



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:29 PM UTC

PDB ID : 3R2A / pdb\_00003r2a  
Title : Crystal structure of RXRalpha ligand-binding domain complexed with corepressor SMRT2 and antagonist rhein  
Authors : Zhang, H.; Chen, L.; Chen, J.; Jiang, H.; Shen, X.  
Deposited on : 2011-03-14  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| 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                                                             |

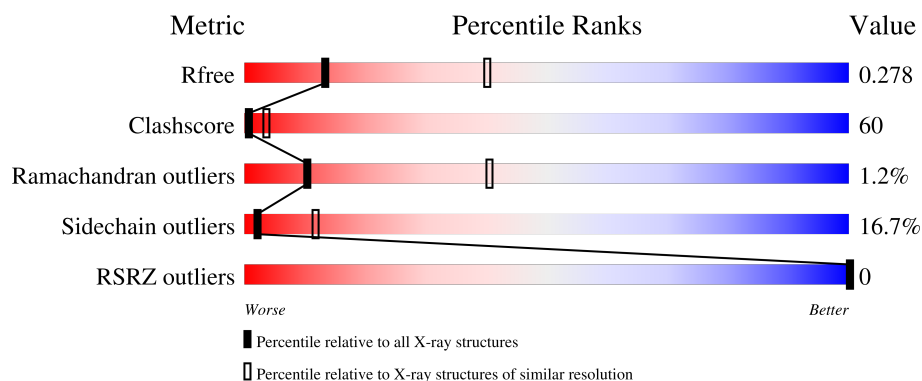
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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                      | 2672 (3.00-3.00)                                      |
| Clashscore            | 190562                      | 2977 (3.00-3.00)                                      |
| Ramachandran outliers | 187476                      | 2877 (3.00-3.00)                                      |
| Sidechain outliers    | 187428                      | 2880 (3.00-3.00)                                      |
| RSRZ outliers         | 180081                      | 2671 (3.00-3.00)                                      |

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     | 240    |                  |
| 1   | B     | 240    |                  |
| 1   | C     | 240    |                  |
| 1   | D     | 240    |                  |
| 2   | E     | 16     |                  |

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| Mol | Chain | Length | Quality of chain                                                                       |
|-----|-------|--------|----------------------------------------------------------------------------------------|
| 2   | F     | 16     | <div><div></div><div></div><div></div><div>25%</div><div>31%</div><div>44%</div></div> |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6940 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.

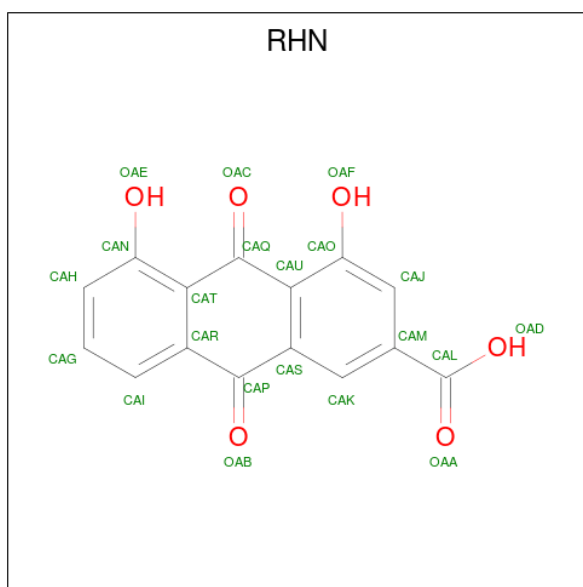
- Molecule 1 is a protein called Retinoic acid receptor RXR-alpha.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 211      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1666  | 1069 | 287 | 301 | 9  |         |         |       |
| 1   | B     | 217      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1717  | 1099 | 296 | 311 | 11 |         |         |       |
| 1   | C     | 203      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1607  | 1034 | 276 | 288 | 9  |         |         |       |
| 1   | D     | 219      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1733  | 1111 | 298 | 313 | 11 |         |         |       |

- Molecule 2 is a protein called Nuclear receptor corepressor 2.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 2   | E     | 7        | Total | C  | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 50    | 31 | 8  | 10 | 1 |         |         |       |
| 2   | F     | 9        | Total | C  | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 65    | 41 | 10 | 13 | 1 |         |         |       |

- Molecule 3 is 4,5-dihydroxy-9,10-dioxo-9,10-dihydroanthracene-2-carboxylic acid (CCD ID: RHN) (formula: C<sub>15</sub>H<sub>8</sub>O<sub>6</sub>).

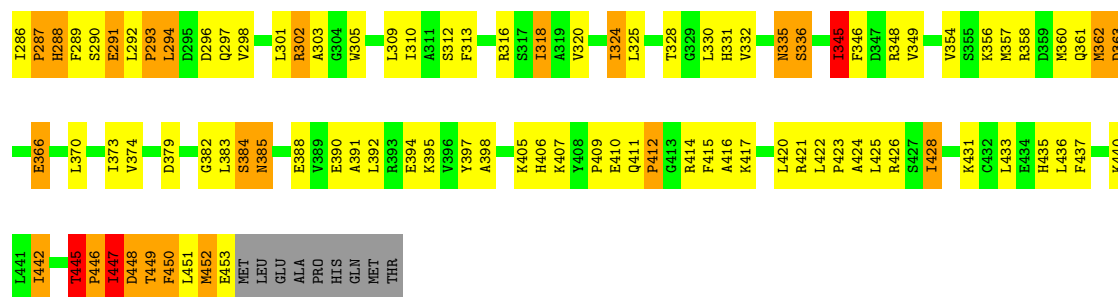


| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 3   | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 21    | 15 | 6 |         |         |
| 3   | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 21    | 15 | 6 |         |         |

- Molecule 4 is water.

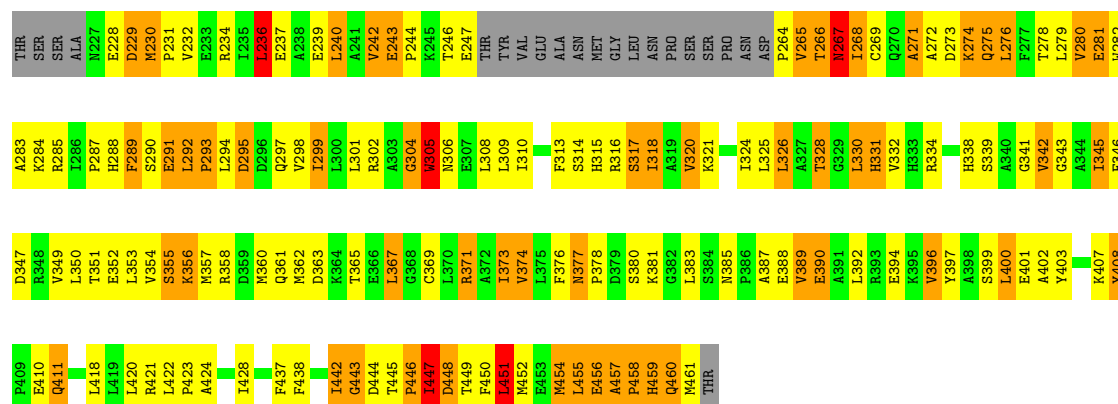
| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 4   | A     | 17       | Total O<br>17 17 | 0       | 0       |
| 4   | B     | 15       | Total O<br>15 15 | 0       | 0       |
| 4   | C     | 13       | Total O<br>13 13 | 0       | 0       |
| 4   | D     | 12       | Total O<br>12 12 | 0       | 0       |
| 4   | E     | 2        | Total O<br>2 2   | 0       | 0       |
| 4   | F     | 1        | Total O<br>1 1   | 0       | 0       |





• Molecule 1: Retinoic acid receptor RXR-alpha

Chain D: 28% 38% 22% 9%



• Molecule 2: Nuclear receptor corepressor 2

Chain E: 31% 12% 56%



• Molecule 2: Nuclear receptor corepressor 2

Chain F: 25% 31% 44%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 85.03Å 117.58Å 117.12Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 42.52 – 3.00<br>42.52 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (42.52-3.00)<br>93.6 (42.52-3.00)                     | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.08                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.22 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0019                                             | Depositor        |
| R, $R_{free}$                                                           | 0.254 , 0.335<br>0.268 , 0.278                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1191 reflections (5.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 72.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.242                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 114.6                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | 0.447 for -h,l,k                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 6940                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 70.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: RHN

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     | 1.91         | 11/1699 (0.6%) | 1.41        | 25/2297 (1.1%)  |
| 1   | B     | 1.71         | 6/1751 (0.3%)  | 1.63        | 46/2367 (1.9%)  |
| 1   | C     | 1.93         | 5/1639 (0.3%)  | 1.59        | 30/2214 (1.4%)  |
| 1   | D     | 1.67         | 6/1768 (0.3%)  | 1.63        | 40/2389 (1.7%)  |
| 2   | E     | 1.31         | 0/49           | 1.58        | 1/64 (1.6%)     |
| 2   | F     | 1.31         | 0/64           | 1.71        | 2/85 (2.4%)     |
| All | All   | 1.80         | 28/6970 (0.4%) | 1.57        | 144/9416 (1.5%) |

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   | D     | 0                   | 1                   |

All (28) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 371 | ARG  | CZ-NH1 | -9.84 | 1.19        | 1.32     |
| 1   | B     | 371 | ARG  | CD-NE  | -8.38 | 1.34        | 1.46     |
| 1   | B     | 371 | ARG  | CG-CD  | -7.64 | 1.29        | 1.52     |
| 1   | A     | 443 | GLY  | CA-C   | -7.34 | 1.45        | 1.51     |
| 1   | D     | 299 | ILE  | CA-CB  | -6.46 | 1.46        | 1.54     |
| 1   | A     | 342 | VAL  | CA-CB  | -6.19 | 1.46        | 1.54     |
| 1   | A     | 299 | ILE  | CA-CB  | -5.92 | 1.47        | 1.54     |
| 1   | D     | 305 | TRP  | CA-C   | -5.91 | 1.44        | 1.52     |
| 1   | D     | 342 | VAL  | CA-C   | -5.84 | 1.45        | 1.52     |
| 1   | D     | 242 | VAL  | CA-CB  | -5.80 | 1.46        | 1.54     |
| 1   | A     | 442 | ILE  | CA-C   | -5.69 | 1.45        | 1.52     |
| 1   | B     | 376 | PHE  | CA-C   | -5.69 | 1.47        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 372 | ALA  | CA-CB | -5.66 | 1.44        | 1.53     |
| 1   | A     | 442 | ILE  | C-N   | -5.58 | 1.30        | 1.33     |
| 1   | B     | 311 | ALA  | CA-CB | -5.52 | 1.44        | 1.53     |
| 1   | A     | 310 | ILE  | CA-CB | -5.52 | 1.47        | 1.54     |
| 1   | D     | 230 | MET  | C-O   | -5.50 | 1.21        | 1.23     |
| 1   | A     | 416 | ALA  | CA-CB | -5.34 | 1.45        | 1.53     |
| 1   | A     | 310 | ILE  | C-O   | -5.33 | 1.18        | 1.24     |
| 1   | B     | 310 | ILE  | CA-C  | -5.30 | 1.46        | 1.52     |
| 1   | C     | 398 | ALA  | CA-CB | -5.19 | 1.45        | 1.53     |
| 1   | C     | 294 | LEU  | CA-C  | -5.11 | 1.46        | 1.52     |
| 1   | A     | 342 | VAL  | CA-C  | -5.10 | 1.47        | 1.53     |
| 1   | D     | 424 | ALA  | CA-CB | -5.09 | 1.45        | 1.53     |
| 1   | C     | 416 | ALA  | CA-CB | -5.09 | 1.45        | 1.53     |
| 1   | C     | 242 | VAL  | CA-CB | -5.01 | 1.47        | 1.54     |
| 1   | C     | 447 | ILE  | CA-CB | -5.01 | 1.47        | 1.54     |
| 1   | A     | 300 | LEU  | C-O   | -5.00 | 1.18        | 1.24     |

