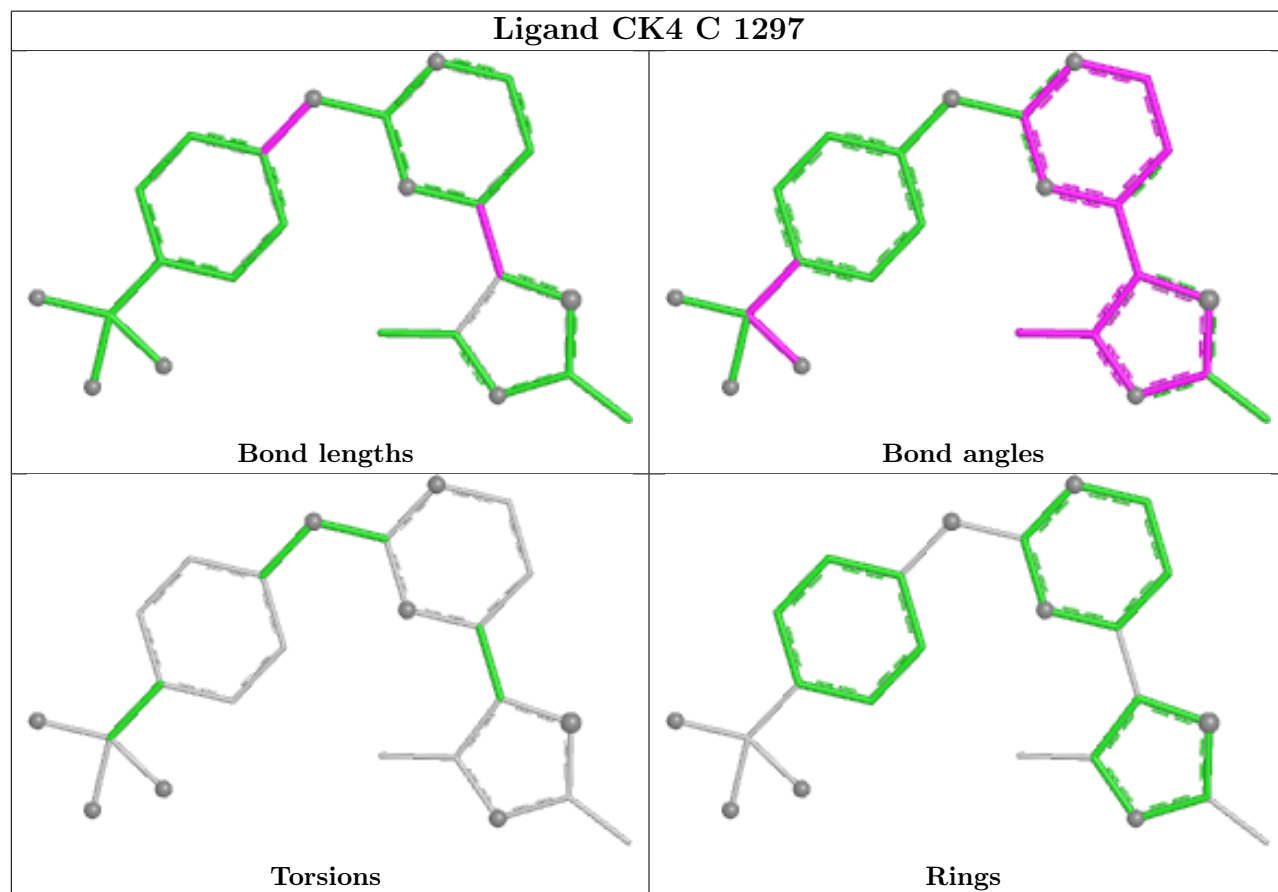
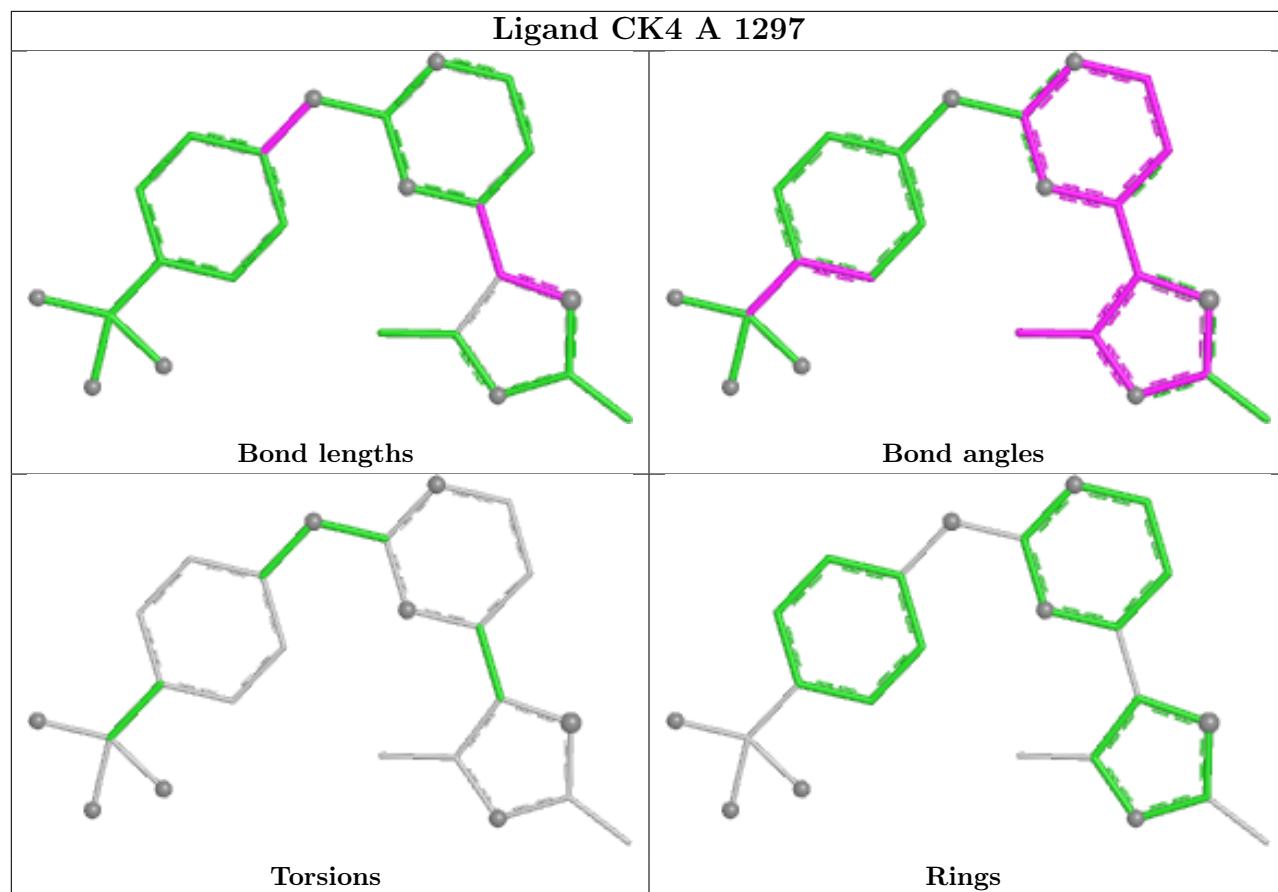
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | A     | 1297 | CK4  | 9       | 0            |
| 4   | C     | 1297 | CK4  | 5       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|-----------------|--------|--------------|-----------------------|--------|
| 1   | A     | 296/298 (99%)   | -0.65  | 3 (1%) 79 73 | 14, 33, 73, 107       | 0      |
| 1   | C     | 296/298 (99%)   | -0.61  | 4 (1%) 73 65 | 13, 33, 74, 106       | 1 (0%) |
| 2   | B     | 258/259 (99%)   | -0.66  | 0 100 100    | 19, 36, 60, 103       | 0      |
| 2   | D     | 258/259 (99%)   | -0.66  | 1 (0%) 88 85 | 16, 36, 58, 102       | 0      |
| 3   | F     | 6/9 (66%)       | -0.68  | 0 100 100    | 45, 47, 54, 58        | 0      |
