



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:32 AM EDT

PDB ID : 3Q5E / pdb\_00003q5e  
Title : crystal structure of human Atlastin-1 (residues 1-447) bound to GDP, crystal form 2  
Authors : Byrnes, L.J.; Sondermann, H.  
Deposited on : 2010-12-28  
Resolution : 3.01 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                                                             |

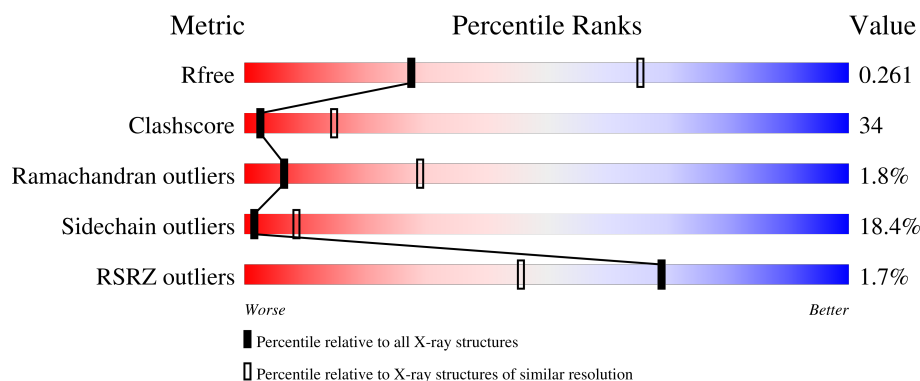
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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                      | 3131 (3.04-3.00)                                      |
| Clashscore            | 190562                      | 3444 (3.04-3.00)                                      |
| Ramachandran outliers | 187476                      | 3319 (3.04-3.00)                                      |
| Sidechain outliers    | 187428                      | 3322 (3.04-3.00)                                      |
| RSRZ outliers         | 180081                      | 3130 (3.04-3.00)                                      |

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     | 447    | <div> <div>38%</div> <div>38%</div> <div>16%</div> <div>8%</div> </div>  |
| 1   | C     | 447    | <div> <div>44%</div> <div>40%</div> <div>7%</div> <div>9%</div> </div>   |
| 1   | E     | 447    | <div> <div>40%</div> <div>35%</div> <div>10%</div> <div>14%</div> </div> |
| 1   | G     | 447    | <div> <div>42%</div> <div>35%</div> <div>9%</div> <div>14%</div> </div>  |

## 2 Entry composition [i](#)

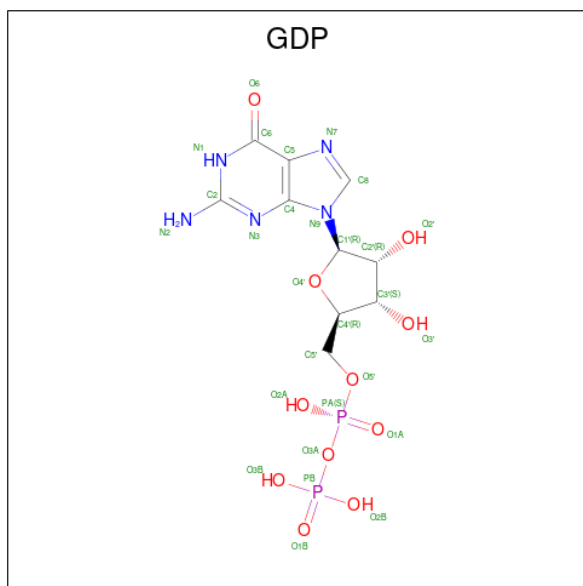
There are 3 unique types of molecules in this entry. The entry contains 12936 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Atlastin-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 411      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3310  | 2116 | 554 | 627 | 13 |         |         |       |
| 1   | C     | 409      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3293  | 2106 | 550 | 624 | 13 |         |         |       |
| 1   | E     | 386      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3116  | 2006 | 514 | 583 | 13 |         |         |       |
| 1   | G     | 384      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3101  | 1995 | 515 | 578 | 13 |         |         |       |

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



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| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |         |
| 2   | G     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |         |

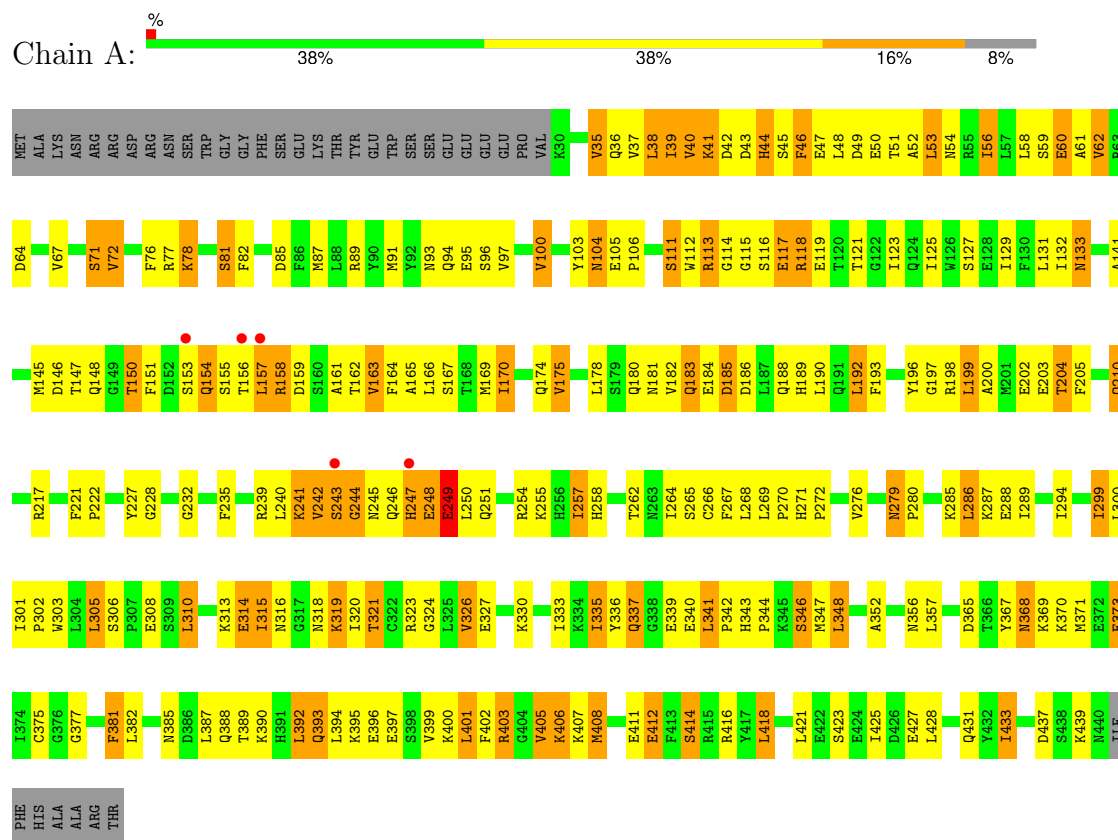
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | C     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | E     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | G     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