All (144) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | C     | 273 | ASP  | N-CA-C     | -17.93 | 91.81       | 111.36   |
| 1   | C     | 449 | THR  | N-CA-C     | -17.78 | 91.90       | 111.28   |
| 1   | C     | 366 | GLU  | CG-CD-OE2  | 15.44  | 153.90      | 118.40   |
| 1   | D     | 452 | MET  | N-CA-C     | 15.27  | 127.41      | 111.07   |
| 1   | C     | 366 | GLU  | OE1-CD-OE2 | -13.80 | 89.78       | 122.90   |
| 1   | A     | 449 | THR  | N-CA-C     | -13.13 | 96.61       | 111.71   |
| 1   | D     | 459 | HIS  | N-CA-C     | -12.93 | 96.88       | 113.17   |
| 1   | B     | 271 | ALA  | N-CA-C     | 12.66  | 125.16      | 111.36   |
| 1   | B     | 371 | ARG  | CG-CD-NE   | 12.17  | 138.77      | 112.00   |
| 1   | B     | 451 | LEU  | N-CA-C     | -11.95 | 92.91       | 110.23   |
| 1   | B     | 266 | THR  | N-CA-C     | -11.63 | 98.35       | 112.54   |
| 1   | D     | 276 | LEU  | N-CA-C     | -11.41 | 98.59       | 111.71   |
| 1   | B     | 276 | LEU  | N-CA-C     | -10.91 | 99.47       | 111.36   |
| 1   | D     | 330 | LEU  | N-CA-C     | 10.79  | 126.29      | 111.39   |
| 1   | D     | 305 | TRP  | CA-C-N     | -10.41 | 106.91      | 120.44   |
| 1   | D     | 305 | TRP  | C-N-CA     | -10.41 | 106.91      | 120.44   |
| 1   | D     | 448 | ASP  | N-CA-C     | -10.05 | 99.14       | 111.40   |
| 1   | C     | 270 | GLN  | N-CA-C     | -10.01 | 95.18       | 110.70   |
| 1   | A     | 442 | ILE  | N-CA-C     | -9.86  | 88.84       | 109.34   |
| 1   | A     | 444 | ASP  | N-CA-C     | -9.85  | 97.53       | 110.53   |
| 1   | D     | 447 | ILE  | CB-CA-C    | -9.74  | 95.32       | 111.29   |
| 1   | D     | 304 | GLY  | N-CA-C     | -9.68  | 97.27       | 112.85   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | D     | 451  | LEU  | N-CA-C   | -9.59 | 94.57       | 109.25   |
| 1   | B     | 459  | HIS  | N-CA-C   | -9.52 | 90.51       | 110.80   |
| 1   | A     | 442  | ILE  | CA-C-N   | -9.44 | 113.89      | 122.29   |
| 1   | A     | 442  | ILE  | C-N-CA   | -9.44 | 113.89      | 122.29   |
| 1   | B     | 408  | TYR  | CA-C-N   | 9.18  | 128.85      | 118.85   |
| 1   | B     | 408  | TYR  | C-N-CA   | 9.18  | 128.85      | 118.85   |
| 1   | D     | 328  | THR  | N-CA-C   | -9.03 | 101.81      | 112.92   |
| 1   | D     | 408  | TYR  | CA-C-N   | 8.91  | 128.95      | 119.05   |
| 1   | D     | 408  | TYR  | C-N-CA   | 8.91  | 128.95      | 119.05   |
| 1   | B     | 371  | ARG  | CD-NE-CZ | -8.89 | 111.95      | 124.40   |
| 1   | D     | 443  | GLY  | CA-C-N   | 8.87  | 134.15      | 120.75   |
| 1   | D     | 443  | GLY  | C-N-CA   | 8.87  | 134.15      | 120.75   |
| 1   | A     | 342  | VAL  | CB-CA-C  | -8.61 | 102.28      | 112.19   |
| 1   | B     | 454  | MET  | N-CA-C   | 8.53  | 122.30      | 109.25   |
| 2   | F     | 2340 | GLY  | N-CA-C   | -8.47 | 102.14      | 113.24   |
| 1   | D     | 274  | LYS  | N-CA-C   | -8.37 | 102.08      | 111.71   |
| 1   | B     | 444  | ASP  | N-CA-C   | 8.19  | 119.44      | 108.38   |
| 1   | D     | 243  | GLU  | N-CA-C   | -8.02 | 97.93       | 109.48   |
| 1   | B     | 452  | MET  | N-CA-C   | 7.93  | 119.62      | 110.97   |
| 2   | E     | 2343 | ALA  | N-CA-C   | -7.93 | 95.80       | 108.73   |
| 1   | A     | 233  | GLU  | N-CA-C   | -7.90 | 101.78      | 111.33   |
| 1   | B     | 445  | THR  | N-CA-C   | -7.87 | 95.82       | 109.58   |
| 1   | B     | 272  | ALA  | N-CA-C   | 7.71  | 121.79      | 112.38   |
| 1   | A     | 388  | GLU  | N-CA-C   | -7.66 | 102.88      | 111.07   |
| 1   | B     | 263  | ASP  | N-CA-C   | 7.53  | 120.57      | 109.50   |
| 1   | B     | 267  | ASN  | CA-C-N   | -7.50 | 110.91      | 121.55   |
| 1   | B     | 267  | ASN  | C-N-CA   | -7.50 | 110.91      | 121.55   |
| 1   | B     | 339  | SER  | N-CA-C   | 7.46  | 122.58      | 113.17   |
| 1   | A     | 412  | PRO  | N-CA-C   | -7.39 | 104.23      | 113.84   |
| 1   | C     | 269  | CYS  | CA-C-N   | -7.21 | 111.54      | 122.21   |
| 1   | C     | 269  | CYS  | C-N-CA   | -7.21 | 111.54      | 122.21   |
| 1   | B     | 382  | GLY  | N-CA-C   | 7.21  | 126.73      | 113.76   |
| 1   | D     | 396  | VAL  | N-CA-C   | 7.17  | 117.27      | 110.53   |
| 1   | D     | 354  | VAL  | CB-CA-C  | -7.03 | 102.81      | 112.02   |
| 1   | D     | 293  | PRO  | N-CA-C   | -7.03 | 100.18      | 111.14   |
| 1   | D     | 446  | PRO  | N-CA-C   | -7.01 | 100.89      | 111.41   |
| 2   | F     | 2342 | GLU  | N-CA-C   | -6.99 | 103.67      | 111.71   |
| 1   | B     | 352  | GLU  | N-CA-C   | 6.88  | 118.86      | 111.36   |
| 1   | A     | 265  | VAL  | N-CA-C   | -6.88 | 103.61      | 110.62   |
| 1   | C     | 442  | ILE  | CA-C-N   | 6.87  | 126.63      | 120.10   |
| 1   | C     | 442  | ILE  | C-N-CA   | 6.87  | 126.63      | 120.10   |
| 1   | A     | 232  | VAL  | CB-CA-C  | -6.85 | 102.90      | 112.14   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | B     | 354 | VAL  | N-CA-C   | 6.76  | 116.89      | 110.53   |
| 1   | B     | 449 | THR  | N-CA-C   | -6.70 | 103.98      | 111.28   |
| 1   | D     | 229 | ASP  | N-CA-C   | -6.68 | 101.71      | 110.53   |
| 1   | B     | 287 | PRO  | N-CA-C   | 6.62  | 122.94      | 113.47   |
| 1   | C     | 366 | GLU  | CB-CG-CD | 6.62  | 123.85      | 112.60   |
| 1   | C     | 286 | ILE  | N-CA-C   | -6.51 | 101.80      | 108.96   |
| 1   | B     | 354 | VAL  | CB-CA-C  | -6.48 | 103.53      | 112.02   |
| 1   | A     | 227 | ASN  | N-CA-C   | -6.41 | 105.28      | 113.23   |
| 1   | B     | 263 | ASP  | CA-C-N   | 6.36  | 125.94      | 119.19   |
| 1   | B     | 263 | ASP  | C-N-CA   | 6.36  | 125.94      | 119.19   |
| 1   | A     | 414 | ARG  | N-CA-C   | 6.36  | 118.21      | 111.28   |
| 1   | D     | 229 | ASP  | CA-C-N   | -6.28 | 116.05      | 122.83   |
| 1   | D     | 229 | ASP  | C-N-CA   | -6.28 | 116.05      | 122.83   |
| 1   | D     | 242 | VAL  | N-CA-C   | -6.27 | 106.40      | 112.29   |
| 1   | D     | 387 | ALA  | N-CA-C   | -6.25 | 104.52      | 111.71   |
| 1   | C     | 293 | PRO  | N-CA-C   | -6.25 | 101.27      | 111.15   |
| 1   | B     | 326 | LEU  | N-CA-C   | 6.19  | 118.70      | 110.53   |
| 1   | A     | 448 | ASP  | N-CA-C   | -6.17 | 100.95      | 113.29   |
| 1   | B     | 443 | GLY  | N-CA-C   | 6.17  | 120.13      | 112.73   |
| 1   | D     | 399 | SER  | N-CA-C   | -6.14 | 104.69      | 111.82   |
| 1   | A     | 329 | GLY  | N-CA-C   | -6.11 | 106.88      | 115.32   |
| 1   | D     | 326 | LEU  | N-CA-C   | 6.09  | 118.39      | 110.53   |
| 1   | D     | 454 | MET  | N-CA-C   | 6.05  | 118.58      | 108.96   |
| 1   | C     | 412 | PRO  | N-CA-C   | -6.03 | 106.32      | 113.86   |
| 1   | D     | 295 | ASP  | N-CA-C   | -5.96 | 104.69      | 111.07   |
| 1   | C     | 287 | PRO  | CA-C-N   | -5.94 | 113.23      | 122.67   |
| 1   | C     | 287 | PRO  | C-N-CA   | -5.94 | 113.23      | 122.67   |
| 1   | D     | 377 | ASN  | CA-C-N   | 5.93  | 125.48      | 119.19   |
| 1   | D     | 377 | ASN  | C-N-CA   | 5.93  | 125.48      | 119.19   |
| 1   | B     | 377 | ASN  | CA-C-N   | 5.93  | 125.55      | 119.56   |
| 1   | B     | 377 | ASN  | C-N-CA   | 5.93  | 125.55      | 119.56   |
| 1   | D     | 354 | VAL  | N-CA-C   | 5.90  | 116.08      | 110.53   |
| 1   | B     | 267 | ASN  | N-CA-C   | -5.87 | 104.88      | 111.28   |
| 1   | A     | 414 | ARG  | CA-C-N   | -5.87 | 112.81      | 120.44   |
| 1   | A     | 414 | ARG  | C-N-CA   | -5.87 | 112.81      | 120.44   |
| 1   | C     | 450 | PHE  | CA-C-N   | -5.86 | 111.94      | 121.26   |
| 1   | C     | 450 | PHE  | C-N-CA   | -5.86 | 111.94      | 121.26   |
| 1   | A     | 310 | ILE  | CB-CA-C  | -5.85 | 104.25      | 112.14   |
| 1   | C     | 289 | PHE  | N-CA-C   | 5.85  | 117.65      | 111.28   |
| 1   | B     | 237 | GLU  | N-CA-C   | -5.78 | 104.98      | 111.28   |
| 1   | C     | 345 | ILE  | CB-CA-C  | -5.78 | 104.25      | 112.22   |
| 1   | B     | 387 | ALA  | N-CA-C   | -5.74 | 105.98      | 112.87   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 448 | ASP  | N-CA-C    | 5.74  | 117.21      | 111.07   |
| 1   | D     | 457 | ALA  | N-CA-C    | -5.67 | 105.74      | 113.57   |
| 1   | C     | 335 | ASN  | N-CA-C    | -5.59 | 105.09      | 111.07   |
| 1   | C     | 362 | MET  | N-CA-C    | -5.58 | 103.12      | 110.43   |
| 1   | C     | 452 | MET  | N-CA-C    | -5.57 | 97.87       | 108.17   |
| 1   | B     | 265 | VAL  | N-CA-C    | 5.56  | 116.29      | 110.62   |
| 1   | B     | 371 | ARG  | NE-CZ-NH1 | -5.56 | 115.94      | 121.50   |
| 1   | B     | 367 | LEU  | N-CA-C    | -5.53 | 105.25      | 111.28   |
| 1   | A     | 294 | LEU  | N-CA-C    | -5.51 | 105.38      | 111.71   |
| 1   | B     | 287 | PRO  | CA-C-N    | -5.50 | 113.85      | 122.65   |
| 1   | B     | 287 | PRO  | C-N-CA    | -5.50 | 113.85      | 122.65   |
| 1   | D     | 271 | ALA  | N-CA-C    | 5.49  | 117.26      | 111.28   |
| 1   | B     | 442 | ILE  | CB-CA-C   | -5.49 | 104.73      | 112.14   |
| 1   | C     | 336 | SER  | N-CA-C    | -5.48 | 105.21      | 111.07   |
| 1   | C     | 417 | LYS  | N-CA-C    | -5.45 | 105.24      | 111.07   |
| 1   | D     | 289 | PHE  | N-CA-C    | 5.42  | 116.87      | 111.07   |
| 1   | B     | 242 | VAL  | N-CA-C    | 5.42  | 117.39      | 112.29   |
| 1   | A     | 312 | SER  | N-CA-C    | 5.41  | 116.98      | 111.14   |
| 1   | D     | 280 | VAL  | N-CA-C    | 5.41  | 116.18      | 110.72   |
| 1   | D     | 374 | VAL  | CB-CA-C   | -5.37 | 104.81      | 112.22   |
| 1   | A     | 319 | ALA  | N-CA-C    | -5.36 | 105.33      | 111.07   |
| 1   | C     | 363 | ASP  | N-CA-CB   | -5.35 | 101.93      | 111.08   |
| 1   | C     | 379 | ASP  | N-CA-C    | -5.35 | 106.53      | 113.16   |
| 1   | A     | 443 | GLY  | N-CA-C    | -5.33 | 100.84      | 111.34   |
| 1   | B     | 289 | PHE  | N-CA-C    | 5.33  | 116.77      | 111.07   |
| 1   | A     | 306 | ASN  | N-CA-C    | 5.32  | 116.76      | 111.07   |
| 1   | D     | 267 | ASN  | N-CA-C    | -5.29 | 105.42      | 111.07   |
| 1   | C     | 354 | VAL  | CB-CA-C   | -5.22 | 105.09      | 112.14   |
| 1   | B     | 458 | PRO  | N-CA-C    | -5.22 | 101.72      | 112.47   |
| 1   | C     | 373 | ILE  | CB-CA-C   | -5.18 | 105.15      | 112.14   |
| 1   | B     | 307 | GLU  | N-CA-C    | 5.08  | 116.90      | 111.36   |
| 1   | A     | 441 | LEU  | N-CA-C    | 5.07  | 116.62      | 111.14   |
| 1   | C     | 291 | GLU  | N-CA-C    | -5.06 | 106.89      | 113.16   |
| 1   | B     | 280 | VAL  | N-CA-C    | 5.05  | 115.82      | 110.72   |
| 1   | A     | 443 | GLY  | CA-C-O    | 5.03  | 125.14      | 120.81   |
| 1   | D     | 236 | LEU  | N-CA-C    | -5.02 | 105.81      | 111.28   |
| 1   | B     | 457 | ALA  | N-CA-C    | -5.02 | 106.64      | 113.57   |
| 1   | C     | 288 | HIS  | N-CA-C    | 5.01  | 118.71      | 112.59   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | D     | 443 | GLY  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1666  | 0        | 1701     | 148     | 0            |
| 1   | B     | 1717  | 0        | 1736     | 268     | 3            |
| 1   | C     | 1607  | 0        | 1639     | 149     | 1            |
| 1   | D     | 1733  | 0        | 1764     | 280     | 2            |
| 2   | E     | 50    | 0        | 50       | 15      | 0            |
| 2   | F     | 65    | 0        | 68       | 17      | 0            |
| 3   | A     | 21    | 0        | 5        | 3       | 0            |
| 3   | C     | 21    | 0        | 6        | 3       | 0            |
| 4   | A     | 17    | 0        | 0        | 3       | 0            |
| 4   | B     | 15    | 0        | 0        | 0       | 0            |
| 4   | C     | 13    | 0        | 0        | 1       | 0            |
| 4   | D     | 12    | 0        | 0        | 3       | 0            |
| 4   | E     | 2     | 0        | 0        | 0       | 0            |
| 4   | F     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 6940  | 0        | 6969     | 830     | 3            |

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 60.