| 3   | H     | 6/9 (66%)       | -0.96  | 0 100 100    | 15, 25, 72, 76        | 0      |
| All | All   | 1120/1132 (98%) | -0.65  | 8 (0%) 84 79 | 13, 35, 67, 107       | 1 (0%) |

All (8) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | D     | 175 | VAL  | 5.1  |
| 1   | C     | 13  | GLY  | 4.7  |
| 1   | C     | 39  | THR  | 3.0  |
| 1   | C     | 72  | THR  | 2.5  |
| 1   | A     | 15  | TYR  | 2.4  |
| 1   | A     | 39  | THR  | 2.4  |
| 1   | A     | 40  | GLU  | 2.2  |
| 1   | C     | 163 | VAL  | 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | ABA  | H     | 503 | 6/7   | 0.91 | 0.07 | 24,37,52,53                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | PFF  | F     | 508 | 12/13 | 0.92 | 0.07 | 56,64,72,72                 | 0     |
| 3   | ABA  | F     | 503 | 6/7   | 0.94 | 0.05 | 12,42,54,56                 | 0     |
| 3   | PFF  | H     | 508 | 12/13 | 0.94 | 0.05 | 25,34,44,44                 | 0     |

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

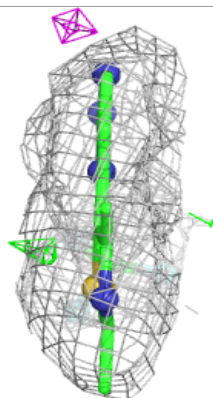
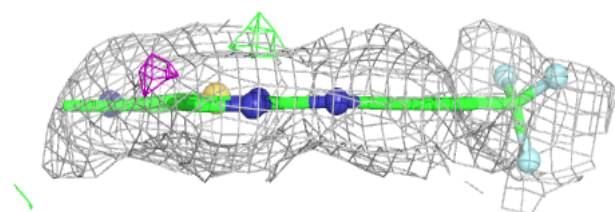
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 4   | CK4  | A     | 1297 | 24/24 | 0.89 | 0.08 | 72,77,80,92                 | 0     |
| 4   | CK4  | C     | 1297 | 24/24 | 0.90 | 0.07 | 42,54,58,59                 | 0     |

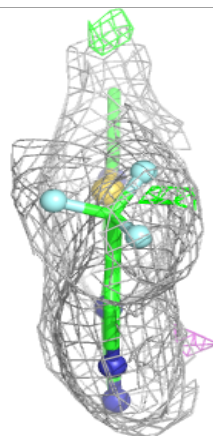
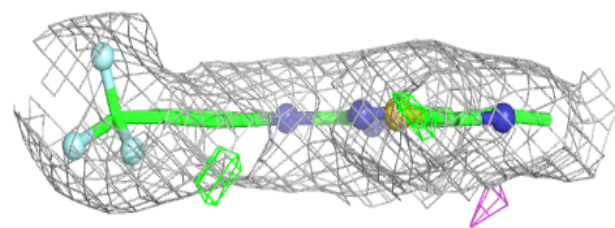
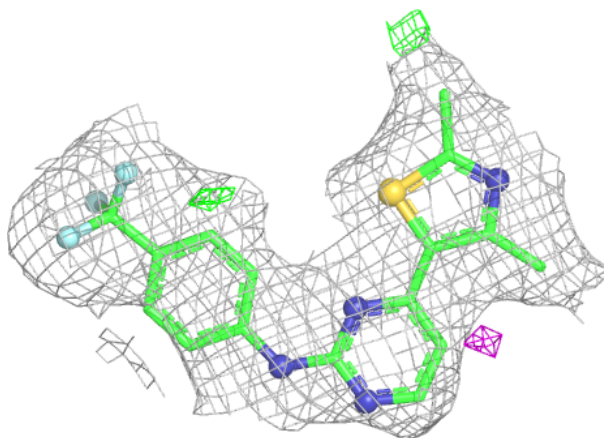
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around CK4 A 1297:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CK4 C 1297:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.