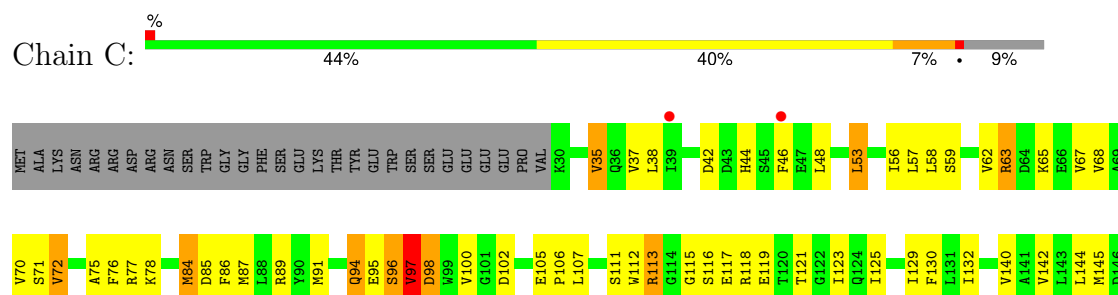
### 3 Residue-property plots [i](#)

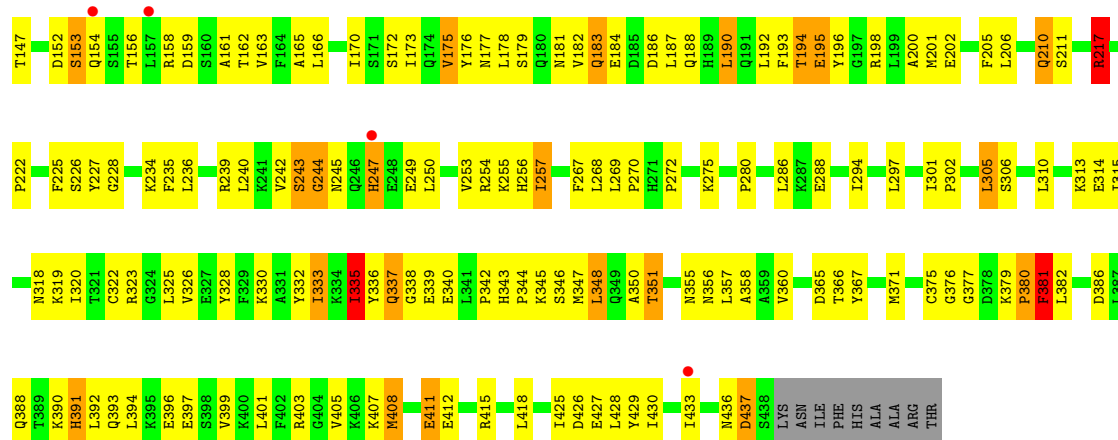
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Atlastin-1