All (830) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:324:ILE:HG13 | 1:B:346:PHE:CE1  | 1.44                     | 1.52              |
| 1:D:385:ASN:CG   | 1:D:388:GLU:HB2  | 1.38                     | 1.47              |
| 1:D:236:LEU:O    | 1:D:240:LEU:CD1  | 1.65                     | 1.43              |
| 1:D:305:TRP:N    | 1:D:308:LEU:HD23 | 1.30                     | 1.38              |
| 1:B:381:LYS:CE   | 1:C:445:THR:OG1  | 1.63                     | 1.37              |
| 1:B:456:GLU:O    | 1:B:459:HIS:CB   | 1.71                     | 1.37              |
| 1:B:264:PRO:O    | 1:B:267:ASN:HB3  | 1.27                     | 1.30              |
| 1:D:385:ASN:ND2  | 1:D:388:GLU:HB2  | 1.46                     | 1.29              |
| 1:D:389:VAL:HA   | 1:D:392:LEU:CD2  | 1.65                     | 1.27              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:400:LEU:O    | 1:D:400:LEU:HD12  | 1.35                     | 1.26              |
| 1:D:385:ASN:CG   | 1:D:388:GLU:CB    | 2.08                     | 1.26              |
| 1:D:385:ASN:OD1  | 1:D:388:GLU:CB    | 1.83                     | 1.25              |
| 1:B:454:MET:HE2  | 1:B:455:LEU:CA    | 1.67                     | 1.24              |
| 1:B:442:ILE:HG21 | 4:D:55:HOH:O      | 1.06                     | 1.23              |
| 1:B:454:MET:HE2  | 1:B:454:MET:C     | 1.63                     | 1.22              |
| 1:A:448:ASP:O    | 1:A:451:LEU:HD12  | 1.38                     | 1.21              |
| 1:D:281:GLU:OE2  | 1:D:285:ARG:NH2   | 1.72                     | 1.21              |
| 1:B:454:MET:CE   | 1:B:455:LEU:HA    | 1.70                     | 1.21              |
| 1:C:410:GLU:O    | 1:C:412:PRO:HD3   | 1.43                     | 1.19              |
| 1:D:236:LEU:O    | 1:D:240:LEU:HD11  | 1.15                     | 1.19              |
| 1:B:267:ASN:OD1  | 1:B:326:LEU:CD1   | 1.91                     | 1.18              |
| 1:D:283:ALA:O    | 1:D:289:PHE:HD2   | 1.28                     | 1.16              |
| 1:B:298:VAL:HG13 | 2:E:2341:LEU:CD1  | 1.74                     | 1.15              |
| 1:B:454:MET:HE2  | 1:B:455:LEU:N     | 1.61                     | 1.15              |
| 1:A:445:THR:HB   | 1:A:446:PRO:HD3   | 1.27                     | 1.15              |
| 1:B:298:VAL:CG1  | 2:E:2341:LEU:HD12 | 1.76                     | 1.14              |
| 1:C:363:ASP:HB2  | 1:C:366:GLU:OE1   | 1.49                     | 1.13              |
| 1:D:236:LEU:HD22 | 1:D:240:LEU:HD11  | 1.25                     | 1.13              |
| 1:A:447:ILE:CD1  | 1:A:448:ASP:H     | 1.59                     | 1.12              |
| 1:C:271:ALA:O    | 1:C:272:ALA:HB3   | 1.37                     | 1.12              |
| 1:A:409:PRO:HD2  | 1:A:410:GLU:OE1   | 1.47                     | 1.12              |
| 1:B:455:LEU:O    | 1:B:455:LEU:HD23  | 1.46                     | 1.12              |
| 1:B:324:ILE:CG1  | 1:B:346:PHE:CE1   | 2.32                     | 1.11              |
| 1:D:389:VAL:HA   | 1:D:392:LEU:HD21  | 1.31                     | 1.11              |
| 1:A:425:LEU:HD12 | 1:A:425:LEU:O     | 1.46                     | 1.11              |
| 1:C:357:MET:HG2  | 1:C:362:MET:HE3   | 1.11                     | 1.11              |
| 1:D:305:TRP:H    | 1:D:308:LEU:CD2   | 1.63                     | 1.11              |
| 1:B:454:MET:CE   | 1:B:455:LEU:CA    | 2.29                     | 1.10              |
| 1:A:451:LEU:HD22 | 1:A:451:LEU:O     | 1.50                     | 1.09              |
| 1:B:348:ARG:HG3  | 1:B:348:ARG:HH11  | 1.02                     | 1.09              |
| 1:B:361:GLN:HE21 | 1:B:361:GLN:HA    | 1.02                     | 1.09              |
| 1:A:447:ILE:HD12 | 1:A:448:ASP:N     | 1.68                     | 1.08              |
| 1:D:456:GLU:O    | 1:D:459:HIS:CD2   | 2.06                     | 1.08              |
| 1:B:361:GLN:HE21 | 1:B:361:GLN:CA    | 1.64                     | 1.07              |
| 1:B:448:ASP:O    | 1:B:451:LEU:O     | 1.72                     | 1.07              |
| 1:D:283:ALA:O    | 1:D:289:PHE:CD2   | 2.07                     | 1.07              |
| 1:D:385:ASN:OD1  | 1:D:388:GLU:HB2   | 1.45                     | 1.07              |
| 1:B:455:LEU:HD23 | 1:B:455:LEU:C     | 1.74                     | 1.06              |
| 1:D:448:ASP:O    | 1:D:451:LEU:O     | 1.71                     | 1.06              |
| 1:B:454:MET:HE3  | 1:B:456:GLU:H     | 1.21                     | 1.06              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:240:LEU:H    | 1:D:240:LEU:HD12  | 0.92                     | 1.05              |
| 1:B:455:LEU:HD22 | 1:B:455:LEU:H     | 0.92                     | 1.05              |
| 1:A:227:ASN:O    | 1:A:231:PRO:HG3   | 1.57                     | 1.05              |
| 1:D:275:GLN:OE1  | 1:D:275:GLN:HA    | 1.54                     | 1.04              |
| 1:A:445:THR:CB   | 1:A:446:PRO:HD3   | 1.86                     | 1.04              |
| 1:D:236:LEU:CD2  | 1:D:240:LEU:HD11  | 1.87                     | 1.04              |
| 1:D:330:LEU:O    | 1:D:330:LEU:HG    | 1.51                     | 1.04              |
| 1:B:347:ASP:O    | 1:B:351:THR:HG23  | 1.56                     | 1.04              |
| 1:A:447:ILE:HD12 | 1:A:448:ASP:H     | 0.89                     | 1.03              |
| 1:C:296:ASP:OD1  | 1:C:384:SER:OG    | 1.77                     | 1.03              |
| 1:C:357:MET:HG2  | 1:C:362:MET:CE    | 1.88                     | 1.03              |
| 1:B:455:LEU:C    | 1:B:455:LEU:CD2   | 2.30                     | 1.03              |
| 1:B:455:LEU:N    | 1:B:455:LEU:HD22  | 1.58                     | 1.02              |
| 1:B:454:MET:HE2  | 1:B:455:LEU:HA    | 1.24                     | 1.02              |
| 1:D:305:TRP:N    | 1:D:308:LEU:CD2   | 2.21                     | 1.02              |
| 1:A:315:HIS:O    | 1:A:318:ILE:HD13  | 1.59                     | 1.02              |
| 1:C:451:LEU:HD12 | 1:C:453:GLU:N     | 1.73                     | 1.02              |
| 1:B:312:SER:OG   | 1:B:371:ARG:NH1   | 1.92                     | 1.01              |
| 1:B:264:PRO:O    | 1:B:267:ASN:CB    | 2.08                     | 1.01              |
| 1:B:324:ILE:CG1  | 1:B:346:PHE:HE1   | 1.69                     | 1.01              |
| 1:C:345:ILE:O    | 1:C:349:VAL:HG23  | 1.61                     | 1.01              |
| 1:D:242:VAL:O    | 1:D:244:PRO:HD3   | 1.60                     | 1.01              |
| 1:B:460:GLN:HA   | 1:C:284:LYS:NZ    | 1.76                     | 1.01              |
| 1:C:269:CYS:C    | 1:C:271:ALA:H     | 1.65                     | 1.01              |
| 1:D:361:GLN:HG2  | 1:D:361:GLN:O     | 1.60                     | 1.00              |
| 1:D:283:ALA:HB1  | 1:D:289:PHE:CE2   | 1.97                     | 1.00              |
| 1:D:240:LEU:CD1  | 1:D:240:LEU:H     | 1.70                     | 0.99              |
| 1:B:229:ASP:O    | 1:B:231:PRO:CD    | 2.11                     | 0.99              |
| 1:B:298:VAL:HG13 | 2:E:2341:LEU:HD12 | 1.00                     | 0.99              |
| 1:B:239:GLU:OE1  | 1:B:282:TRP:NE1   | 1.94                     | 0.99              |
| 1:D:385:ASN:OD1  | 1:D:388:GLU:N     | 1.93                     | 0.99              |
| 1:B:456:GLU:O    | 1:B:459:HIS:HB3   | 0.82                     | 0.99              |
| 1:C:271:ALA:O    | 1:C:272:ALA:CB    | 2.01                     | 0.98              |
| 1:D:240:LEU:HD12 | 1:D:240:LEU:N     | 1.77                     | 0.98              |
| 1:A:296:ASP:OD1  | 1:A:384:SER:OG    | 1.80                     | 0.98              |
| 1:D:304:GLY:HA3  | 1:D:308:LEU:HD21  | 1.46                     | 0.98              |
| 1:B:454:MET:HE2  | 1:B:454:MET:O     | 1.62                     | 0.98              |
| 1:B:348:ARG:HH11 | 1:B:348:ARG:CG    | 1.74                     | 0.97              |
| 1:D:264:PRO:O    | 1:D:267:ASN:ND2   | 1.77                     | 0.97              |
| 1:A:450:PHE:HE2  | 1:D:450:PHE:CD1   | 1.83                     | 0.97              |
| 1:B:457:ALA:HB3  | 1:B:458:PRO:HD3   | 1.46                     | 0.97              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:325:LEU:O    | 1:D:325:LEU:HD12  | 1.63                     | 0.97              |
| 1:B:460:GLN:HA   | 1:C:284:LYS:HZ1   | 1.23                     | 0.97              |
| 1:A:363:ASP:OD2  | 1:A:366:GLU:HG3   | 1.64                     | 0.96              |
| 1:D:389:VAL:O    | 1:D:392:LEU:HD23  | 1.64                     | 0.96              |
| 1:B:381:LYS:HE2  | 1:C:445:THR:OG1   | 0.84                     | 0.96              |
| 2:E:2344:ILE:O   | 2:E:2344:ILE:HG22 | 1.63                     | 0.96              |
| 1:C:445:THR:HB   | 1:C:446:PRO:HD3   | 1.49                     | 0.95              |
| 1:C:410:GLU:C    | 1:C:412:PRO:HD3   | 1.92                     | 0.95              |
| 1:D:444:ASP:O    | 1:D:445:THR:HG22  | 1.65                     | 0.95              |
| 1:D:266:THR:HA   | 1:D:269:CYS:HB2   | 1.49                     | 0.94              |
| 1:A:363:ASP:OD2  | 1:A:366:GLU:OE2   | 1.86                     | 0.94              |
| 1:D:454:MET:SD   | 1:D:454:MET:C     | 2.50                     | 0.94              |
| 1:D:236:LEU:O    | 1:D:240:LEU:HD12  | 1.68                     | 0.93              |
| 1:D:284:LYS:HG2  | 4:D:6:HOH:O       | 1.66                     | 0.93              |
| 1:D:400:LEU:HD12 | 1:D:400:LEU:C     | 1.81                     | 0.92              |
| 1:D:389:VAL:CA   | 1:D:392:LEU:CD2   | 2.48                     | 0.92              |
| 1:B:229:ASP:O    | 1:B:231:PRO:HD3   | 1.68                     | 0.91              |
| 1:B:454:MET:HE3  | 1:B:456:GLU:N     | 1.85                     | 0.91              |
| 1:C:445:THR:HB   | 1:C:446:PRO:CD    | 2.01                     | 0.91              |
| 1:B:267:ASN:OD1  | 1:B:326:LEU:HD13  | 1.71                     | 0.90              |
| 1:B:361:GLN:CA   | 1:B:361:GLN:NE2   | 2.30                     | 0.90              |
| 1:D:454:MET:SD   | 1:D:454:MET:O     | 2.30                     | 0.90              |
| 1:D:279:LEU:HD23 | 1:D:305:TRP:CE3   | 2.05                     | 0.90              |
| 1:B:385:ASN:ND2  | 1:B:388:GLU:HB2   | 1.84                     | 0.90              |
| 1:C:424:ALA:O    | 1:C:428:ILE:HG13  | 1.72                     | 0.90              |
| 1:C:269:CYS:O    | 1:C:269:CYS:SG    | 2.30                     | 0.89              |
| 1:B:361:GLN:HA   | 1:B:361:GLN:NE2   | 1.85                     | 0.89              |
| 1:B:324:ILE:HG13 | 1:B:346:PHE:CZ    | 2.07                     | 0.89              |
| 1:B:454:MET:C    | 1:B:454:MET:CE    | 2.44                     | 0.89              |
| 1:A:445:THR:CB   | 1:A:446:PRO:CD    | 2.51                     | 0.89              |
| 1:B:457:ALA:O    | 1:B:460:GLN:HG3   | 1.73                     | 0.88              |
| 1:B:460:GLN:CA   | 1:C:284:LYS:HZ1   | 1.86                     | 0.88              |
| 1:D:456:GLU:O    | 1:D:459:HIS:HD2   | 1.48                     | 0.88              |
| 1:D:448:ASP:OD2  | 1:D:449:THR:HG23  | 1.73                     | 0.87              |
| 1:B:334:ARG:HG3  | 1:B:338:HIS:HD2   | 1.37                     | 0.87              |
| 1:B:334:ARG:HG3  | 1:B:338:HIS:CD2   | 2.10                     | 0.87              |
| 1:C:449:THR:CG2  | 1:C:450:PHE:N     | 2.37                     | 0.87              |
| 1:D:239:GLU:O    | 1:D:242:VAL:HG22  | 1.73                     | 0.87              |
| 1:A:425:LEU:HD12 | 1:A:425:LEU:C     | 1.88                     | 0.87              |
| 1:B:229:ASP:C    | 1:B:231:PRO:HD3   | 2.00                     | 0.87              |
| 1:A:264:PRO:O    | 1:A:268:ILE:HG13  | 1.75                     | 0.87              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:342:VAL:O    | 1:A:342:VAL:HG23  | 1.74                     | 0.87              |
| 1:B:456:GLU:C    | 1:B:459:HIS:HB3   | 1.97                     | 0.87              |
| 1:A:447:ILE:CD1  | 1:A:448:ASP:N     | 2.29                     | 0.86              |
| 1:A:450:PHE:CE2  | 1:D:450:PHE:CD1   | 2.63                     | 0.86              |
| 1:B:442:ILE:CG2  | 4:D:55:HOH:O      | 1.81                     | 0.86              |
| 1:C:447:ILE:O    | 1:C:448:ASP:OD1   | 1.94                     | 0.86              |
| 1:B:455:LEU:N    | 1:B:455:LEU:CD2   | 2.37                     | 0.86              |
| 1:A:440:LYS:HG2  | 1:D:450:PHE:HE1   | 1.40                     | 0.85              |
| 1:D:350:LEU:O    | 1:D:355:SER:OG    | 1.93                     | 0.85              |
| 1:A:232:VAL:HG23 | 1:A:233:GLU:N     | 1.91                     | 0.85              |
| 1:C:272:ALA:HA   | 1:C:275:GLN:HB2   | 1.59                     | 0.85              |
| 1:D:247:GLU:H    | 1:D:247:GLU:CD    | 1.85                     | 0.85              |
| 1:D:457:ALA:HB3  | 1:D:458:PRO:HD3   | 1.59                     | 0.85              |
| 1:B:267:ASN:OD1  | 1:B:326:LEU:HD12  | 1.76                     | 0.85              |
| 1:C:451:LEU:HD12 | 1:C:451:LEU:O     | 1.77                     | 0.84              |
| 1:C:410:GLU:O    | 1:C:412:PRO:CD    | 2.24                     | 0.84              |
| 1:D:410:GLU:HG3  | 1:D:411:GLN:HG3   | 1.56                     | 0.84              |
| 1:A:345:ILE:HD11 | 1:A:428:ILE:CG2   | 2.06                     | 0.84              |
| 1:D:455:LEU:C    | 1:D:455:LEU:HD12  | 2.02                     | 0.84              |
| 1:D:330:LEU:O    | 1:D:330:LEU:CG    | 2.26                     | 0.84              |
| 1:D:385:ASN:OD1  | 1:D:388:GLU:CA    | 2.26                     | 0.84              |
| 1:D:385:ASN:ND2  | 1:D:388:GLU:CB    | 2.36                     | 0.83              |
| 1:D:230:MET:N    | 1:D:231:PRO:HD3   | 1.92                     | 0.83              |
| 1:D:385:ASN:CG   | 1:D:388:GLU:HB3   | 2.03                     | 0.83              |
| 1:A:452:MET:SD   | 2:F:2338:ASN:OD1  | 2.36                     | 0.83              |
| 1:D:447:ILE:O    | 1:D:451:LEU:HB2   | 1.76                     | 0.83              |
| 1:B:229:ASP:O    | 1:B:231:PRO:HD2   | 1.76                     | 0.82              |
| 1:D:304:GLY:C    | 1:D:308:LEU:HD23  | 2.04                     | 0.82              |
| 1:D:457:ALA:HB3  | 1:D:458:PRO:CD    | 2.09                     | 0.82              |
| 1:B:348:ARG:HG3  | 1:B:348:ARG:NH1   | 1.85                     | 0.82              |
| 1:D:389:VAL:C    | 1:D:392:LEU:HD23  | 2.03                     | 0.82              |
| 1:A:302:ARG:HD2  | 1:D:445:THR:OG1   | 1.80                     | 0.82              |
| 1:D:304:GLY:CA   | 1:D:308:LEU:HD21  | 2.10                     | 0.81              |
| 1:C:451:LEU:HD12 | 1:C:451:LEU:C     | 2.04                     | 0.81              |
| 1:D:298:VAL:HG23 | 2:F:2341:LEU:HD22 | 1.61                     | 0.81              |
| 1:C:331:HIS:HE1  | 4:C:32:HOH:O      | 1.62                     | 0.81              |
| 1:D:342:VAL:HB   | 1:D:345:ILE:CG2   | 2.11                     | 0.81              |
| 1:B:444:ASP:OD2  | 1:B:445:THR:N     | 2.14                     | 0.81              |
| 1:D:265:VAL:O    | 1:D:268:ILE:HG13  | 1.79                     | 0.81              |
| 1:A:442:ILE:CG2  | 1:A:442:ILE:O     | 2.28                     | 0.81              |
| 1:A:345:ILE:HD11 | 1:A:428:ILE:HG23  | 1.62                     | 0.81              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:283:ALA:O   | 1:B:289:PHE:CD2  | 2.34                     | 0.81              |
| 1:C:447:ILE:C   | 1:C:449:THR:H    | 1.89                     | 0.81              |
| 1:D:385:ASN:OD1 | 1:D:388:GLU:HB3  | 1.81                     | 0.81              |
| 1:A:232:VAL:CG2 | 1:A:233:GLU:N    | 2.44                     | 0.81              |
| 1:A:451:LEU:O   | 1:A:451:LEU:CD2  | 2.29                     | 0.81              |
| 1:D:276:LEU:O   | 1:D:280:VAL:HG23 | 1.80                     | 0.81              |
| 1:D:295:ASP:O   | 1:D:298:VAL:HG12 | 1.81                     | 0.81              |
| 1:A:447:ILE:CG1 | 1:A:448:ASP:N    | 2.44                     | 0.80              |
| 1:B:320:VAL:CG1 | 1:B:321:LYS:N    | 2.44                     | 0.80              |
| 1:A:452:MET:O   | 1:A:453:GLU:O    | 1.98                     | 0.80              |
| 1:C:451:LEU:O   | 1:C:451:LEU:HG   | 1.81                     | 0.80              |
| 1:A:445:THR:OG1 | 1:A:446:PRO:CD   | 2.30                     | 0.80              |
| 1:D:455:LEU:O   | 1:D:455:LEU:CD1  | 2.30                     | 0.80              |
| 1:C:451:LEU:CD1 | 1:C:453:GLU:N    | 2.44                     | 0.80              |
| 2:E:2338:ASN:O  | 2:E:2342:GLU:HG2 | 1.81                     | 0.80              |
| 1:D:446:PRO:O   | 1:D:447:ILE:CG1  | 2.29                     | 0.80              |
| 1:B:454:MET:CE  | 1:B:455:LEU:N    | 2.42                     | 0.80              |
| 1:D:275:GLN:OE1 | 1:D:275:GLN:CA   | 2.29                     | 0.80              |
| 1:B:459:HIS:ND1 | 1:B:460:GLN:N    | 2.28                     | 0.80              |
| 1:C:451:LEU:O   | 1:C:451:LEU:CD1  | 2.30                     | 0.80              |
| 1:D:236:LEU:O   | 1:D:236:LEU:CD2  | 2.30                     | 0.80              |
| 1:D:304:GLY:O   | 1:D:305:TRP:CB   | 2.30                     | 0.80              |
| 1:D:455:LEU:O   | 1:D:455:LEU:HD13 | 1.80                     | 0.80              |
| 1:D:460:GLN:NE2 | 1:D:460:GLN:N    | 2.30                     | 0.80              |
| 1:B:267:ASN:CG  | 1:B:326:LEU:HD12 | 2.07                     | 0.79              |
| 1:C:451:LEU:CD1 | 1:C:453:GLU:CA   | 2.60                     | 0.79              |
| 1:D:285:ARG:O   | 1:D:287:PRO:HD3  | 1.82                     | 0.79              |
| 2:E:2344:ILE:O  | 2:E:2344:ILE:CG2 | 2.30                     | 0.79              |
| 1:D:236:LEU:CD2 | 1:D:236:LEU:C    | 2.55                     | 0.79              |
| 1:A:424:ALA:O   | 1:A:428:ILE:HG13 | 1.82                     | 0.79              |
| 1:C:366:GLU:OE2 | 1:C:414:ARG:NH2  | 2.15                     | 0.79              |
| 1:D:315:HIS:O   | 1:D:318:ILE:HG23 | 1.81                     | 0.79              |
| 1:C:296:ASP:CG  | 1:C:384:SER:OG   | 2.25                     | 0.79              |
| 1:C:363:ASP:HB2 | 1:C:366:GLU:CD   | 2.07                     | 0.79              |
| 1:C:451:LEU:O   | 1:C:451:LEU:CG   | 2.30                     | 0.78              |
| 1:D:266:THR:CA  | 1:D:269:CYS:HB2  | 2.13                     | 0.78              |
| 1:B:283:ALA:O   | 1:B:289:PHE:HD2  | 1.66                     | 0.78              |
| 1:A:425:LEU:O   | 1:A:425:LEU:CD1  | 2.30                     | 0.78              |
| 1:D:287:PRO:O   | 1:D:288:HIS:HB2  | 1.82                     | 0.78              |
| 1:A:363:ASP:OD2 | 1:A:366:GLU:CG   | 2.30                     | 0.78              |
| 1:C:445:THR:CB  | 1:C:446:PRO:HD3  | 2.13                     | 0.78              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:236:LEU:C     | 1:D:240:LEU:HD11 | 2.07                     | 0.78              |
| 1:B:454:MET:CE    | 1:B:454:MET:O    | 2.30                     | 0.78              |
| 1:B:267:ASN:CG    | 1:B:326:LEU:CD1  | 2.57                     | 0.77              |
| 1:B:320:VAL:HG12  | 1:B:321:LYS:N    | 1.98                     | 0.77              |
| 1:B:348:ARG:HD3   | 1:B:352:GLU:OE2  | 1.83                     | 0.77              |
| 1:B:298:VAL:CG1   | 2:E:2341:LEU:CD1 | 2.48                     | 0.77              |
| 1:D:455:LEU:C     | 1:D:455:LEU:CD1  | 2.57                     | 0.77              |
| 1:D:361:GLN:O     | 1:D:361:GLN:CG   | 2.30                     | 0.77              |
| 1:A:328:THR:OG1   | 1:A:330:LEU:N    | 2.16                     | 0.76              |
| 1:D:310:ILE:O     | 1:D:314:SER:OG   | 2.03                     | 0.76              |
| 1:A:445:THR:HB    | 1:A:446:PRO:CD   | 2.11                     | 0.76              |
| 1:C:449:THR:HG22  | 1:C:450:PHE:N    | 2.01                     | 0.76              |
| 1:B:361:GLN:NE2   | 1:B:361:GLN:N    | 2.34                     | 0.76              |
| 1:B:456:GLU:O     | 1:B:459:HIS:N    | 2.18                     | 0.76              |
| 1:B:264:PRO:HA    | 1:B:267:ASN:HB2  | 1.68                     | 0.76              |
| 1:D:342:VAL:O     | 1:D:345:ILE:HG22 | 1.86                     | 0.76              |
| 1:D:385:ASN:HD21  | 1:D:388:GLU:HB2  | 1.43                     | 0.75              |
| 1:D:316:ARG:HB3   | 1:D:325:LEU:HD11 | 1.68                     | 0.75              |
| 1:B:363:ASP:OD2   | 1:B:363:ASP:C    | 2.30                     | 0.75              |
| 1:B:442:ILE:HG22  | 1:B:443:GLY:N    | 2.01                     | 0.75              |
| 1:C:316:ARG:NH1   | 1:C:325:LEU:O    | 2.19                     | 0.75              |
| 1:B:457:ALA:HB3   | 1:B:458:PRO:CD   | 2.15                     | 0.75              |
| 1:C:448:ASP:OD1   | 1:C:448:ASP:C    | 2.29                     | 0.75              |
| 1:A:447:ILE:O     | 1:A:448:ASP:HB3  | 1.85                     | 0.75              |
| 1:B:283:ALA:HB1   | 1:B:289:PHE:CE2  | 2.22                     | 0.75              |
| 1:D:363:ASP:C     | 1:D:363:ASP:OD2  | 2.30                     | 0.75              |
| 2:E:2341:LEU:HD13 | 2:E:2341:LEU:O   | 1.86                     | 0.75              |
| 1:B:442:ILE:CG2   | 1:B:443:GLY:N    | 2.49                     | 0.74              |
| 1:D:304:GLY:CA    | 1:D:308:LEU:CD2  | 2.65                     | 0.74              |
| 1:D:446:PRO:C     | 1:D:447:ILE:HG13 | 2.11                     | 0.74              |
| 1:A:436:LEU:HB2   | 3:A:1:RHN:OAE    | 1.88                     | 0.74              |
| 1:D:236:LEU:O     | 1:D:236:LEU:HD22 | 1.87                     | 0.74              |
| 1:D:271:ALA:O     | 1:D:275:GLN:HB2  | 1.87                     | 0.74              |
| 1:B:381:LYS:HG3   | 1:B:381:LYS:O    | 1.85                     | 0.74              |
| 1:A:409:PRO:CD    | 1:A:410:GLU:OE1  | 2.34                     | 0.74              |
| 1:D:228:GLU:CG    | 1:D:228:GLU:O    | 2.31                     | 0.74              |
| 2:F:2338:ASN:O    | 2:F:2339:MET:SD  | 2.45                     | 0.74              |
| 1:B:242:VAL:O     | 1:B:243:GLU:C    | 2.29                     | 0.74              |
| 1:B:324:ILE:HG13  | 1:B:346:PHE:HE1  | 0.96                     | 0.73              |
| 1:B:444:ASP:OD2   | 1:B:445:THR:HG23 | 1.88                     | 0.73              |
| 1:D:448:ASP:OD2   | 1:D:449:THR:N    | 2.19                     | 0.73              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:345:ILE:HG22 | 1:C:346:PHE:N     | 2.04                     | 0.73              |
| 1:D:444:ASP:O    | 1:D:445:THR:CG2   | 2.34                     | 0.73              |
| 1:B:385:ASN:CG   | 1:B:388:GLU:HB2   | 2.11                     | 0.73              |
| 1:D:455:LEU:HD12 | 1:D:455:LEU:H     | 1.54                     | 0.72              |
| 1:B:438:PHE:HD2  | 1:B:439:PHE:CE2   | 2.06                     | 0.72              |
| 1:B:457:ALA:C    | 1:B:459:HIS:H     | 1.96                     | 0.72              |
| 1:C:451:LEU:CD1  | 1:C:453:GLU:HA    | 2.19                     | 0.72              |
| 1:A:232:VAL:O    | 1:A:233:GLU:C     | 2.27                     | 0.72              |
| 1:D:445:THR:N    | 1:D:446:PRO:HD2   | 2.04                     | 0.72              |
| 1:A:433:LEU:HD21 | 1:D:447:ILE:HG12  | 1.69                     | 0.72              |
| 1:A:440:LYS:HG2  | 1:D:450:PHE:CE1   | 2.24                     | 0.72              |
| 1:B:444:ASP:CG   | 1:B:445:THR:H     | 1.98                     | 0.72              |
| 1:D:304:GLY:O    | 1:D:305:TRP:HB2   | 1.88                     | 0.71              |
| 1:B:264:PRO:C    | 1:B:267:ASN:HB3   | 2.13                     | 0.71              |
| 1:D:279:LEU:HD23 | 1:D:305:TRP:CZ3   | 2.24                     | 0.71              |
| 1:D:445:THR:N    | 1:D:446:PRO:CD    | 2.54                     | 0.71              |
| 1:A:441:LEU:C    | 1:A:443:GLY:N     | 2.41                     | 0.71              |
| 1:B:267:ASN:ND2  | 1:B:326:LEU:HD12  | 2.05                     | 0.71              |
| 1:B:456:GLU:O    | 1:B:459:HIS:CA    | 2.37                     | 0.71              |
| 1:D:236:LEU:HD22 | 1:D:236:LEU:C     | 2.16                     | 0.71              |
| 1:D:236:LEU:HD22 | 1:D:240:LEU:CD1   | 2.15                     | 0.71              |
| 1:D:295:ASP:O    | 1:D:298:VAL:CG1   | 2.39                     | 0.71              |
| 2:F:2341:LEU:O   | 2:F:2345:ILE:HG13 | 1.89                     | 0.71              |
| 1:B:407:LYS:NZ   | 1:B:408:TYR:OH    | 2.23                     | 0.71              |
| 1:D:242:VAL:O    | 1:D:244:PRO:CD    | 2.38                     | 0.70              |
| 1:B:227:ASN:HB2  | 1:B:231:PRO:HA    | 1.72                     | 0.70              |
| 1:C:409:PRO:HD2  | 1:C:410:GLU:OE1   | 1.91                     | 0.70              |
| 1:B:263:ASP:OD1  | 1:B:263:ASP:C     | 2.34                     | 0.70              |
| 1:B:348:ARG:O    | 1:B:352:GLU:HB2   | 1.91                     | 0.70              |
| 1:B:454:MET:HE1  | 1:B:455:LEU:HA    | 1.70                     | 0.70              |
| 1:D:320:VAL:CG1  | 1:D:321:LYS:N     | 2.54                     | 0.70              |
| 1:D:397:TYR:O    | 1:D:400:LEU:HB3   | 1.92                     | 0.70              |
| 2:F:2340:GLY:O   | 2:F:2343:ALA:HB3  | 1.91                     | 0.70              |
| 1:D:334:ARG:O    | 1:D:338:HIS:HD2   | 1.75                     | 0.70              |
| 1:A:447:ILE:HG13 | 1:A:448:ASP:N     | 2.06                     | 0.70              |
| 1:B:324:ILE:CD1  | 1:B:346:PHE:CE1   | 2.75                     | 0.69              |
| 1:C:447:ILE:HG13 | 1:C:448:ASP:HB3   | 1.73                     | 0.69              |
| 1:D:342:VAL:HB   | 1:D:345:ILE:HG22  | 1.73                     | 0.69              |
| 1:B:381:LYS:O    | 1:B:381:LYS:CG    | 2.40                     | 0.69              |
| 1:B:348:ARG:CD   | 1:B:352:GLU:OE2   | 2.41                     | 0.69              |
| 1:C:269:CYS:C    | 1:C:271:ALA:N     | 2.35                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:288:HIS:HB2   | 1:C:392:LEU:HD21  | 1.75                     | 0.69              |
| 1:D:446:PRO:O     | 1:D:447:ILE:CB    | 2.41                     | 0.69              |
| 1:A:452:MET:O     | 1:A:453:GLU:C     | 2.34                     | 0.69              |
| 1:A:263:ASP:N     | 1:A:264:PRO:CD    | 2.55                     | 0.68              |
| 1:C:447:ILE:C     | 1:C:449:THR:N     | 2.49                     | 0.68              |
| 1:A:335:ASN:OD1   | 1:A:336:SER:N     | 2.26                     | 0.68              |
| 1:A:347:ASP:O     | 1:A:351:THR:HG23  | 1.92                     | 0.68              |
| 1:D:305:TRP:H     | 1:D:308:LEU:HD23  | 0.87                     | 0.68              |
| 2:E:2338:ASN:OD1  | 2:E:2338:ASN:C    | 2.37                     | 0.68              |
| 1:D:290:SER:O     | 1:D:297:GLN:NE2   | 2.26                     | 0.68              |
| 1:D:279:LEU:CD2   | 1:D:305:TRP:CE3   | 2.77                     | 0.68              |
| 1:B:457:ALA:CB    | 1:B:458:PRO:HD3   | 2.19                     | 0.67              |
| 1:C:370:LEU:O     | 1:C:374:VAL:HG23  | 1.95                     | 0.67              |
| 1:D:316:ARG:NH1   | 1:D:325:LEU:O     | 2.27                     | 0.67              |
| 1:D:273:ASP:OD1   | 1:D:273:ASP:C     | 2.37                     | 0.67              |
| 1:B:455:LEU:O     | 1:B:455:LEU:CD2   | 2.30                     | 0.67              |
| 1:C:288:HIS:HB2   | 1:C:392:LEU:CD2   | 2.24                     | 0.67              |
| 1:A:442:ILE:O     | 1:A:442:ILE:HG23  | 1.94                     | 0.67              |
| 1:B:227:ASN:C     | 1:B:227:ASN:HD22  | 2.03                     | 0.67              |
| 2:F:2341:LEU:HD21 | 2:F:2345:ILE:HD11 | 1.77                     | 0.67              |
| 1:C:335:ASN:OD1   | 1:C:336:SER:N     | 2.27                     | 0.66              |
| 1:D:229:ASP:OD2   | 1:D:230:MET:N     | 2.28                     | 0.66              |
| 1:C:363:ASP:CB    | 1:C:366:GLU:HG3   | 2.25                     | 0.66              |
| 1:B:438:PHE:HD2   | 1:B:439:PHE:CD2   | 2.13                     | 0.66              |
| 1:C:421:ARG:NE    | 1:C:421:ARG:HA    | 2.10                     | 0.66              |
| 1:D:234:ARG:O     | 1:D:237:GLU:HB2   | 1.96                     | 0.66              |
| 1:D:325:LEU:HB3   | 1:D:331:HIS:HB2   | 1.77                     | 0.66              |
| 1:D:389:VAL:CA    | 1:D:392:LEU:HD23  | 2.24                     | 0.66              |
| 1:A:363:ASP:CG    | 1:A:366:GLU:HG3   | 2.20                     | 0.66              |
| 1:D:446:PRO:O     | 1:D:447:ILE:HD12  | 1.95                     | 0.66              |
| 1:D:455:LEU:HD12  | 1:D:455:LEU:N     | 2.10                     | 0.66              |
| 1:A:385:ASN:C     | 1:A:385:ASN:OD1   | 2.38                     | 0.66              |
| 1:A:231:PRO:O     | 1:A:234:ARG:HB2   | 1.96                     | 0.66              |
| 1:D:403:TYR:OH    | 1:D:407:LYS:HD2   | 1.95                     | 0.66              |
| 1:A:345:ILE:O     | 1:A:349:VAL:HG23  | 1.95                     | 0.66              |
| 1:B:348:ARG:CG    | 1:B:348:ARG:NH1   | 2.42                     | 0.66              |
| 1:D:272:ALA:CB    | 1:D:309:LEU:HD11  | 2.26                     | 0.65              |
| 1:A:363:ASP:OD2   | 1:A:366:GLU:CD    | 2.39                     | 0.65              |
| 1:C:269:CYS:O     | 1:C:271:ALA:N     | 2.29                     | 0.65              |
| 1:D:369:CYS:O     | 1:D:373:ILE:HG13  | 1.97                     | 0.65              |
| 1:C:363:ASP:HB2   | 1:C:366:GLU:CG    | 2.25                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:291:GLU:N     | 1:D:291:GLU:OE1   | 2.30                     | 0.65              |
| 1:D:283:ALA:HB1   | 1:D:289:PHE:HE2   | 1.57                     | 0.65              |
| 1:D:228:GLU:O     | 1:D:228:GLU:HG3   | 1.96                     | 0.65              |
| 1:D:236:LEU:O     | 1:D:236:LEU:HD23  | 1.95                     | 0.65              |
| 1:D:390:GLU:O     | 1:D:394:GLU:HG3   | 1.96                     | 0.65              |
| 1:D:420:LEU:O     | 1:D:423:PRO:HD2   | 1.97                     | 0.65              |
| 1:A:450:PHE:CE2   | 1:D:450:PHE:CE1   | 2.85                     | 0.65              |
| 1:B:381:LYS:HB3   | 1:C:445:THR:HA    | 1.77                     | 0.65              |
| 1:A:350:LEU:O     | 1:A:355:SER:OG    | 2.07                     | 0.64              |
| 1:C:363:ASP:HB3   | 1:C:366:GLU:H     | 1.62                     | 0.64              |
| 1:C:385:ASN:ND2   | 1:C:385:ASN:O     | 2.30                     | 0.64              |
| 1:A:441:LEU:O     | 1:A:443:GLY:N     | 2.30                     | 0.64              |
| 1:A:444:ASP:HA    | 1:C:348:ARG:HH11  | 1.62                     | 0.64              |
| 1:A:263:ASP:O     | 1:A:266:THR:HB    | 1.97                     | 0.64              |
| 1:D:345:ILE:O     | 1:D:349:VAL:HG23  | 1.98                     | 0.64              |
| 1:D:460:GLN:N     | 1:D:460:GLN:HE21  | 1.94                     | 0.64              |
| 1:B:373:ILE:HD11  | 1:B:397:TYR:HB3   | 1.80                     | 0.64              |
| 1:D:230:MET:N     | 1:D:231:PRO:CD    | 2.60                     | 0.64              |
| 1:A:345:ILE:HD11  | 1:A:428:ILE:HG22  | 1.79                     | 0.64              |
| 1:B:455:LEU:H     | 1:B:455:LEU:CD2   | 1.85                     | 0.64              |
| 1:B:403:TYR:O     | 1:B:406:HIS:HB2   | 1.98                     | 0.64              |
| 1:B:227:ASN:ND2   | 1:B:227:ASN:O     | 2.30                     | 0.64              |
| 1:B:444:ASP:CG    | 1:B:445:THR:N     | 2.51                     | 0.64              |
| 1:B:448:ASP:OD2   | 1:B:448:ASP:N     | 2.30                     | 0.64              |
| 1:D:274:LYS:C     | 1:D:275:GLN:OE1   | 2.41                     | 0.64              |
| 1:D:389:VAL:CA    | 1:D:392:LEU:HD21  | 2.15                     | 0.64              |
| 1:A:440:LYS:CG    | 1:D:450:PHE:HE1   | 2.11                     | 0.63              |
| 1:B:236:LEU:HD22  | 1:B:240:LEU:CD1   | 2.29                     | 0.63              |
| 1:D:390:GLU:OE2   | 1:D:394:GLU:OE2   | 2.16                     | 0.63              |
| 1:D:457:ALA:O     | 1:D:460:GLN:NE2   | 2.30                     | 0.63              |
| 1:A:449:THR:HG22  | 1:A:450:PHE:N     | 2.13                     | 0.63              |
| 1:B:236:LEU:CD2   | 1:B:240:LEU:HG    | 2.28                     | 0.63              |
| 1:C:268:ILE:O     | 1:C:268:ILE:HG22  | 1.97                     | 0.63              |
| 1:A:321:LYS:HE2   | 1:A:322:ASP:OD1   | 1.97                     | 0.63              |
| 1:A:447:ILE:O     | 1:A:448:ASP:CB    | 2.47                     | 0.63              |
| 1:B:342:VAL:HG23  | 1:B:342:VAL:O     | 1.99                     | 0.62              |
| 1:A:442:ILE:HG12  | 1:C:435:HIS:NE2   | 2.13                     | 0.62              |
| 1:B:363:ASP:N     | 1:B:366:GLU:OE2   | 2.32                     | 0.62              |
| 2:F:2337:THR:HG23 | 2:F:2338:ASN:H    | 1.64                     | 0.62              |
| 1:A:296:ASP:CG    | 1:A:384:SER:OG    | 2.42                     | 0.62              |
| 2:F:2341:LEU:CD2  | 2:F:2345:ILE:HD11 | 2.29                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:389:VAL:O    | 1:D:392:LEU:CD2  | 2.44                     | 0.62              |
| 1:B:459:HIS:ND1  | 1:B:459:HIS:C    | 2.58                     | 0.61              |
| 1:C:236:LEU:HD22 | 1:C:236:LEU:O    | 1.99                     | 0.61              |
| 1:D:356:LYS:O    | 1:D:360:MET:HG2  | 1.99                     | 0.61              |
| 1:C:229:ASP:OD1  | 1:C:229:ASP:N    | 2.30                     | 0.61              |
| 1:D:305:TRP:O    | 1:D:306:ASN:C    | 2.39                     | 0.61              |
| 1:D:446:PRO:O    | 1:D:447:ILE:HG13 | 1.98                     | 0.61              |
| 1:B:361:GLN:NE2  | 1:B:361:GLN:H    | 1.99                     | 0.61              |
| 1:B:264:PRO:HA   | 1:B:267:ASN:CB   | 2.31                     | 0.61              |
| 1:B:315:HIS:O    | 1:B:318:ILE:HG23 | 2.01                     | 0.61              |
| 1:B:312:SER:OG   | 1:B:371:ARG:CZ   | 2.48                     | 0.61              |
| 1:A:229:ASP:HB3  | 1:A:395:LYS:HD3  | 1.83                     | 0.60              |
| 1:D:266:THR:O    | 1:D:269:CYS:HB2  | 2.01                     | 0.60              |
| 1:B:377:ASN:OD1  | 1:B:377:ASN:C    | 2.44                     | 0.60              |
| 1:B:454:MET:O    | 1:B:454:MET:SD   | 2.59                     | 0.60              |
| 1:D:266:THR:C    | 1:D:269:CYS:HB2  | 2.26                     | 0.60              |
| 1:A:447:ILE:C    | 1:A:449:THR:H    | 2.09                     | 0.60              |
| 1:D:446:PRO:O    | 1:D:447:ILE:CD1  | 2.50                     | 0.60              |
| 1:A:227:ASN:O    | 1:A:231:PRO:CG   | 2.42                     | 0.60              |
| 1:B:362:MET:HE2  | 1:B:418:LEU:CD2  | 2.32                     | 0.60              |
| 1:D:369:CYS:HB2  | 1:D:400:LEU:HD22 | 1.84                     | 0.60              |
| 1:C:272:ALA:HA   | 1:C:275:GLN:H    | 1.67                     | 0.60              |
| 1:B:236:LEU:HD22 | 1:B:240:LEU:HG   | 1.84                     | 0.60              |
| 1:C:410:GLU:OE1  | 1:C:410:GLU:N    | 2.30                     | 0.60              |
| 1:D:272:ALA:HB2  | 1:D:309:LEU:HD11 | 1.84                     | 0.60              |
| 1:D:362:MET:HE2  | 1:D:418:LEU:CD2  | 2.32                     | 0.60              |
| 1:C:363:ASP:CB   | 1:C:366:GLU:CG   | 2.79                     | 0.59              |
| 1:B:239:GLU:OE1  | 1:B:282:TRP:CD1  | 2.54                     | 0.59              |
| 1:D:369:CYS:CB   | 1:D:400:LEU:HD22 | 2.32                     | 0.59              |
| 1:D:457:ALA:CB   | 1:D:458:PRO:HD3  | 2.32                     | 0.59              |
| 1:A:350:LEU:HA   | 1:A:354:VAL:HB   | 1.84                     | 0.59              |
| 1:B:232:VAL:HG22 | 1:B:399:SER:HB3  | 1.83                     | 0.59              |
| 1:B:457:ALA:CB   | 1:B:458:PRO:CD   | 2.78                     | 0.59              |
| 1:C:391:ALA:O    | 1:C:395:LYS:HG3  | 2.02                     | 0.59              |
| 1:B:447:ILE:O    | 1:B:451:LEU:N    | 2.25                     | 0.59              |
| 1:A:315:HIS:O    | 1:A:318:ILE:HG23 | 2.03                     | 0.58              |
| 1:C:447:ILE:O    | 1:C:449:THR:N    | 2.35                     | 0.58              |
| 1:A:445:THR:OG1  | 1:A:446:PRO:HD3  | 1.99                     | 0.58              |
| 1:B:459:HIS:CG   | 1:B:460:GLN:N    | 2.71                     | 0.58              |
| 1:C:363:ASP:HB3  | 1:C:366:GLU:HG3  | 1.84                     | 0.58              |
| 1:C:450:PHE:O    | 1:C:451:LEU:C    | 2.45                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:274:LYS:O    | 1:D:275:GLN:OE1  | 2.21                     | 0.58              |
| 1:D:304:GLY:C    | 1:D:308:LEU:CD2  | 2.73                     | 0.58              |
| 1:D:320:VAL:HG13 | 1:D:321:LYS:N    | 2.18                     | 0.58              |
| 1:A:445:THR:OG1  | 1:A:446:PRO:HD2  | 2.02                     | 0.58              |
| 1:A:446:PRO:CG   | 1:A:446:PRO:O    | 2.50                     | 0.58              |
| 1:D:444:ASP:C    | 1:D:445:THR:HG22 | 2.29                     | 0.58              |
| 1:D:460:GLN:HE21 | 1:D:460:GLN:H    | 1.50                     | 0.58              |
| 1:D:400:LEU:O    | 1:D:400:LEU:CD1  | 2.30                     | 0.58              |
| 1:D:458:PRO:HB3  | 1:D:461:MET:HG2  | 1.85                     | 0.58              |
| 1:B:457:ALA:N    | 1:B:458:PRO:HD2  | 2.17                     | 0.58              |
| 1:C:449:THR:HG23 | 1:C:450:PHE:N    | 2.15                     | 0.58              |
| 1:B:453:GLU:O    | 1:B:455:LEU:HD13 | 2.03                     | 0.58              |
| 1:C:449:THR:HG22 | 1:C:450:PHE:H    | 1.69                     | 0.57              |
| 1:C:425:LEU:HD12 | 1:C:425:LEU:O    | 2.04                     | 0.57              |
| 1:A:395:LYS:NZ   | 4:A:48:HOH:O     | 2.37                     | 0.57              |
| 1:D:342:VAL:HB   | 1:D:345:ILE:HG21 | 1.86                     | 0.57              |
| 1:C:233:GLU:O    | 1:C:237:GLU:HG3  | 2.03                     | 0.57              |
| 1:D:334:ARG:O    | 1:D:338:HIS:CD2  | 2.57                     | 0.57              |
| 1:A:449:THR:CG2  | 1:A:450:PHE:N    | 2.62                     | 0.57              |
| 1:D:407:LYS:HD3  | 1:D:408:TYR:CE1  | 2.40                     | 0.57              |
| 1:D:458:PRO:HA   | 1:D:460:GLN:H    | 1.69                     | 0.57              |
| 1:A:353:LEU:O    | 1:A:357:MET:HG3  | 2.05                     | 0.57              |
| 1:B:275:GLN:OE1  | 1:B:275:GLN:HA   | 1.99                     | 0.57              |
| 1:D:283:ALA:CB   | 1:D:289:PHE:CE2  | 2.81                     | 0.57              |
| 1:A:351:THR:OG1  | 1:A:352:GLU:N    | 2.35                     | 0.56              |
| 1:B:362:MET:CE   | 1:B:418:LEU:HD23 | 2.35                     | 0.56              |
| 1:B:457:ALA:N    | 1:B:458:PRO:CD   | 2.64                     | 0.56              |
| 1:C:290:SER:HA   | 1:C:297:GLN:NE2  | 2.19                     | 0.56              |
| 1:C:357:MET:HE2  | 1:C:362:MET:HE1  | 1.87                     | 0.56              |
| 1:D:367:LEU:O    | 1:D:367:LEU:HD12 | 2.05                     | 0.56              |
| 1:D:394:GLU:HA   | 1:D:397:TYR:CZ   | 2.41                     | 0.56              |
| 1:D:291:GLU:OE1  | 1:D:291:GLU:CA   | 2.53                     | 0.56              |
| 1:D:341:GLY:C    | 1:D:343:GLY:H    | 2.13                     | 0.56              |
| 1:A:284:LYS:HE2  | 1:D:459:HIS:O    | 2.05                     | 0.56              |
| 1:B:376:PHE:CZ   | 1:B:392:LEU:HD12 | 2.40                     | 0.56              |
| 1:A:345:ILE:CD1  | 1:A:428:ILE:HG23 | 2.34                     | 0.56              |
| 1:D:458:PRO:HA   | 1:D:460:GLN:HB2  | 1.87                     | 0.56              |
| 1:A:280:VAL:HG22 | 1:A:301:LEU:CD1  | 2.35                     | 0.56              |
| 1:B:320:VAL:CG1  | 1:B:321:LYS:H    | 2.18                     | 0.56              |
| 1:A:242:VAL:HG11 | 1:A:282:TRP:HB2  | 1.87                     | 0.56              |
| 1:A:444:ASP:HA   | 1:C:348:ARG:NH1  | 2.20                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:325:LEU:CD1   | 1:B:331:HIS:CD2  | 2.88                     | 0.56              |
| 1:B:438:PHE:CD2   | 1:B:439:PHE:CD2  | 2.93                     | 0.56              |
| 1:D:275:GLN:NE2   | 1:D:278:THR:OG1  | 2.39                     | 0.56              |
| 1:D:353:LEU:CD1   | 1:D:428:ILE:HD12 | 2.36                     | 0.56              |
| 1:D:447:ILE:O     | 1:D:447:ILE:HG22 | 2.05                     | 0.56              |
| 1:A:233:GLU:O     | 1:A:237:GLU:HG3  | 2.06                     | 0.55              |
| 1:B:385:ASN:ND2   | 1:B:388:GLU:CB   | 2.64                     | 0.55              |
| 1:D:421:ARG:HA    | 1:D:421:ARG:NE   | 2.21                     | 0.55              |
| 1:C:268:ILE:HD12  | 1:C:268:ILE:N    | 2.22                     | 0.55              |
| 1:D:373:ILE:CD1   | 1:D:397:TYR:HB3  | 2.36                     | 0.55              |
| 1:D:376:PHE:CZ    | 1:D:392:LEU:HD12 | 2.40                     | 0.55              |
| 1:A:411:GLN:C     | 1:A:413:GLY:N    | 2.63                     | 0.55              |
| 1:B:342:VAL:HB    | 1:B:345:ILE:HG22 | 1.87                     | 0.55              |
| 1:D:390:GLU:O     | 1:D:394:GLU:CG   | 2.55                     | 0.55              |
| 1:A:349:VAL:O     | 1:A:353:LEU:HB2  | 2.06                     | 0.55              |
| 1:B:351:THR:OG1   | 1:B:352:GLU:N    | 2.38                     | 0.55              |
| 1:B:229:ASP:C     | 1:B:231:PRO:CD   | 2.72                     | 0.55              |
| 1:D:304:GLY:HA3   | 1:D:308:LEU:CD2  | 2.27                     | 0.55              |
| 1:D:438:PHE:O     | 1:D:442:ILE:HB   | 2.06                     | 0.55              |
| 1:B:264:PRO:O     | 1:B:267:ASN:N    | 2.40                     | 0.55              |
| 1:D:283:ALA:C     | 1:D:289:PHE:CD2  | 2.85                     | 0.55              |
| 2:E:2341:LEU:HD13 | 2:E:2341:LEU:C   | 2.31                     | 0.55              |
| 1:D:240:LEU:O     | 1:D:243:GLU:CB   | 2.55                     | 0.55              |
| 1:D:373:ILE:HD11  | 1:D:397:TYR:HB3  | 1.89                     | 0.54              |
| 1:C:451:LEU:HD13  | 1:C:453:GLU:C    | 2.32                     | 0.54              |
| 1:B:264:PRO:C     | 1:B:267:ASN:H    | 2.15                     | 0.54              |
| 1:A:348:ARG:O     | 1:A:352:GLU:HB2  | 2.07                     | 0.54              |
| 1:D:242:VAL:O     | 1:D:243:GLU:C    | 2.46                     | 0.54              |
| 1:D:289:PHE:O     | 1:D:292:LEU:HD12 | 2.08                     | 0.54              |
| 1:A:357:MET:HG2   | 1:A:362:MET:HE3  | 1.88                     | 0.54              |
| 1:B:273:ASP:OD1   | 1:B:273:ASP:C    | 2.49                     | 0.54              |
| 1:C:324:ILE:HG12  | 1:C:332:VAL:HB   | 1.90                     | 0.54              |
| 1:D:266:THR:HA    | 1:D:269:CYS:CB   | 2.32                     | 0.54              |
| 1:D:385:ASN:OD1   | 1:D:385:ASN:C    | 2.51                     | 0.54              |
| 1:A:328:THR:HG1   | 1:A:330:LEU:N    | 2.06                     | 0.54              |
| 1:B:450:PHE:HA    | 1:C:450:PHE:HZ   | 1.73                     | 0.54              |
| 1:B:376:PHE:CE1   | 1:B:392:LEU:HD12 | 2.43                     | 0.53              |
| 1:D:247:GLU:CD    | 1:D:247:GLU:N    | 2.58                     | 0.53              |
| 1:B:310:ILE:HA    | 1:B:313:PHE:CE2  | 2.43                     | 0.53              |
| 1:B:456:GLU:N     | 1:B:456:GLU:OE2  | 2.41                     | 0.53              |
| 1:C:448:ASP:C     | 1:C:450:PHE:N    | 2.53                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:451:LEU:HD11  | 1:C:453:GLU:HA   | 1.90                     | 0.53              |
| 1:D:320:VAL:O     | 1:D:358:ARG:NH2  | 2.41                     | 0.53              |
| 1:C:277:PHE:O     | 1:C:281:GLU:HG2  | 2.09                     | 0.53              |
| 1:A:425:LEU:C     | 1:A:425:LEU:CD1  | 2.60                     | 0.53              |
| 1:B:362:MET:HE1   | 1:B:370:LEU:HD11 | 1.91                     | 0.53              |
| 1:B:363:ASP:OD2   | 1:B:365:THR:N    | 2.42                     | 0.53              |
| 1:C:356:LYS:O     | 1:C:360:MET:HG2  | 2.08                     | 0.53              |
| 1:B:376:PHE:CE1   | 1:B:392:LEU:HB3  | 2.44                     | 0.53              |
| 1:D:283:ALA:CB    | 1:D:289:PHE:HE2  | 2.21                     | 0.53              |
| 1:B:265:VAL:C     | 1:B:267:ASN:N    | 2.62                     | 0.53              |
| 1:D:275:GLN:O     | 1:D:279:LEU:HB2  | 2.08                     | 0.53              |
| 1:D:376:PHE:CE2   | 1:D:392:LEU:HD11 | 2.44                     | 0.53              |
| 1:A:442:ILE:O     | 1:A:442:ILE:HG22 | 2.08                     | 0.53              |
| 1:D:240:LEU:O     | 1:D:243:GLU:HB2  | 2.08                     | 0.53              |
| 1:A:440:LYS:HD3   | 1:D:450:PHE:CE1  | 2.44                     | 0.52              |
| 1:B:454:MET:C     | 1:B:454:MET:SD   | 2.91                     | 0.52              |
| 1:B:450:PHE:O     | 1:B:451:LEU:C    | 2.49                     | 0.52              |
| 1:C:292:LEU:O     | 1:C:293:PRO:C    | 2.46                     | 0.52              |
| 1:D:392:LEU:O     | 1:D:396:VAL:HG23 | 2.09                     | 0.52              |
| 1:B:438:PHE:CD2   | 1:B:439:PHE:CE2  | 2.94                     | 0.52              |
| 1:B:451:LEU:HD21  | 1:C:305:TRP:CZ2  | 2.44                     | 0.52              |
| 1:A:451:LEU:O     | 1:A:451:LEU:CG   | 2.57                     | 0.52              |
| 1:A:277:PHE:O     | 1:A:281:GLU:HG2  | 2.10                     | 0.52              |
| 1:A:280:VAL:O     | 1:A:284:LYS:HG3  | 2.10                     | 0.52              |
| 1:A:360:MET:HE1   | 1:A:418:LEU:CD2  | 2.39                     | 0.52              |
| 1:A:410:GLU:OE1   | 1:A:410:GLU:N    | 2.30                     | 0.52              |
| 1:D:237:GLU:HA    | 1:D:240:LEU:HD13 | 1.91                     | 0.52              |
| 1:D:240:LEU:O     | 1:D:243:GLU:N    | 2.37                     | 0.52              |
| 1:C:451:LEU:HD13  | 1:C:453:GLU:CA   | 2.39                     | 0.51              |
| 1:D:445:THR:O     | 1:D:448:ASP:OD1  | 2.29                     | 0.51              |
| 1:B:459:HIS:CG    | 1:B:460:GLN:H    | 2.29                     | 0.51              |
| 1:D:446:PRO:O     | 1:D:447:ILE:HB   | 2.08                     | 0.51              |
| 2:E:2338:ASN:OD1  | 2:E:2340:GLY:N   | 2.44                     | 0.51              |
| 1:D:310:ILE:HA    | 1:D:313:PHE:CE2  | 2.45                     | 0.51              |
| 1:B:320:VAL:HG13  | 1:B:321:LYS:H    | 1.75                     | 0.51              |
| 1:D:383:LEU:HD13  | 1:D:389:VAL:HG21 | 1.91                     | 0.51              |
| 1:B:391:ALA:HA    | 1:B:394:GLU:CD   | 2.36                     | 0.51              |
| 1:D:229:ASP:O     | 1:D:230:MET:C    | 2.51                     | 0.51              |
| 1:A:382:GLY:O     | 1:A:383:LEU:C    | 2.51                     | 0.51              |
| 1:C:280:VAL:HG22  | 1:C:301:LEU:HD13 | 1.92                     | 0.51              |
| 2:F:2341:LEU:HD21 | 2:F:2345:ILE:CD1 | 2.41                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:273:ASP:OD1  | 1:B:273:ASP:O    | 2.29                     | 0.51              |
| 1:B:298:VAL:CG1  | 2:E:2341:LEU:CG  | 2.89                     | 0.51              |
| 1:B:437:PHE:HD2  | 1:C:437:PHE:HD2  | 1.58                     | 0.51              |
| 1:C:269:CYS:HB2  | 1:C:271:ALA:HB3  | 1.91                     | 0.51              |
| 1:C:302:ARG:HG3  | 1:C:303:ALA:N    | 2.25                     | 0.51              |
| 1:A:305:TRP:CD1  | 1:A:305:TRP:C    | 2.88                     | 0.51              |
| 1:A:446:PRO:O    | 1:A:446:PRO:HG2  | 2.11                     | 0.51              |
| 1:B:362:MET:CE   | 1:B:418:LEU:CD2  | 2.89                     | 0.51              |