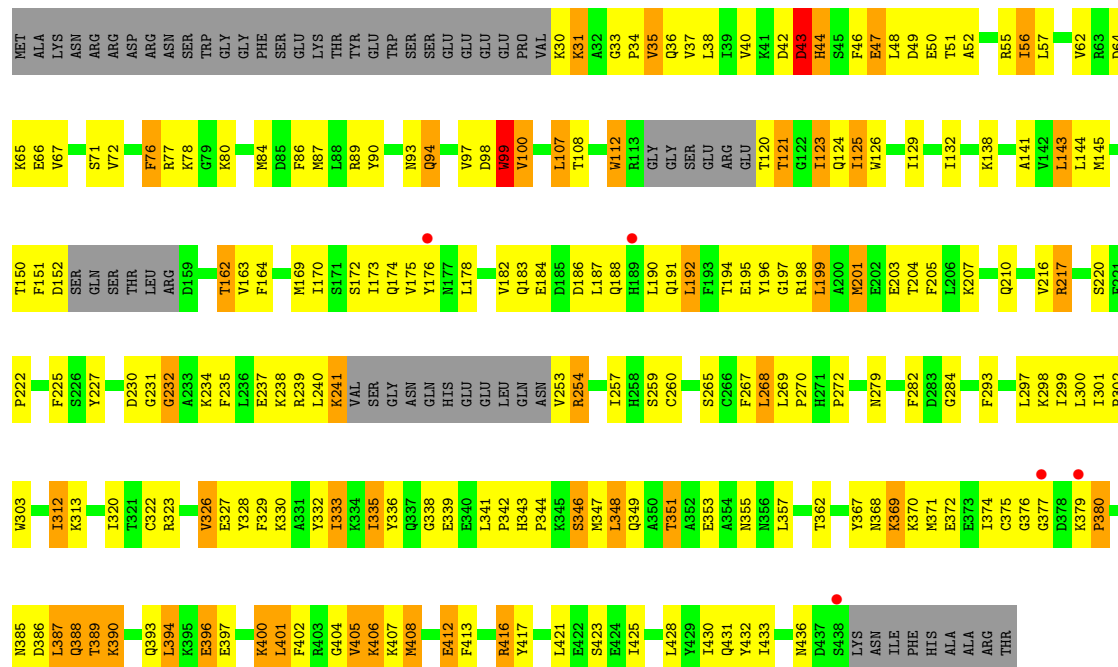


#### • Molecule 1: Atlastin-1

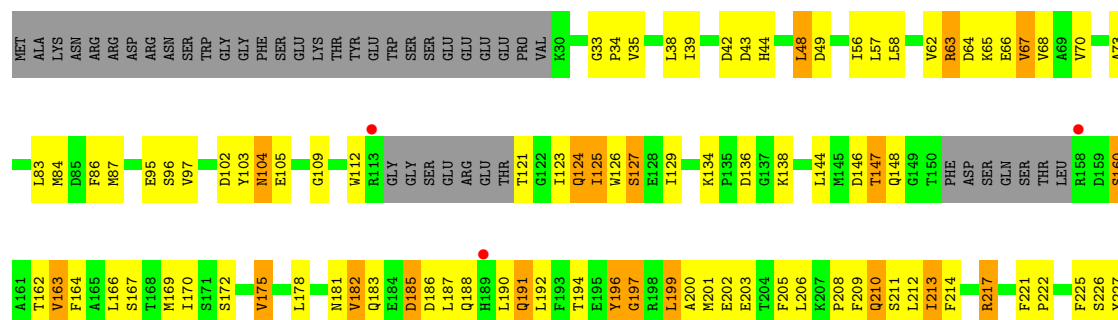
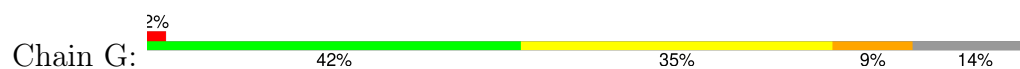


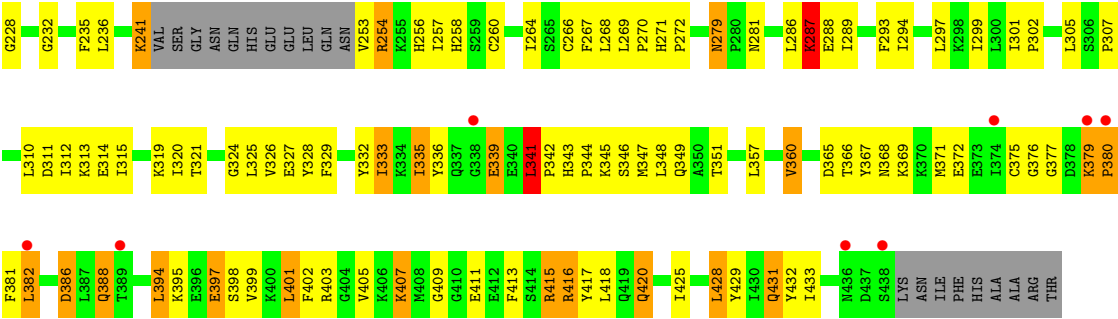


### • Molecule 1: Atlastin-1



### • Molecule 1: Atlastin-1





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 104.39Å 133.55Å 175.84Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 42.54 – 3.01<br>42.54 – 3.01                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 94.2 (42.54-3.01)<br>93.1 (42.54-3.01)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.70 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.6.4_486)                           | Depositor        |
| R, $R_{free}$                                                           | 0.197 , 0.273<br>0.190 , 0.261                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2000 reflections (4.10%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 54.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.735                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 70.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 12936                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 74.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: GDP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.58         | 0/3379      | 0.92        | 6/4556 (0.1%)   |
| 1   | C     | 0.55         | 0/3362      | 0.93        | 12/4534 (0.3%)  |
| 1   | E     | 0.60         | 0/3181      | 0.99        | 9/4287 (0.2%)   |
| 1   | G     | 0.55         | 0/3165      | 0.98        | 12/4264 (0.3%)  |
| All | All   | 0.57         | 0/13087     | 0.95        | 39/17641 (0.2%) |

There are no bond length outliers.