| 1:C:445:THR:CG2  | 1:C:446:PRO:HD3  | 2.41                     | 0.51              |
| 1:D:385:ASN:O    | 1:D:388:GLU:HB3  | 2.11                     | 0.51              |
| 1:B:276:LEU:HD23 | 1:B:276:LEU:O    | 2.11                     | 0.50              |
| 1:B:386:PRO:C    | 1:B:388:GLU:N    | 2.67                     | 0.50              |
| 1:D:236:LEU:C    | 1:D:240:LEU:CD1  | 2.70                     | 0.50              |
| 1:A:413:GLY:HA3  | 4:A:40:HOH:O     | 2.11                     | 0.50              |
| 1:B:407:LYS:HB3  | 1:B:408:TYR:CD1  | 2.47                     | 0.50              |
| 1:A:316:ARG:HH12 | 1:A:326:LEU:C    | 2.19                     | 0.50              |
| 1:A:441:LEU:C    | 1:A:443:GLY:H    | 2.11                     | 0.50              |
| 1:D:292:LEU:HB2  | 1:D:297:GLN:HG2  | 1.94                     | 0.50              |
| 1:D:273:ASP:OD1  | 1:D:273:ASP:O    | 2.30                     | 0.50              |
| 1:B:362:MET:CE   | 1:B:370:LEU:HD11 | 2.40                     | 0.50              |
| 1:C:335:ASN:O    | 1:C:336:SER:C    | 2.52                     | 0.50              |
| 1:A:448:ASP:O    | 1:A:448:ASP:OD2  | 2.30                     | 0.50              |
| 1:B:264:PRO:O    | 1:B:267:ASN:CA   | 2.58                     | 0.50              |
| 1:B:409:PRO:CD   | 1:B:410:GLU:H    | 2.25                     | 0.50              |
| 1:B:460:GLN:HG2  | 1:C:294:LEU:HD11 | 1.93                     | 0.50              |
| 1:C:310:ILE:HA   | 1:C:313:PHE:CE2  | 2.47                     | 0.50              |
| 1:D:265:VAL:C    | 1:D:268:ILE:HG13 | 2.36                     | 0.50              |
| 1:D:385:ASN:OD1  | 1:D:385:ASN:O    | 2.30                     | 0.50              |
| 1:A:446:PRO:CD   | 1:A:446:PRO:O    | 2.60                     | 0.50              |
| 1:B:460:GLN:HA   | 1:C:284:LYS:CE   | 2.42                     | 0.50              |
| 1:D:320:VAL:HG13 | 1:D:321:LYS:H    | 1.75                     | 0.50              |
| 1:B:266:THR:O    | 1:B:267:ASN:C    | 2.53                     | 0.50              |
| 1:B:271:ALA:CB   | 1:B:328:THR:HG21 | 2.42                     | 0.50              |
| 1:B:460:GLN:O    | 1:B:460:GLN:OE1  | 2.30                     | 0.50              |
| 1:A:232:VAL:C    | 1:A:234:ARG:N    | 2.68                     | 0.49              |
| 1:A:411:GLN:C    | 1:A:413:GLY:H    | 2.19                     | 0.49              |
| 1:C:296:ASP:OD2  | 1:C:384:SER:OG   | 2.30                     | 0.49              |
| 1:C:309:LEU:O    | 1:C:312:SER:HB2  | 2.12                     | 0.49              |
| 1:D:285:ARG:O    | 1:D:287:PRO:CD   | 2.58                     | 0.49              |
| 1:D:308:LEU:HD22 | 1:D:308:LEU:H    | 1.76                     | 0.49              |
| 1:D:367:LEU:HD12 | 1:D:367:LEU:C    | 2.37                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:2344:ILE:O   | 2:F:2345:ILE:O    | 2.30                     | 0.49              |
| 1:B:455:LEU:C    | 1:B:455:LEU:HD22  | 2.24                     | 0.49              |
| 1:C:452:MET:O    | 1:C:453:GLU:O     | 2.30                     | 0.49              |
| 1:D:266:THR:C    | 1:D:269:CYS:H     | 2.21                     | 0.49              |
| 1:D:362:MET:HE2  | 1:D:418:LEU:HD23  | 1.94                     | 0.49              |
| 2:F:2341:LEU:C   | 2:F:2341:LEU:HD23 | 2.37                     | 0.49              |
| 1:A:280:VAL:HG22 | 1:A:301:LEU:HD11  | 1.94                     | 0.49              |
| 1:B:280:VAL:HG12 | 1:B:284:LYS:HE3   | 1.94                     | 0.49              |
| 1:C:242:VAL:HG11 | 1:C:282:TRP:HB2   | 1.93                     | 0.49              |
| 1:C:360:MET:O    | 1:C:361:GLN:C     | 2.51                     | 0.49              |
| 1:B:242:VAL:O    | 1:B:243:GLU:O     | 2.30                     | 0.49              |
| 1:B:271:ALA:HB2  | 1:B:328:THR:HG21  | 1.94                     | 0.49              |
| 1:B:448:ASP:HA   | 1:B:451:LEU:HB2   | 1.94                     | 0.49              |
| 1:B:456:GLU:C    | 1:B:459:HIS:H     | 2.18                     | 0.49              |
| 1:B:263:ASP:OD1  | 1:B:263:ASP:O     | 2.30                     | 0.49              |
| 1:A:360:MET:O    | 1:A:361:GLN:C     | 2.52                     | 0.49              |
| 1:B:236:LEU:HD22 | 1:B:240:LEU:CG    | 2.42                     | 0.49              |
| 1:B:282:TRP:HZ3  | 1:B:375:LEU:HD13  | 1.77                     | 0.49              |
| 1:D:353:LEU:HD12 | 1:D:428:ILE:HD12  | 1.94                     | 0.49              |
| 1:B:376:PHE:CE1  | 1:B:392:LEU:CD1   | 2.96                     | 0.49              |
| 1:C:451:LEU:C    | 1:C:451:LEU:CD1   | 2.69                     | 0.49              |
| 1:B:409:PRO:HD2  | 1:B:410:GLU:H     | 1.78                     | 0.48              |
| 1:C:420:LEU:CD1  | 1:D:397:TYR:CE2   | 2.95                     | 0.48              |
| 1:A:391:ALA:O    | 1:A:395:LYS:HG3   | 2.12                     | 0.48              |
| 1:A:445:THR:HA   | 1:D:381:LYS:HG3   | 1.94                     | 0.48              |
| 1:C:436:LEU:HD13 | 3:C:2:RHN:OAC     | 2.12                     | 0.48              |
| 1:A:346:PHE:CD2  | 1:A:346:PHE:C     | 2.91                     | 0.48              |
| 1:B:390:GLU:O    | 1:B:393:ARG:HB3   | 2.13                     | 0.48              |
| 1:C:272:ALA:CA   | 1:C:275:GLN:H     | 2.26                     | 0.48              |
| 1:B:295:ASP:O    | 1:B:299:ILE:HG13  | 2.13                     | 0.48              |
| 1:B:438:PHE:HD2  | 1:B:439:PHE:HE2   | 1.58                     | 0.48              |
| 1:C:236:LEU:HD22 | 1:C:236:LEU:C     | 2.37                     | 0.48              |
| 1:D:389:VAL:HA   | 1:D:392:LEU:HD22  | 1.80                     | 0.48              |
| 1:D:265:VAL:O    | 1:D:269:CYS:N     | 2.47                     | 0.48              |
| 1:B:437:PHE:CD2  | 1:C:437:PHE:HD2   | 2.30                     | 0.48              |
| 1:C:231:PRO:HG2  | 1:C:234:ARG:HB2   | 1.94                     | 0.48              |
| 1:C:452:MET:O    | 1:C:453:GLU:C     | 2.57                     | 0.48              |
| 1:D:357:MET:HG2  | 1:D:362:MET:SD    | 2.53                     | 0.48              |
| 1:D:281:GLU:CD   | 1:D:285:ARG:NH2   | 2.64                     | 0.48              |
| 1:D:363:ASP:OD2  | 1:D:365:THR:N     | 2.46                     | 0.48              |
| 1:D:376:PHE:CZ   | 1:D:392:LEU:CD1   | 2.96                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:230:MET:HE2  | 1:A:230:MET:HB2  | 1.70                     | 0.48              |
| 1:A:315:HIS:ND1  | 4:A:24:HOH:O     | 2.35                     | 0.48              |
| 1:B:447:ILE:H    | 1:B:447:ILE:HG13 | 1.25                     | 0.48              |
| 1:C:324:ILE:HD13 | 1:C:346:PHE:CD1  | 2.48                     | 0.48              |
| 1:D:275:GLN:O    | 1:D:279:LEU:N    | 2.35                     | 0.48              |
| 1:A:370:LEU:O    | 1:A:374:VAL:HG23 | 2.13                     | 0.48              |
| 1:D:455:LEU:CD1  | 1:D:455:LEU:H    | 2.18                     | 0.48              |
| 1:D:292:LEU:O    | 1:D:293:PRO:C    | 2.54                     | 0.48              |
| 1:A:440:LYS:O    | 1:A:443:GLY:HA3  | 2.14                     | 0.47              |
| 1:C:420:LEU:HD11 | 1:D:397:TYR:CD2  | 2.50                     | 0.47              |
| 1:C:451:LEU:HD12 | 1:C:452:MET:C    | 2.34                     | 0.47              |
| 1:B:460:GLN:CB   | 1:C:284:LYS:HZ1  | 2.25                     | 0.47              |
| 1:C:288:HIS:CB   | 1:C:392:LEU:HD21 | 2.44                     | 0.47              |
| 1:D:345:ILE:HG23 | 1:D:346:PHE:N    | 2.28                     | 0.47              |
| 1:B:397:TYR:O    | 1:B:400:LEU:HB3  | 2.14                     | 0.47              |
| 1:A:238:ALA:O    | 1:A:242:VAL:HG22 | 2.14                     | 0.47              |
| 1:C:320:VAL:O    | 1:C:358:ARG:NH2  | 2.47                     | 0.47              |
| 1:A:434:GLU:OE1  | 1:B:434:GLU:OE1  | 2.32                     | 0.47              |
| 1:B:457:ALA:C    | 1:B:459:HIS:N    | 2.65                     | 0.47              |
| 1:D:265:VAL:HA   | 1:D:268:ILE:CG1  | 2.45                     | 0.47              |
| 1:A:448:ASP:C    | 1:A:450:PHE:N    | 2.62                     | 0.47              |
| 1:B:298:VAL:HG12 | 2:E:2341:LEU:HG  | 1.95                     | 0.47              |
| 1:B:439:PHE:CD2  | 1:B:439:PHE:N    | 2.83                     | 0.47              |
| 1:B:454:MET:CE   | 1:B:455:LEU:C    | 2.86                     | 0.47              |
| 1:D:228:GLU:O    | 1:D:228:GLU:HG2  | 2.13                     | 0.47              |
| 1:D:438:PHE:O    | 1:D:442:ILE:N    | 2.39                     | 0.47              |
| 2:F:2344:ILE:C   | 2:F:2345:ILE:O   | 2.54                     | 0.47              |
| 1:A:305:TRP:NE1  | 1:A:309:LEU:HD11 | 2.29                     | 0.47              |
| 1:B:312:SER:OG   | 1:B:371:ARG:NE   | 2.48                     | 0.47              |
| 1:B:376:PHE:CD1  | 1:B:392:LEU:HB3  | 2.50                     | 0.47              |
| 1:C:409:PRO:CD   | 1:C:410:GLU:OE1  | 2.62                     | 0.47              |
| 1:B:227:ASN:HA   | 1:B:399:SER:OG   | 2.14                     | 0.47              |
| 1:B:437:PHE:CE1  | 1:C:447:ILE:HG12 | 2.50                     | 0.47              |
| 1:C:290:SER:HA   | 1:C:297:GLN:HE22 | 1.80                     | 0.47              |
| 1:D:282:TRP:CE2  | 1:D:371:ARG:NH1  | 2.84                     | 0.47              |
| 1:B:460:GLN:O    | 1:B:460:GLN:CD   | 2.58                     | 0.46              |
| 1:D:376:PHE:O    | 1:D:378:PRO:HD3  | 2.16                     | 0.46              |
| 1:A:447:ILE:C    | 1:A:449:THR:N    | 2.66                     | 0.46              |
| 1:B:454:MET:HE3  | 1:B:455:LEU:C    | 2.38                     | 0.46              |
| 1:D:444:ASP:O    | 1:D:444:ASP:OD2  | 2.34                     | 0.46              |
| 2:F:2338:ASN:C   | 2:F:2339:MET:SD  | 2.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:381:LYS:HE3  | 1:C:445:THR:HB   | 1.45                     | 0.46              |
| 1:B:438:PHE:CD2  | 1:B:439:PHE:HD2  | 2.33                     | 0.46              |
| 1:D:345:ILE:CG2  | 1:D:346:PHE:N    | 2.78                     | 0.46              |
| 1:B:297:GLN:O    | 1:B:301:LEU:HD12 | 2.16                     | 0.46              |
| 1:B:442:ILE:HA   | 1:B:442:ILE:HD12 | 1.51                     | 0.46              |
| 1:C:272:ALA:O    | 1:C:273:ASP:C    | 2.54                     | 0.46              |
| 1:D:320:VAL:HG12 | 1:D:321:LYS:N    | 2.29                     | 0.46              |
| 1:A:452:MET:C    | 1:A:453:GLU:O    | 2.58                     | 0.46              |
| 1:B:324:ILE:CD1  | 1:B:346:PHE:CD1  | 2.99                     | 0.46              |
| 1:D:229:ASP:C    | 1:D:231:PRO:HD3  | 2.39                     | 0.46              |
| 1:A:414:ARG:O    | 1:A:415:PHE:C    | 2.52                     | 0.46              |
| 1:D:313:PHE:O    | 1:D:317:SER:OG   | 2.33                     | 0.46              |
| 1:B:271:ALA:HB1  | 1:B:328:THR:CG2  | 2.45                     | 0.46              |
| 1:C:335:ASN:CG   | 1:C:336:SER:N    | 2.74                     | 0.45              |
| 1:C:268:ILE:N    | 1:C:268:ILE:CD1  | 2.79                     | 0.45              |
| 1:C:421:ARG:NE   | 1:C:421:ARG:CA   | 2.78                     | 0.45              |
| 1:A:299:ILE:O    | 1:A:303:ALA:HB2  | 2.16                     | 0.45              |
| 1:B:381:LYS:O    | 1:B:381:LYS:CD   | 2.63                     | 0.45              |
| 1:B:342:VAL:HB   | 1:B:345:ILE:CG2  | 2.46                     | 0.45              |
| 1:B:345:ILE:O    | 1:B:349:VAL:HG23 | 2.17                     | 0.45              |
| 1:C:431:LYS:O    | 1:C:435:HIS:HD2  | 2.00                     | 0.45              |
| 1:C:448:ASP:O    | 1:C:448:ASP:CG   | 2.54                     | 0.45              |
| 1:D:457:ALA:HB3  | 1:D:458:PRO:HD2  | 1.96                     | 0.45              |
| 1:B:264:PRO:C    | 1:B:267:ASN:CB   | 2.80                     | 0.45              |
| 1:B:460:GLN:O    | 1:B:460:GLN:CG   | 2.64                     | 0.45              |
| 1:B:377:ASN:HA   | 1:B:378:PRO:HD3  | 1.75                     | 0.45              |
| 1:B:437:PHE:HE1  | 1:C:447:ILE:HG12 | 1.80                     | 0.45              |
| 1:D:325:LEU:HD12 | 1:D:325:LEU:C    | 2.39                     | 0.45              |
| 1:D:422:LEU:N    | 1:D:423:PRO:CD   | 2.80                     | 0.45              |
| 1:B:279:LEU:HD12 | 1:B:279:LEU:HA   | 1.79                     | 0.45              |
| 1:B:362:MET:HE1  | 1:B:370:LEU:CD1  | 2.46                     | 0.45              |
| 1:B:430:LEU:O    | 1:B:434:GLU:HG3  | 2.16                     | 0.45              |
| 1:C:348:ARG:O    | 1:C:349:VAL:C    | 2.59                     | 0.45              |
| 1:B:394:GLU:H    | 1:B:394:GLU:HG3  | 1.60                     | 0.45              |
| 1:B:420:LEU:HA   | 1:B:420:LEU:HD23 | 1.71                     | 0.45              |
| 1:D:389:VAL:HG13 | 1:D:392:LEU:HD21 | 1.97                     | 0.45              |
| 1:B:267:ASN:OD1  | 1:B:326:LEU:HD11 | 2.04                     | 0.45              |
| 1:B:362:MET:HE3  | 1:B:418:LEU:HD23 | 1.99                     | 0.45              |
| 1:D:420:LEU:C    | 1:D:423:PRO:HD2  | 2.41                     | 0.45              |
| 1:B:447:ILE:HG21 | 3:C:2:RHN:HAH    | 1.99                     | 0.45              |
| 1:D:460:GLN:NE2  | 1:D:460:GLN:CA   | 2.78                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:347:ASP:OD2  | 1:B:347:ASP:N    | 2.50                     | 0.44              |
| 1:D:267:ASN:ND2  | 1:D:267:ASN:H    | 2.13                     | 0.44              |
| 1:A:385:ASN:OD1  | 1:A:387:ALA:N    | 2.50                     | 0.44              |
| 1:A:433:LEU:HD21 | 1:D:447:ILE:CG1  | 2.42                     | 0.44              |
| 1:B:353:LEU:O    | 1:B:357:MET:HB2  | 2.17                     | 0.44              |
| 1:D:347:ASP:O    | 1:D:351:THR:HG23 | 2.17                     | 0.44              |
| 1:B:422:LEU:N    | 1:B:423:PRO:CD   | 2.80                     | 0.44              |
| 1:D:383:LEU:CD1  | 1:D:389:VAL:HG21 | 2.47                     | 0.44              |
| 1:A:444:ASP:C    | 1:A:445:THR:HG1  | 2.19                     | 0.44              |
| 1:B:386:PRO:C    | 1:B:388:GLU:H    | 2.26                     | 0.44              |
| 1:C:385:ASN:HD21 | 1:C:388:GLU:HB2  | 1.82                     | 0.44              |
| 1:D:456:GLU:O    | 1:D:459:HIS:NE2  | 2.47                     | 0.44              |
| 1:B:274:LYS:O    | 1:B:277:PHE:HB3  | 2.17                     | 0.44              |
| 1:C:345:ILE:HD12 | 1:C:345:ILE:HG23 | 1.68                     | 0.44              |
| 2:F:2341:LEU:C   | 2:F:2343:ALA:N   | 2.74                     | 0.44              |
| 1:B:294:LEU:O    | 1:B:298:VAL:HG23 | 2.17                     | 0.44              |
| 1:C:405:LYS:O    | 1:C:406:HIS:C    | 2.58                     | 0.44              |
| 1:D:289:PHE:CD1  | 1:D:289:PHE:C    | 2.95                     | 0.44              |
| 1:D:378:PRO:C    | 1:D:380:SER:H    | 2.25                     | 0.44              |
| 1:C:363:ASP:CB   | 1:C:366:GLU:OE1  | 2.42                     | 0.44              |
| 1:C:451:LEU:HD12 | 1:C:453:GLU:H    | 1.69                     | 0.44              |
| 1:D:400:LEU:C    | 1:D:400:LEU:CD1  | 2.56                     | 0.44              |
| 1:B:265:VAL:C    | 1:B:267:ASN:H    | 2.26                     | 0.43              |
| 1:D:228:GLU:OE2  | 1:D:231:PRO:HA   | 2.18                     | 0.43              |
| 1:D:240:LEU:C    | 1:D:243:GLU:H    | 2.23                     | 0.43              |
| 2:F:2341:LEU:CD2 | 2:F:2345:ILE:CD1 | 2.95                     | 0.43              |
| 1:A:317:SER:O    | 1:A:320:VAL:HB   | 2.19                     | 0.43              |
| 1:D:265:VAL:HA   | 1:D:268:ILE:HG13 | 2.00                     | 0.43              |
| 1:D:315:HIS:HB2  | 1:D:367:LEU:HD21 | 1.29                     | 0.43              |
| 1:A:422:LEU:HB2  | 1:A:423:PRO:HD3  | 2.01                     | 0.43              |
| 1:B:421:ARG:HA   | 1:B:421:ARG:NE   | 2.33                     | 0.43              |
| 1:C:360:MET:O    | 1:C:361:GLN:HB2  | 2.16                     | 0.43              |
| 1:D:326:LEU:HD12 | 1:D:330:LEU:HD23 | 2.00                     | 0.43              |
| 1:A:232:VAL:HB   | 1:A:365:THR:HG23 | 2.00                     | 0.43              |
| 1:A:263:ASP:N    | 1:A:263:ASP:OD1  | 2.52                     | 0.43              |
| 1:B:234:ARG:O    | 1:B:237:GLU:HB2  | 2.18                     | 0.43              |
| 1:C:397:TYR:HB2  | 1:C:415:PHE:HZ   | 1.82                     | 0.43              |
| 1:B:264:PRO:HG3  | 1:B:332:VAL:HG13 | 1.99                     | 0.43              |
| 2:E:2341:LEU:CD1 | 2:E:2341:LEU:C   | 2.91                     | 0.43              |
| 1:B:268:ILE:O    | 1:B:268:ILE:HG22 | 2.18                     | 0.43              |
| 1:A:277:PHE:O    | 1:A:281:GLU:HB2  | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:401:GLU:HG2  | 1:A:405:LYS:HE2   | 1.99                     | 0.43              |
| 1:B:458:PRO:O    | 1:B:459:HIS:C     | 2.58                     | 0.43              |
| 1:B:450:PHE:HE1  | 1:C:440:LYS:HG3   | 1.84                     | 0.43              |
| 1:B:454:MET:CE   | 1:B:456:GLU:N     | 2.69                     | 0.43              |
| 1:B:454:MET:HG2  | 1:B:456:GLU:OE2   | 2.19                     | 0.43              |
| 1:D:351:THR:OG1  | 1:D:352:GLU:N     | 2.51                     | 0.43              |
| 1:A:440:LYS:CG   | 1:D:450:PHE:CE1   | 2.95                     | 0.42              |
| 1:C:230:MET:HB2  | 1:C:230:MET:HE2   | 1.66                     | 0.42              |
| 1:D:351:THR:OG1  | 1:D:352:GLU:HG3   | 2.19                     | 0.42              |
| 1:D:461:MET:HE2  | 1:D:461:MET:HB3   | 1.69                     | 0.42              |
| 1:B:449:THR:O    | 1:B:451:LEU:O     | 2.36                     | 0.42              |
| 1:D:301:LEU:HB3  | 2:F:2341:LEU:HD11 | 2.01                     | 0.42              |
| 1:B:439:PHE:N    | 1:B:439:PHE:HD2   | 2.17                     | 0.42              |
| 1:B:449:THR:OG1  | 1:B:450:PHE:N     | 2.51                     | 0.42              |
| 1:D:374:VAL:O    | 1:D:377:ASN:HB2   | 2.19                     | 0.42              |
| 1:D:445:THR:O    | 1:D:445:THR:HG23  | 2.20                     | 0.42              |
| 1:A:447:ILE:CD1  | 1:D:437:PHE:HZ    | 2.33                     | 0.42              |
| 1:B:267:ASN:OD1  | 1:B:267:ASN:C     | 2.62                     | 0.42              |
| 1:B:360:MET:O    | 1:B:361:GLN:C     | 2.62                     | 0.42              |
| 1:B:430:LEU:HD23 | 1:B:433:LEU:HD12  | 2.00                     | 0.42              |
| 1:D:240:LEU:CD1  | 1:D:240:LEU:N     | 2.49                     | 0.42              |
| 1:D:389:VAL:CG1  | 1:D:392:LEU:HD21  | 2.49                     | 0.42              |
| 1:B:394:GLU:HA   | 1:B:397:TYR:CZ    | 2.55                     | 0.42              |
| 1:D:275:GLN:OE1  | 1:D:275:GLN:N     | 2.52                     | 0.42              |
| 1:B:409:PRO:CG   | 1:B:410:GLU:N     | 2.82                     | 0.42              |
| 1:C:272:ALA:C    | 1:C:274:LYS:N     | 2.69                     | 0.42              |
| 1:A:263:ASP:N    | 1:A:264:PRO:HD2   | 2.35                     | 0.42              |
| 1:B:312:SER:HG   | 1:B:371:ARG:NH1   | 2.10                     | 0.42              |
| 1:B:348:ARG:HD3  | 1:B:352:GLU:CD    | 2.45                     | 0.42              |
| 1:B:407:LYS:NZ   | 1:B:408:TYR:CZ    | 2.86                     | 0.42              |
| 1:B:458:PRO:O    | 1:B:459:HIS:O     | 2.37                     | 0.42              |
| 1:C:305:TRP:CD1  | 1:C:305:TRP:C     | 2.98                     | 0.42              |
| 1:D:302:ARG:HE   | 1:D:302:ARG:HB3   | 1.58                     | 0.42              |
| 3:A:1:RHN:OAE    | 3:A:1:RHN:OAC     | 2.37                     | 0.42              |
| 1:B:355:SER:O    | 1:B:359:ASP:OD1   | 2.38                     | 0.42              |
| 1:D:237:GLU:CA   | 1:D:240:LEU:HD13  | 2.50                     | 0.42              |
| 1:A:299:ILE:O    | 1:A:303:ALA:CB    | 2.68                     | 0.41              |
| 1:B:456:GLU:HB3  | 1:B:459:HIS:HB2   | 2.02                     | 0.41              |
| 1:C:328:THR:H    | 1:C:328:THR:HG23  | 1.57                     | 0.41              |
| 1:B:334:ARG:HG2  | 1:B:335:ASN:N     | 2.33                     | 0.41              |
| 1:D:397:TYR:O    | 1:D:401:GLU:N     | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:442:ILE:HD12 | 1:D:442:ILE:HA   | 1.62                     | 0.41              |
| 1:A:286:ILE:HG23 | 1:A:286:ILE:HD12 | 1.77                     | 0.41              |
| 1:D:324:ILE:O    | 1:D:324:ILE:HG13 | 2.20                     | 0.41              |
| 1:B:298:VAL:CG1  | 2:E:2341:LEU:HG  | 2.50                     | 0.41              |
| 1:C:288:HIS:HB2  | 1:C:392:LEU:HD22 | 1.99                     | 0.41              |
| 1:D:444:ASP:C    | 1:D:446:PRO:CD   | 2.93                     | 0.41              |
| 1:C:433:LEU:HD23 | 1:C:433:LEU:HA   | 1.86                     | 0.41              |
| 2:F:2340:GLY:O   | 2:F:2343:ALA:CB  | 2.64                     | 0.41              |
| 1:A:360:MET:HE1  | 1:A:418:LEU:HD21 | 2.01                     | 0.41              |
| 1:A:369:CYS:CB   | 1:A:400:LEU:HD13 | 2.50                     | 0.41              |
| 1:A:440:LYS:CD   | 1:D:450:PHE:HE1  | 2.33                     | 0.41              |
| 1:B:345:ILE:CG2  | 1:B:346:PHE:N    | 2.83                     | 0.41              |
| 1:A:436:LEU:HD22 | 3:A:1:RHN:HAH    | 2.03                     | 0.41              |
| 1:B:420:LEU:O    | 1:B:423:PRO:HD2  | 2.20                     | 0.41              |
| 1:C:422:LEU:HB2  | 1:C:423:PRO:HD3  | 2.03                     | 0.41              |
| 1:D:376:PHE:CE1  | 1:D:392:LEU:HD12 | 2.56                     | 0.41              |
| 1:A:232:VAL:O    | 1:A:235:ILE:N    | 2.54                     | 0.41              |
| 1:A:363:ASP:OD2  | 1:A:363:ASP:N    | 2.54                     | 0.41              |
| 1:B:351:THR:HG23 | 1:B:351:THR:H    | 1.54                     | 0.41              |
| 1:B:397:TYR:O    | 1:B:401:GLU:N    | 2.52                     | 0.41              |
| 1:B:438:PHE:CD2  | 1:B:439:PHE:HE2  | 2.37                     | 0.41              |
| 1:B:455:LEU:N    | 1:B:455:LEU:HD13 | 2.35                     | 0.41              |
| 1:C:436:LEU:HD22 | 3:C:2:RHN:OAE    | 2.20                     | 0.41              |
| 1:A:302:ARG:HG3  | 1:A:303:ALA:N    | 2.36                     | 0.41              |
| 1:D:402:ALA:O    | 1:D:403:TYR:C    | 2.61                     | 0.41              |
| 1:B:236:LEU:CD2  | 1:B:236:LEU:O    | 2.70                     | 0.40              |
| 1:C:242:VAL:O    | 1:C:243:GLU:C    | 2.61                     | 0.40              |
| 1:C:318:ILE:HD13 | 1:C:318:ILE:HG21 | 1.66                     | 0.40              |
| 1:C:363:ASP:CB   | 1:C:366:GLU:CD   | 2.87                     | 0.40              |
| 1:A:243:GLU:HA   | 1:A:244:PRO:HD3  | 1.85                     | 0.40              |
| 1:C:288:HIS:ND1  | 1:C:291:GLU:OE2  | 2.48                     | 0.40              |
| 1:C:382:GLY:O    | 1:C:383:LEU:C    | 2.61                     | 0.40              |
| 1:C:411:GLN:HB3  | 1:C:414:ARG:HB2  | 2.03                     | 0.40              |
| 1:B:263:ASP:HA   | 1:B:264:PRO:HD3  | 1.65                     | 0.40              |
| 1:B:239:GLU:O    | 1:B:242:VAL:HG22 | 2.21                     | 0.40              |
| 1:B:358:ARG:O    | 1:B:361:GLN:NE2  | 2.55                     | 0.40              |
| 1:B:369:CYS:O    | 1:B:373:ILE:HG13 | 2.22                     | 0.40              |
| 1:B:446:PRO:O    | 1:B:447:ILE:C    | 2.63                     | 0.40              |
| 1:D:308:LEU:HD22 | 1:D:308:LEU:N    | 2.35                     | 0.40              |
| 1:B:232:VAL:HG12 | 1:B:365:THR:CG2  | 2.52                     | 0.40              |
| 1:B:373:ILE:HG23 | 1:B:373:ILE:HD13 | 1.78                     | 0.40              |

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| Atom-1        | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|----------------|--------------------------|-------------------|
| 1:D:287:PRO:O | 1:D:288:HIS:CB | 2.58                     | 0.40              |

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:B:285:ARG:NH1 | 1:D:237:GLU:OE1[1_655] | 2.00                     | 0.20              |
| 1:B:285:ARG:NH1 | 1:D:237:GLU:OE2[1_655] | 2.15                     | 0.05              |
| 1:B:321:LYS:NZ  | 1:C:273:ASP:OD1[3_454] | 2.18                     | 0.02              |

## 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     | 207/240 (86%) | 199 (96%) | 6 (3%)  | 2 (1%)   | 12          | 45  |
| 1   | B     | 213/240 (89%) | 203 (95%) | 8 (4%)  | 2 (1%)   | 14          | 48  |
| 1   | C     | 199/240 (83%) | 189 (95%) | 6 (3%)  | 4 (2%)   | 6           | 28  |
| 1   | D     | 215/240 (90%) | 208 (97%) | 5 (2%)  | 2 (1%)   | 14          | 48  |
| 2   | E     | 5/16 (31%)    | 4 (80%)   | 1 (20%) | 0        | 100         | 100 |
| 2   | F     | 7/16 (44%)    | 6 (86%)   | 1 (14%) | 0        | 100         | 100 |
| All | All   | 846/992 (85%) | 809 (96%) | 27 (3%) | 10 (1%)  | 10          | 40  |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 445 | THR  |
| 1   | C     | 445 | THR  |
| 1   | D     | 305 | TRP  |
| 1   | D     | 447 | ILE  |
| 1   | A     | 446 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 272 | ALA  |
| 1   | B     | 446 | PRO  |
| 1   | B     | 460 | GLN  |
| 1   | C     | 446 | PRO  |
| 1   | C     | 231 | 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     | 181/207 (87%) | 163 (90%) | 18 (10%)  | 7           | 30 |
| 1   | B     | 187/207 (90%) | 147 (79%) | 40 (21%)  | 1           | 6  |
| 1   | C     | 174/207 (84%) | 152 (87%) | 22 (13%)  | 4           | 20 |
| 1   | D     | 189/207 (91%) | 152 (80%) | 37 (20%)  | 1           | 8  |
| 2   | E     | 5/12 (42%)    | 2 (40%)   | 3 (60%)   | 0           | 0  |
| 2   | F     | 7/12 (58%)    | 3 (43%)   | 4 (57%)   | 0           | 0  |
| All | All   | 743/852 (87%) | 619 (83%) | 124 (17%) | 2           | 12 |