All (39) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 244 | GLY  | N-CA-C  | -11.08 | 102.48      | 114.67   |
| 1   | A     | 217 | ARG  | N-CA-C  | 9.92   | 121.86      | 111.14   |
| 1   | G     | 217 | ARG  | N-CA-C  | 8.40   | 120.21      | 111.14   |
| 1   | E     | 217 | ARG  | N-CA-C  | 8.34   | 120.45      | 111.36   |
| 1   | C     | 200 | ALA  | N-CA-C  | -7.87  | 104.28      | 114.04   |
| 1   | C     | 172 | SER  | N-CA-C  | -7.75  | 104.35      | 113.88   |
| 1   | C     | 244 | GLY  | N-CA-C  | -7.57  | 105.81      | 115.42   |
| 1   | G     | 328 | TYR  | N-CA-C  | -7.54  | 104.06      | 113.55   |
| 1   | G     | 109 | GLY  | N-CA-C  | -6.60  | 105.41      | 112.08   |
| 1   | C     | 217 | ARG  | N-CA-C  | 6.34   | 121.27      | 112.45   |
| 1   | C     | 161 | ALA  | N-CA-C  | -6.27  | 105.76      | 113.41   |
| 1   | A     | 67  | VAL  | N-CA-C  | 6.16   | 117.35      | 108.48   |
| 1   | E     | 67  | VAL  | N-CA-C  | 6.02   | 117.15      | 108.48   |
| 1   | G     | 67  | VAL  | N-CA-C  | 5.97   | 117.19      | 108.53   |
| 1   | C     | 335 | ILE  | CB-CA-C | -5.82  | 104.52      | 111.97   |
| 1   | C     | 67  | VAL  | N-CA-C  | 5.80   | 116.94      | 108.53   |
| 1   | E     | 328 | TYR  | N-CA-C  | -5.80  | 104.56      | 111.69   |
| 1   | E     | 232 | GLY  | N-CA-C  | -5.77  | 105.80      | 112.83   |
| 1   | E     | 99  | TRP  | N-CA-C  | -5.65  | 106.23      | 113.01   |
| 1   | A     | 377 | GLY  | N-CA-C  | -5.65  | 105.84      | 113.24   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | G     | 172 | SER  | N-CA-C  | -5.65 | 107.02      | 114.31   |
| 1   | G     | 403 | ARG  | N-CA-C  | -5.63 | 102.58      | 110.35   |
| 1   | G     | 279 | ASN  | CA-C-N  | 5.51  | 125.16      | 119.05   |
| 1   | G     | 279 | ASN  | C-N-CA  | 5.51  | 125.16      | 119.05   |
| 1   | G     | 341 | LEU  | CA-C-N  | 5.44  | 126.93      | 120.23   |
| 1   | G     | 341 | LEU  | C-N-CA  | 5.44  | 126.93      | 120.23   |
| 1   | C     | 388 | GLN  | N-CA-C  | -5.43 | 106.70      | 113.55   |
| 1   | E     | 173 | ILE  | CB-CA-C | -5.42 | 105.08      | 111.09   |
| 1   | C     | 243 | SER  | CB-CA-C | -5.37 | 109.93      | 117.23   |
| 1   | E     | 408 | MET  | N-CA-C  | 5.32  | 119.70      | 112.04   |
| 1   | E     | 112 | TRP  | N-CA-C  | -5.23 | 105.22      | 111.03   |
| 1   | C     | 179 | SER  | N-CA-C  | 5.23  | 119.56      | 111.56   |
| 1   | A     | 97  | VAL  | N-CA-C  | -5.21 | 105.40      | 113.16   |
| 1   | E     | 93  | ASN  | N-CA-C  | 5.17  | 119.00      | 109.24   |
| 1   | A     | 249 | GLU  | N-CA-C  | -5.10 | 106.30      | 112.88   |
| 1   | G     | 211 | SER  | N-CA-C  | 5.10  | 117.88      | 109.72   |
| 1   | G     | 388 | GLN  | N-CA-C  | -5.08 | 107.06      | 114.12   |
| 1   | C     | 428 | LEU  | N-CA-C  | -5.08 | 107.09      | 113.28   |
| 1   | C     | 158 | ARG  | N-CA-C  | -5.01 | 107.00      | 112.72   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3310  | 0        | 3291     | 302     | 0            |
| 1   | C     | 3293  | 0        | 3272     | 191     | 0            |
| 1   | E     | 3116  | 0        | 3109     | 202     | 0            |
| 1   | G     | 3101  | 0        | 3102     | 196     | 0            |
| 2   | A     | 28    | 0        | 12       | 2       | 0            |
| 2   | C     | 28    | 0        | 12       | 3       | 0            |
| 2   | E     | 28    | 0        | 12       | 2       | 0            |
| 2   | G     | 28    | 0        | 12       | 1       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | E     | 1     | 0        | 0        | 0       | 0            |
| 3   | G     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 12936 | 0        | 12822    | 873     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (873) 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:A:37:VAL:HG21  | 1:A:53:LEU:HD23  | 1.22                     | 1.14              |
| 1:A:403:ARG:HH11 | 1:A:403:ARG:HG2  | 1.09                     | 1.14              |
| 1:C:48:LEU:HB2   | 1:C:333:ILE:HG13 | 1.26                     | 1.14              |
| 1:A:341:LEU:HG   | 1:A:342:PRO:HD2  | 1.31                     | 1.12              |
| 1:A:381:PHE:HB2  | 1:A:439:LYS:HD3  | 1.32                     | 1.11              |
| 1:C:245:ASN:HD21 | 1:G:397:GLU:HA   | 1.09                     | 1.11              |
| 1:G:379:LYS:HB3  | 1:G:380:PRO:HD3  | 1.36                     | 1.05              |
| 1:A:154:GLN:O    | 1:A:158:ARG:HG2  | 1.61                     | 1.01              |
| 1:A:111:SER:HA   | 1:A:113:ARG:NH1  | 1.78                     | 0.98              |
| 1:G:196:TYR:HB2  | 1:G:347:MET:HE1  | 1.44                     | 0.98              |
| 1:E:56:ILE:HD13  | 1:E:125:ILE:HD11 | 1.44                     | 0.98              |
| 1:C:379:LYS:HB3  | 1:C:380:PRO:HD3  | 1.46                     | 0.97              |
| 1:A:269:LEU:HD12 | 1:A:270:PRO:HD2  | 1.44                     | 0.96              |
| 1:A:39:ILE:HG23  | 1:A:47:GLU:HG3   | 1.47                     | 0.94              |
| 1:E:343:HIS:CD2  | 1:E:344:PRO:HD2  | 2.02                     | 0.94              |
| 1:A:158:ARG:O    | 1:A:162:THR:HG23 | 1.68                     | 0.94              |
| 1:G:196:TYR:HB2  | 1:G:347:MET:CE   | 1.97                     | 0.94              |
| 1:A:200:ALA:O    | 1:A:204:THR:HG23 | 1.68                     | 0.93              |
| 1:A:316:ASN:O    | 1:A:406:LYS:HE2  | 1.72                     | 0.90              |
| 1:G:190:LEU:HD23 | 1:G:257:ILE:HD11 | 1.52                     | 0.90              |
| 1:G:332:TYR:OH   | 1:G:351:THR:HG22 | 1.72                     | 0.90              |
| 1:E:269:LEU:HD12 | 1:E:270:PRO:HD2  | 1.53                     | 0.89              |
| 1:A:50:GLU:HG2   | 1:A:54:ASN:HD21  | 1.35                     | 0.89              |
| 1:A:117:GLU:HB2  | 1:A:119:GLU:HB3  | 1.54                     | 0.88              |
| 1:E:120:THR:HB   | 1:E:151:PHE:CE2  | 2.09                     | 0.88              |
| 1:A:241:LYS:HD3  | 1:A:242:VAL:N    | 1.88                     | 0.88              |
| 1:C:117:GLU:HG2  | 1:C:119:GLU:HB3  | 1.56                     | 0.87              |
| 1:E:379:LYS:HB2  | 1:E:380:PRO:HD3  | 1.56                     | 0.87              |
| 1:A:105:GLU:HG3  | 1:A:106:PRO:HD2  | 1.55                     | 0.86              |
| 1:A:46:PHE:HD2   | 1:A:46:PHE:N     | 1.73                     | 0.86              |
| 1:C:196:TYR:CB   | 1:C:347:MET:HE2  | 2.06                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:400:LYS:HA   | 1:A:403:ARG:HD2  | 1.59                     | 0.84              |
| 1:A:112:TRP:H    | 1:A:113:ARG:NH1  | 1.75                     | 0.84              |
| 1:A:316:ASN:CG   | 1:A:406:LYS:HD2  | 2.03                     | 0.83              |
| 1:A:403:ARG:HG2  | 1:A:403:ARG:NH1  | 1.86                     | 0.82              |
| 1:C:87:MET:HE3   | 1:C:305:LEU:HD11 | 1.60                     | 0.82              |
| 1:A:321:THR:HG22 | 1:A:324:GLY:H    | 1.43                     | 0.82              |
| 1:A:389:THR:HA   | 1:A:392:LEU:HD11 | 1.60                     | 0.82              |
| 1:A:243:SER:HB3  | 1:E:401:LEU:HD13 | 1.62                     | 0.82              |
| 1:C:183:GLN:O    | 1:C:186:ASP:HB2  | 1.79                     | 0.82              |
| 1:C:245:ASN:ND2  | 1:G:397:GLU:HA   | 1.93                     | 0.82              |
| 1:E:40:VAL:HG22  | 1:E:46:PHE:HD1   | 1.43                     | 0.82              |
| 1:A:72:VAL:HG13  | 1:A:175:VAL:HG22 | 1.61                     | 0.82              |
| 1:C:196:TYR:HB2  | 1:C:347:MET:HE2  | 1.60                     | 0.81              |
| 1:E:40:VAL:HG22  | 1:E:46:PHE:CD1   | 2.14                     | 0.81              |
| 1:E:86:PHE:CD2   | 1:E:297:LEU:HD21 | 2.15                     | 0.81              |
| 1:A:412:GLU:CD   | 1:A:412:GLU:H    | 1.87                     | 0.80              |
| 1:C:247:HIS:CE1  | 1:C:254:ARG:CZ   | 2.64                     | 0.80              |
| 1:E:402:PHE:CE2  | 1:E:407:LYS:HE3  | 2.16                     | 0.80              |
| 1:A:153:SER:C    | 1:A:157:LEU:HD12 | 2.07                     | 0.80              |
| 1:A:46:PHE:N     | 1:A:46:PHE:CD2   | 2.47                     | 0.80              |
| 1:A:243:SER:N    | 1:A:247:HIS:NE2  | 2.30                     | 0.79              |
| 1:A:368:ASN:C    | 1:A:368:ASN:HD22 | 1.90                     | 0.79              |
| 1:G:123:ILE:HG12 | 1:G:147:THR:HG22 | 1.62                     | 0.79              |
| 1:E:413:PHE:O    | 1:E:416:ARG:HG3  | 1.83                     | 0.78              |
| 1:A:316:ASN:CB   | 1:A:406:LYS:HD2  | 2.13                     | 0.78              |
| 1:C:244:GLY:O    | 1:C:245:ASN:HB2  | 1.83                     | 0.78              |
| 1:G:210:GLN:NE2  | 1:G:313:LYS:HA   | 1.98                     | 0.78              |
| 1:A:421:LEU:O    | 1:A:425:ILE:HG13 | 1.82                     | 0.78              |
| 1:E:327:GLU:HA   | 1:E:330:LYS:HB2  | 1.65                     | 0.78              |
| 1:C:332:TYR:HE1  | 1:C:351:THR:HG22 | 1.48                     | 0.78              |
| 1:G:332:TYR:CE1  | 1:G:351:THR:HG22 | 2.20                     | 0.77              |
| 1:A:401:LEU:C    | 1:A:401:LEU:HD12 | 2.09                     | 0.77              |
| 1:C:335:ILE:HG22 | 1:C:336:TYR:N    | 2.00                     | 0.77              |
| 1:G:227:TYR:CE1  | 1:G:270:PRO:HB3  | 2.19                     | 0.77              |
| 1:C:245:ASN:HD21 | 1:G:397:GLU:CA   | 1.95                     | 0.77              |
| 1:A:111:SER:HA   | 1:A:113:ARG:HH11 | 1.49                     | 0.76              |