All (124) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 228 | GLU  |
| 1   | A     | 236 | LEU  |
| 1   | A     | 242 | VAL  |
| 1   | A     | 274 | LYS  |
| 1   | A     | 276 | LEU  |
| 1   | A     | 302 | ARG  |
| 1   | A     | 318 | ILE  |
| 1   | A     | 322 | ASP  |
| 1   | A     | 351 | THR  |
| 1   | A     | 358 | ARG  |
| 1   | A     | 384 | SER  |
| 1   | A     | 385 | ASN  |
| 1   | A     | 428 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 441 | LEU  |
| 1   | A     | 442 | ILE  |
| 1   | A     | 447 | ILE  |
| 1   | A     | 449 | THR  |
| 1   | A     | 451 | LEU  |
| 1   | B     | 227 | ASN  |
| 1   | B     | 230 | MET  |
| 1   | B     | 232 | VAL  |
| 1   | B     | 236 | LEU  |
| 1   | B     | 263 | ASP  |
| 1   | B     | 265 | VAL  |
| 1   | B     | 269 | CYS  |
| 1   | B     | 273 | ASP  |
| 1   | B     | 275 | GLN  |
| 1   | B     | 276 | LEU  |
| 1   | B     | 281 | GLU  |
| 1   | B     | 298 | VAL  |
| 1   | B     | 299 | ILE  |
| 1   | B     | 301 | LEU  |
| 1   | B     | 302 | ARG  |
| 1   | B     | 324 | ILE  |
| 1   | B     | 325 | LEU  |
| 1   | B     | 330 | LEU  |
| 1   | B     | 332 | VAL  |
| 1   | B     | 345 | ILE  |
| 1   | B     | 348 | ARG  |
| 1   | B     | 351 | THR  |
| 1   | B     | 361 | GLN  |
| 1   | B     | 367 | LEU  |
| 1   | B     | 373 | ILE  |
| 1   | B     | 381 | LYS  |
| 1   | B     | 390 | GLU  |
| 1   | B     | 392 | LEU  |
| 1   | B     | 406 | HIS  |
| 1   | B     | 427 | SER  |
| 1   | B     | 436 | LEU  |
| 1   | B     | 440 | LYS  |
| 1   | B     | 442 | ILE  |
| 1   | B     | 445 | THR  |
| 1   | B     | 447 | ILE  |
| 1   | B     | 448 | ASP  |
| 1   | B     | 454 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 455 | LEU  |
| 1   | B     | 459 | HIS  |
| 1   | B     | 460 | GLN  |
| 1   | C     | 229 | ASP  |
| 1   | C     | 235 | ILE  |
| 1   | C     | 236 | LEU  |
| 1   | C     | 278 | THR  |
| 1   | C     | 287 | PRO  |
| 1   | C     | 298 | VAL  |
| 1   | C     | 302 | ARG  |
| 1   | C     | 318 | ILE  |
| 1   | C     | 324 | ILE  |
| 1   | C     | 330 | LEU  |
| 1   | C     | 345 | ILE  |
| 1   | C     | 384 | SER  |
| 1   | C     | 385 | ASN  |
| 1   | C     | 390 | GLU  |
| 1   | C     | 394 | GLU  |
| 1   | C     | 407 | LYS  |
| 1   | C     | 426 | ARG  |
| 1   | C     | 428 | ILE  |
| 1   | C     | 442 | ILE  |
| 1   | C     | 445 | THR  |
| 1   | C     | 447 | ILE  |
| 1   | C     | 448 | ASP  |
| 1   | D     | 232 | VAL  |
| 1   | D     | 236 | LEU  |
| 1   | D     | 240 | LEU  |
| 1   | D     | 246 | THR  |
| 1   | D     | 265 | VAL  |
| 1   | D     | 266 | THR  |
| 1   | D     | 267 | ASN  |
| 1   | D     | 268 | ILE  |
| 1   | D     | 275 | GLN  |
| 1   | D     | 281 | GLU  |
| 1   | D     | 291 | GLU  |
| 1   | D     | 292 | LEU  |
| 1   | D     | 294 | LEU  |
| 1   | D     | 299 | ILE  |
| 1   | D     | 317 | SER  |
| 1   | D     | 318 | ILE  |
| 1   | D     | 320 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 328  | THR  |
| 1   | D     | 331  | HIS  |
| 1   | D     | 332  | VAL  |
| 1   | D     | 339  | SER  |
| 1   | D     | 345  | ILE  |
| 1   | D     | 355  | SER  |
| 1   | D     | 356  | LYS  |
| 1   | D     | 367  | LEU  |
| 1   | D     | 371  | ARG  |
| 1   | D     | 373  | ILE  |
| 1   | D     | 389  | VAL  |
| 1   | D     | 390  | GLU  |
| 1   | D     | 400  | LEU  |
| 1   | D     | 411  | GLN  |
| 1   | D     | 442  | ILE  |
| 1   | D     | 451  | LEU  |
| 1   | D     | 455  | LEU  |
| 1   | D     | 456  | GLU  |
| 1   | D     | 458  | PRO  |
| 1   | D     | 460  | GLN  |
| 2   | E     | 2338 | ASN  |
| 2   | E     | 2339 | MET  |
| 2   | E     | 2344 | ILE  |
| 2   | F     | 2337 | THR  |
| 2   | F     | 2339 | MET  |
| 2   | F     | 2344 | ILE  |
| 2   | F     | 2345 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 267 | ASN  |
| 1   | A     | 338 | HIS  |
| 1   | B     | 331 | HIS  |
| 1   | B     | 338 | HIS  |
| 1   | B     | 361 | GLN  |
| 1   | B     | 411 | GLN  |
| 1   | C     | 315 | HIS  |
| 1   | C     | 385 | ASN  |
| 1   | D     | 227 | ASN  |
| 1   | D     | 338 | HIS  |
| 1   | D     | 411 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 459 | HIS  |
| 1   | D     | 460 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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 | $\# Z  > 2$ |
| 3   | RHN  | C     | 2   | -    | 23,23,23     | 1.82 | 5 (21%)     | 35,35,35    | 0.92 | 3 (8%)      |
| 3   | RHN  | A     | 1   | -    | 23,23,23     | 1.85 | 5 (21%)     | 35,35,35    | 0.90 | 3 (8%)      |