| 1:C:46:PHE:H     | 1:C:337:GLN:HB2  | 1.48                     | 0.76              |
| 1:E:241:LYS:HE2  | 1:E:241:LYS:HA   | 1.66                     | 0.76              |
| 1:C:335:ILE:HD11 | 1:C:347:MET:HA   | 1.66                     | 0.75              |
| 1:G:394:LEU:O    | 1:G:397:GLU:HB3  | 1.87                     | 0.75              |
| 1:A:38:LEU:HD23  | 1:A:38:LEU:C     | 2.09                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:154:GLN:HG3  | 1:C:105:GLU:OE2  | 1.87                     | 0.75              |
| 1:G:48:LEU:HD12  | 1:G:49:ASP:N     | 2.02                     | 0.75              |
| 1:G:321:THR:HG23 | 1:G:324:GLY:H    | 1.49                     | 0.75              |
| 1:C:76:PHE:CE1   | 1:C:119:GLU:HG3  | 2.21                     | 0.74              |
| 1:A:316:ASN:HB3  | 1:A:406:LYS:HD2  | 1.69                     | 0.74              |
| 1:A:111:SER:CA   | 1:A:113:ARG:NH1  | 2.50                     | 0.74              |
| 1:G:332:TYR:CZ   | 1:G:351:THR:HG22 | 2.21                     | 0.74              |
| 1:G:254:ARG:HH21 | 1:G:258:HIS:HE1  | 1.32                     | 0.74              |
| 1:C:269:LEU:HD12 | 1:C:270:PRO:HD2  | 1.68                     | 0.74              |
| 1:E:371:MET:O    | 1:E:375:CYS:HB3  | 1.87                     | 0.74              |
| 1:G:254:ARG:HH21 | 1:G:258:HIS:CE1  | 2.05                     | 0.74              |
| 1:E:232:GLY:HA2  | 1:E:268:LEU:HD22 | 1.70                     | 0.74              |
| 1:A:41:LYS:HE2   | 1:A:41:LYS:HA    | 1.68                     | 0.73              |
| 1:A:118:ARG:HG3  | 1:A:118:ARG:O    | 1.86                     | 0.73              |
| 1:A:111:SER:CA   | 1:A:113:ARG:HH11 | 2.01                     | 0.73              |
| 1:E:335:ILE:HG22 | 1:E:336:TYR:CD1  | 2.24                     | 0.73              |
| 1:A:41:LYS:HA    | 1:A:41:LYS:CE    | 2.17                     | 0.72              |
| 1:E:240:LEU:HB3  | 1:E:254:ARG:HG2  | 1.69                     | 0.72              |
| 1:G:214:PHE:HD2  | 1:G:236:LEU:HD21 | 1.54                     | 0.72              |
| 1:A:154:GLN:HA   | 1:A:157:LEU:HB2  | 1.71                     | 0.72              |
| 1:G:254:ARG:HD3  | 1:G:254:ARG:C    | 2.13                     | 0.72              |
| 1:A:117:GLU:HB2  | 1:A:119:GLU:CB   | 2.20                     | 0.72              |
| 1:A:241:LYS:HE3  | 1:A:241:LYS:HA   | 1.70                     | 0.72              |
| 1:G:123:ILE:HG12 | 1:G:147:THR:CG2  | 2.19                     | 0.72              |
| 1:E:56:ILE:HD13  | 1:E:125:ILE:CD1  | 2.19                     | 0.72              |
| 1:C:332:TYR:CE1  | 1:C:351:THR:HG22 | 2.25                     | 0.71              |
| 1:G:84:MET:HE3   | 1:G:87:MET:HE2   | 1.71                     | 0.71              |
| 1:E:71:SER:HB3   | 1:E:174:GLN:NE2  | 2.04                     | 0.71              |
| 1:A:240:LEU:O    | 1:A:254:ARG:HD3  | 1.90                     | 0.71              |
| 1:G:196:TYR:O    | 1:G:199:LEU:HD12 | 1.91                     | 0.71              |
| 1:A:50:GLU:HG2   | 1:A:54:ASN:ND2   | 2.05                     | 0.71              |
| 1:A:104:ASN:HD22 | 1:A:285:LYS:HE2  | 1.55                     | 0.71              |
| 1:C:247:HIS:CE1  | 1:C:254:ARG:NE   | 2.58                     | 0.71              |
| 1:G:48:LEU:HD12  | 1:G:49:ASP:H     | 1.56                     | 0.71              |
| 1:G:196:TYR:OH   | 1:G:351:THR:HG21 | 1.90                     | 0.71              |
| 1:A:269:LEU:HD12 | 1:A:270:PRO:CD   | 2.20                     | 0.70              |
| 1:C:343:HIS:HD2  | 1:C:345:LYS:H    | 1.38                     | 0.70              |
| 1:C:222:PRO:HG3  | 1:C:227:TYR:CZ   | 2.26                     | 0.70              |
| 1:E:120:THR:C    | 1:E:151:PHE:HZ   | 2.00                     | 0.70              |
| 1:C:381:PHE:HD2  | 1:C:381:PHE:C    | 1.99                     | 0.70              |
| 1:E:376:GLY:HA3  | 1:E:377:GLY:C    | 2.16                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:205:PHE:O    | 1:C:206:LEU:HD23 | 1.92                     | 0.70              |
| 1:A:381:PHE:CB   | 1:A:439:LYS:HD3  | 2.17                     | 0.69              |
| 1:C:72:VAL:HG13  | 1:C:175:VAL:HG22 | 1.74                     | 0.69              |
| 1:G:199:LEU:HA   | 1:G:202:GLU:HG2  | 1.74                     | 0.69              |
| 1:C:188:GLN:HE21 | 1:C:250:LEU:HG   | 1.56                     | 0.69              |
| 1:G:104:ASN:HD22 | 1:G:287:LYS:NZ   | 1.91                     | 0.69              |
| 1:A:244:GLY:C    | 1:A:246:GLN:H    | 2.00                     | 0.69              |
| 1:G:379:LYS:CB   | 1:G:380:PRO:HD3  | 2.17                     | 0.69              |
| 1:E:207:LYS:HG2  | 1:E:259:SER:O    | 1.92                     | 0.69              |
| 1:A:150:THR:C    | 1:A:151:PHE:HD1  | 2.00                     | 0.69              |
| 1:A:403:ARG:HH11 | 1:A:403:ARG:CG   | 1.97                     | 0.69              |
| 1:C:117:GLU:CG   | 1:C:119:GLU:HB3  | 2.23                     | 0.69              |
| 1:A:106:PRO:HA   | 1:A:285:LYS:HA   | 1.74                     | 0.69              |
| 1:A:112:TRP:H    | 1:A:113:ARG:CZ   | 2.05                     | 0.69              |
| 1:G:147:THR:HG21 | 1:G:167:SER:HB2  | 1.74                     | 0.69              |
| 1:E:387:LEU:HD21 | 1:E:433:ILE:HG22 | 1.75                     | 0.69              |
| 1:C:390:LYS:O    | 1:C:394:LEU:HD13 | 1.92                     | 0.69              |
| 1:A:154:GLN:H    | 1:A:154:GLN:NE2  | 1.90                     | 0.68              |
| 1:C:84:MET:HB2   | 1:C:112:TRP:CD1  | 2.28                     | 0.68              |
| 1:E:343:HIS:CD2  | 1:E:344:PRO:CD   | 2.75                     | 0.68              |
| 1:G:241:LYS:HE2  | 1:G:241:LYS:HA   | 1.73                     | 0.68              |
| 1:A:341:LEU:HG   | 1:A:342:PRO:CD   | 2.17                     | 0.68              |
| 1:C:115:GLY:O    | 1:C:118:ARG:HD3  | 1.92                     | 0.68              |
| 1:C:343:HIS:CD2  | 1:C:345:LYS:H    | 2.11                     | 0.68              |
| 1:C:202:GLU:HB2  | 1:G:205:PHE:CD1  | 2.29                     | 0.68              |
| 1:C:379:LYS:CB   | 1:C:380:PRO:HD3  | 2.22                     | 0.68              |
| 1:E:94:GLN:HE21  | 1:E:94:GLN:H     | 1.40                     | 0.68              |
| 1:C:381:PHE:C    | 1:C:381:PHE:CD2  | 2.72                     | 0.68              |
| 1:G:409:GLY:HA3  | 1:G:413:PHE:HD2  | 1.59                     | 0.68              |
| 1:C:247:HIS:CD2  | 1:C:250:LEU:HB2  | 2.29                     | 0.68              |
| 1:G:170:ILE:O    | 1:G:313:LYS:HE2  | 1.94                     | 0.68              |
| 1:A:85:ASP:OD1   | 1:A:113:ARG:NH1  | 2.27                     | 0.68              |
| 1:E:48:LEU:HD22  | 1:E:333:ILE:HG13 | 1.76                     | 0.68              |
| 1:G:401:LEU:HD12 | 1:G:401:LEU:O    | 1.94                     | 0.68              |
| 1:A:76:PHE:HE2   | 1:A:148:GLN:NE2  | 1.92                     | 0.67              |
| 1:A:112:TRP:N    | 1:A:113:ARG:NH1  | 2.42                     | 0.67              |
| 1:E:240:LEU:O    | 1:E:254:ARG:HG3  | 1.94                     | 0.67              |
| 1:E:412:GLU:HG2  | 1:G:95:GLU:O     | 1.95                     | 0.67              |
| 1:E:120:THR:C    | 1:E:151:PHE:CZ   | 2.73                     | 0.67              |
| 1:C:96:SER:O     | 1:C:97:VAL:HB    | 1.94                     | 0.66              |
| 1:E:336:TYR:OH   | 1:E:347:MET:HE3  | 1.94                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:267:PHE:CD2  | 1:A:300:LEU:HD13 | 2.31                     | 0.66              |
| 1:A:227:TYR:CZ   | 1:A:270:PRO:HB3  | 2.30                     | 0.66              |
| 1:C:315:ILE:HD13 | 1:C:328:TYR:CE2  | 2.30                     | 0.66              |
| 1:G:222:PRO:HG3  | 1:G:227:TYR:CZ   | 2.30                     | 0.66              |
| 1:A:111:SER:HB2  | 1:A:113:ARG:HH11 | 1.61                     | 0.66              |
| 1:E:270:PRO:HG2  | 1:E:293:PHE:HA   | 1.77                     | 0.65              |
| 1:A:154:GLN:N    | 1:A:157:LEU:HD12 | 2.12                     | 0.65              |
| 1:C:115:GLY:O    | 1:C:116:SER:HB3  | 1.94                     | 0.65              |
| 1:G:236:LEU:HD22 | 1:G:266:CYS:HB2  | 1.78                     | 0.65              |
| 1:C:210:GLN:HE22 | 1:C:314:GLU:H    | 1.44                     | 0.65              |
| 1:G:301:ILE:HB   | 1:G:302:PRO:HD3  | 1.79                     | 0.65              |
| 1:E:97:VAL:O     | 1:E:98:ASP:HB3   | 1.97                     | 0.65              |
| 1:G:84:MET:HE2   | 1:G:112:TRP:CZ2  | 2.32                     | 0.64              |
| 1:G:196:TYR:O    | 1:G:197:GLY:C    | 2.40                     | 0.64              |
| 1:G:200:ALA:HA   | 1:G:348:LEU:HD12 | 1.78                     | 0.64              |
| 1:A:87:MET:O     | 1:A:91:MET:HG2   | 1.97                     | 0.64              |
| 1:G:170:ILE:HG23 | 1:G:325:LEU:HD11 | 1.79                     | 0.64              |
| 1:G:269:LEU:HD12 | 1:G:270:PRO:HD2  | 1.80                     | 0.64              |
| 1:A:316:ASN:O    | 1:A:406:LYS:CE   | 2.45                     | 0.64              |
| 1:A:315:ILE:N    | 1:A:315:ILE:HD12 | 2.12                     | 0.64              |
| 1:A:52:ALA:O     | 1:A:56:ILE:HG13  | 1.98                     | 0.64              |
| 1:G:394:LEU:HA   | 1:G:397:GLU:HB3  | 1.80                     | 0.64              |
| 1:C:347:MET:O    | 1:C:351:THR:HG23 | 1.98                     | 0.63              |
| 1:C:222:PRO:HG3  | 1:C:227:TYR:CE1  | 2.33                     | 0.63              |
| 1:E:225:PHE:CD2  | 1:E:235:PHE:HB2  | 2.33                     | 0.63              |