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   | RHN  | C     | 2   | -    | -       | 0/4/20/20 | 0/3/3/3 |
| 3   | RHN  | A     | 1   | -    | -       | 4/4/20/20 | 0/3/3/3 |



All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | A     | 1   | RHN  | CAM-CAL | -4.46 | 1.40        | 1.49     |
| 3   | C     | 2   | RHN  | CAR-CAP | -4.30 | 1.39        | 1.48     |
| 3   | C     | 2   | RHN  | CAM-CAL | -4.05 | 1.40        | 1.49     |
| 3   | A     | 1   | RHN  | CAR-CAP | -4.04 | 1.40        | 1.48     |
| 3   | C     | 2   | RHN  | CAS-CAP | -3.95 | 1.40        | 1.48     |
| 3   | A     | 1   | RHN  | CAS-CAP | -3.94 | 1.40        | 1.48     |
| 3   | A     | 1   | RHN  | CAT-CAQ | -3.16 | 1.40        | 1.47     |
| 3   | A     | 1   | RHN  | CAU-CAQ | -3.14 | 1.40        | 1.47     |
| 3   | C     | 2   | RHN  | CAU-CAQ | -3.03 | 1.40        | 1.47     |
| 3   | C     | 2   | RHN  | CAT-CAQ | -2.99 | 1.40        | 1.47     |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | A     | 1   | RHN  | OAE-CAN-CAT | -2.37 | 116.76      | 121.14   |
| 3   | C     | 2   | RHN  | OAD-CAL-CAM | 2.34  | 120.85      | 114.84   |
| 3   | C     | 2   | RHN  | OAD-CAL-OAA | -2.15 | 118.72      | 123.35   |
| 3   | C     | 2   | RHN  | OAE-CAN-CAT | -2.10 | 117.26      | 121.14   |
| 3   | A     | 1   | RHN  | OAD-CAL-CAM | 2.07  | 120.14      | 114.84   |
| 3   | A     | 1   | RHN  | OAF-CAO-CAU | -2.02 | 117.40      | 121.14   |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | A     | 1   | RHN  | OAA-CAL-CAM-CAK |
| 3   | A     | 1   | RHN  | OAA-CAL-CAM-CAJ |
| 3   | A     | 1   | RHN  | OAD-CAL-CAM-CAJ |
| 3   | A     | 1   | RHN  | OAD-CAL-CAM-CAK |

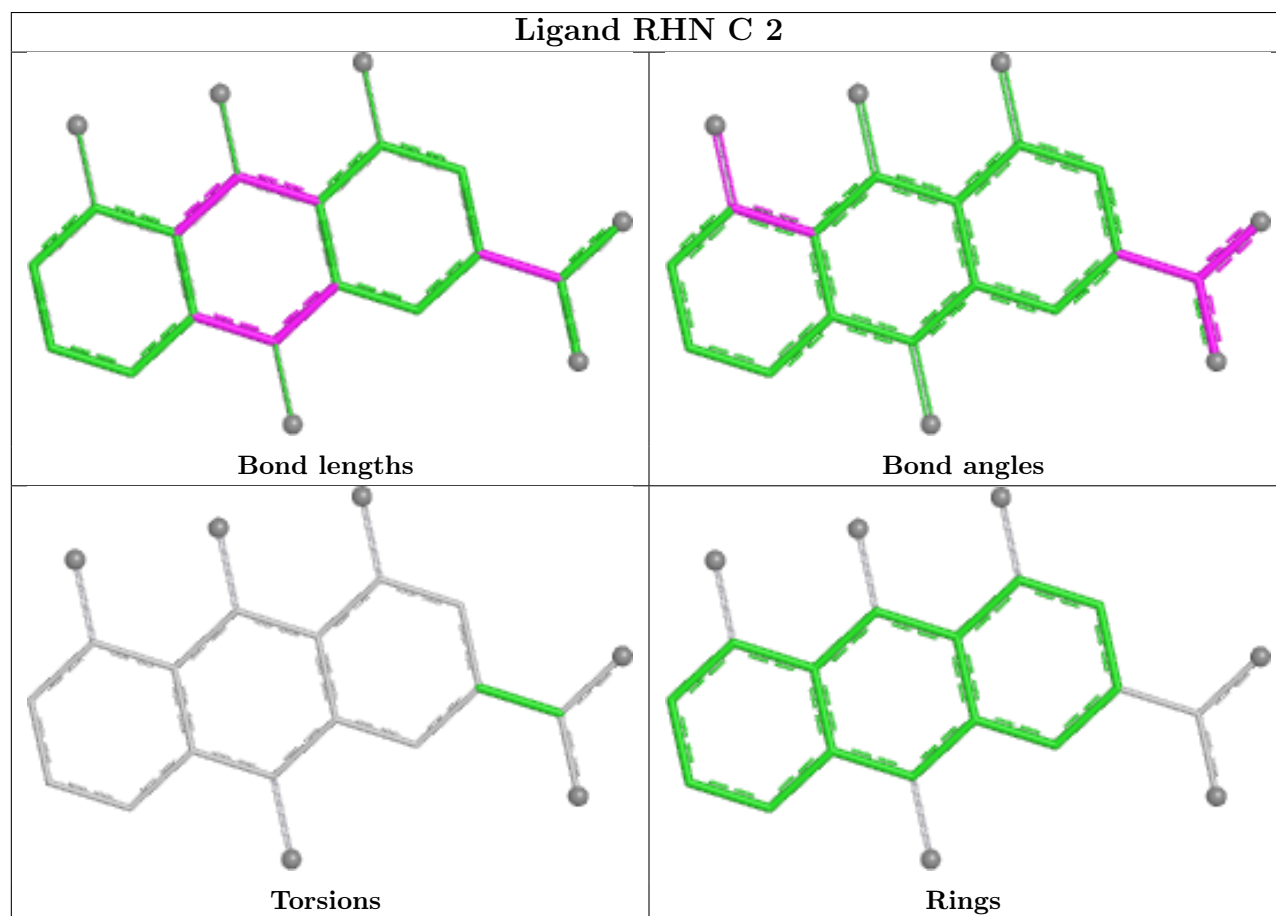
There are no ring outliers.

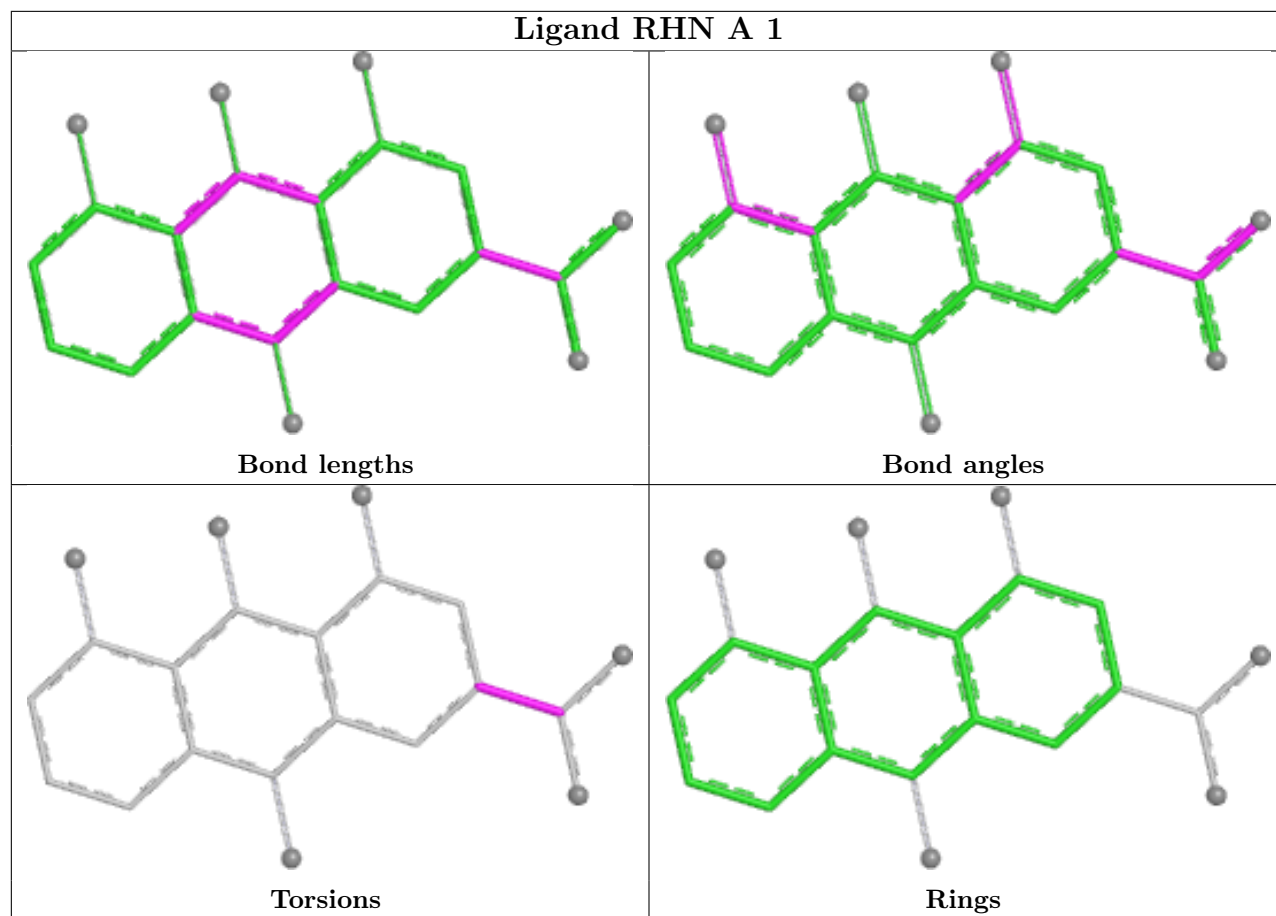
2 monomers are involved in 6 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | C     | 2   | RHN  | 3       | 0            |
| 3   | A     | 1   | RHN  | 3       | 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     | 211/240 (87%) | -1.07  | 0 100 100 | 20, 62, 94, 103       | 0     |
| 1   | B     | 217/240 (90%) | -0.96  | 0 100 100 | 20, 75, 112, 122      | 0     |
| 1   | C     | 203/240 (84%) | -1.08  | 0 100 100 | 20, 61, 86, 99        | 0     |
| 1   | D     | 219/240 (91%) | -1.00  | 0 100 100 | 20, 75, 104, 116      | 0     |
| 2   | E     | 7/16 (43%)    | -1.07  | 0 100 100 | 101, 102, 103, 104    | 0     |
| 2   | F     | 9/16 (56%)    | -0.88  | 0 100 100 | 99, 100, 100, 101     | 0     |
| All | All   | 866/992 (87%) | -1.02  | 0 100 100 | 20, 68, 100, 122      | 0     |

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

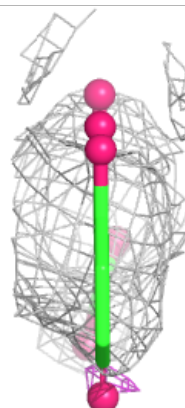
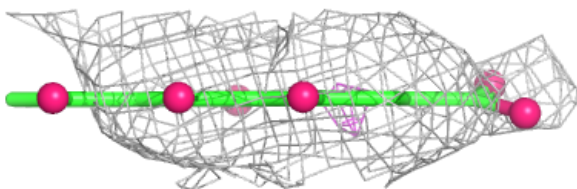
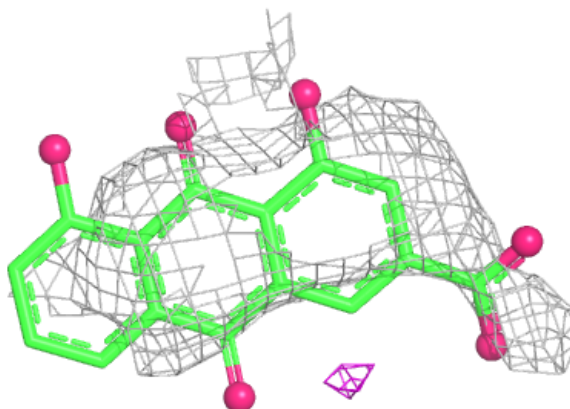
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

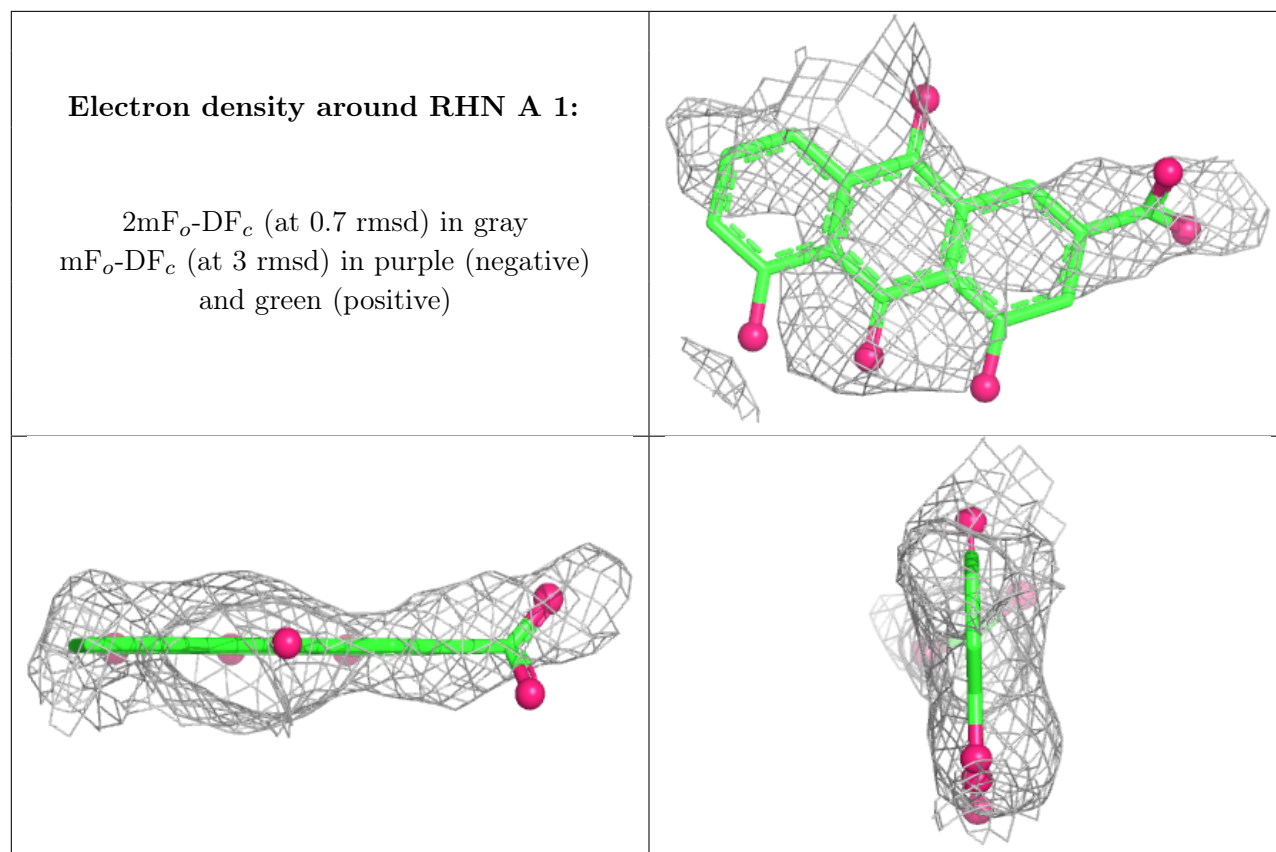
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | RHN  | C     | 2   | 21/21 | 0.97 | 0.12 | 138,139,139,139            | 0     |
| 3   | RHN  | A     | 1   | 21/21 | 0.99 | 0.07 | 129,129,129,129            | 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 RHN C 2:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.