| 1:A:111:SER:CB   | 1:A:113:ARG:HH11 | 2.11                     | 0.63              |
| 1:G:381:PHE:C    | 1:G:381:PHE:CD2  | 2.76                     | 0.63              |
| 1:A:165:ALA:HA   | 1:A:193:PHE:HE1  | 1.64                     | 0.63              |
| 1:E:99:TRP:HE3   | 1:E:99:TRP:O     | 1.81                     | 0.63              |
| 1:A:115:GLY:HA3  | 1:A:118:ARG:HH11 | 1.63                     | 0.62              |
| 1:A:115:GLY:HA3  | 1:A:118:ARG:NH1  | 2.13                     | 0.62              |
| 1:A:241:LYS:HD3  | 1:A:242:VAL:H    | 1.59                     | 0.62              |
| 1:C:343:HIS:CD2  | 1:C:345:LYS:HB2  | 2.33                     | 0.62              |
| 1:C:336:TYR:O    | 1:C:337:GLN:HB3  | 1.99                     | 0.62              |
| 1:A:116:SER:O    | 1:A:118:ARG:HB3  | 1.99                     | 0.62              |
| 1:G:214:PHE:CD2  | 1:G:236:LEU:HD21 | 2.34                     | 0.62              |
| 1:C:76:PHE:CZ    | 1:C:119:GLU:HG3  | 2.33                     | 0.62              |
| 1:C:343:HIS:HD2  | 1:C:345:LYS:HB2  | 1.63                     | 0.62              |
| 1:E:42:ASP:C     | 1:E:44:HIS:H     | 2.08                     | 0.62              |
| 1:E:379:LYS:CB   | 1:E:380:PRO:HD3  | 2.28                     | 0.62              |
| 1:A:356:ASN:OD1  | 1:A:407:LYS:HG2  | 1.99                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:239:ARG:HG2  | 1:E:239:ARG:HH11 | 1.64                     | 0.62              |
| 1:E:176:TYR:CE1  | 1:E:178:LEU:HD21 | 2.35                     | 0.61              |
| 1:A:56:ILE:HD12  | 1:A:125:ILE:HD11 | 1.81                     | 0.61              |
| 1:G:210:GLN:HE21 | 1:G:313:LYS:HA   | 1.63                     | 0.61              |
| 1:G:270:PRO:HG2  | 1:G:293:PHE:HA   | 1.82                     | 0.61              |
| 1:E:72:VAL:HG12  | 1:E:80:LYS:HG2   | 1.83                     | 0.61              |
| 1:E:387:LEU:HD21 | 1:E:433:ILE:CG2  | 2.31                     | 0.61              |
| 1:G:314:GLU:OE2  | 1:G:319:LYS:HE2  | 2.00                     | 0.61              |
| 1:A:45:SER:C     | 1:A:46:PHE:HD2   | 2.09                     | 0.61              |
| 1:A:313:LYS:HE3  | 1:A:315:ILE:HD11 | 1.82                     | 0.61              |
| 1:A:85:ASP:OD2   | 1:A:113:ARG:CZ   | 2.48                     | 0.61              |
| 1:A:183:GLN:O    | 1:A:186:ASP:HB2  | 2.00                     | 0.61              |
| 1:E:90:TYR:HB2   | 1:E:99:TRP:CE3   | 2.36                     | 0.61              |
| 1:A:87:MET:HE3   | 1:A:305:LEU:HD11 | 1.80                     | 0.61              |
| 1:G:286:LEU:HD22 | 1:G:294:ILE:HD11 | 1.82                     | 0.61              |
| 1:G:409:GLY:HA3  | 1:G:413:PHE:CD2  | 2.35                     | 0.61              |
| 1:A:100:VAL:HG13 | 1:A:286:LEU:HD11 | 1.81                     | 0.61              |
| 1:C:196:TYR:CB   | 1:C:347:MET:CE   | 2.78                     | 0.61              |
| 1:A:154:GLN:HG3  | 1:C:105:GLU:CD   | 2.26                     | 0.61              |
| 1:C:275:LYS:HD3  | 1:C:288:GLU:HB3  | 1.83                     | 0.61              |
| 1:C:113:ARG:O    | 1:C:113:ARG:HG2  | 2.00                     | 0.61              |
| 1:E:99:TRP:O     | 1:E:99:TRP:CE3   | 2.53                     | 0.61              |
| 1:A:279:ASN:HD22 | 1:A:279:ASN:C    | 2.08                     | 0.60              |
| 1:E:84:MET:HE3   | 1:E:87:MET:HE2   | 1.83                     | 0.60              |
| 1:A:205:PHE:HE1  | 1:E:201:MET:O    | 1.85                     | 0.60              |
| 1:C:411:GLU:N    | 1:C:411:GLU:CD   | 2.59                     | 0.60              |
| 1:A:37:VAL:HG21  | 1:A:53:LEU:CD2   | 2.15                     | 0.60              |
| 1:A:401:LEU:HD12 | 1:A:401:LEU:O    | 2.01                     | 0.60              |
| 1:G:343:HIS:O    | 1:G:346:SER:HB3  | 2.01                     | 0.60              |
| 1:G:379:LYS:HB3  | 1:G:380:PRO:CD   | 2.21                     | 0.60              |
| 1:C:255:LYS:HG2  | 1:C:256:HIS:CE1  | 2.36                     | 0.60              |
| 1:A:111:SER:CB   | 1:A:113:ARG:HD2  | 2.32                     | 0.60              |
| 1:E:86:PHE:CD1   | 1:E:89:ARG:NH1   | 2.70                     | 0.60              |
| 1:A:369:LYS:HD2  | 1:A:369:LYS:N    | 2.16                     | 0.60              |
| 1:E:396:GLU:O    | 1:E:396:GLU:HG2  | 2.01                     | 0.60              |
| 1:A:327:GLU:OE1  | 1:A:357:LEU:HD13 | 2.02                     | 0.60              |
| 1:G:56:ILE:HG22  | 1:G:129:ILE:HD11 | 1.84                     | 0.60              |
| 1:A:38:LEU:HD23  | 1:A:39:ILE:N     | 2.16                     | 0.59              |
| 1:A:39:ILE:HG23  | 1:A:47:GLU:CG    | 2.26                     | 0.59              |
| 1:G:371:MET:HG2  | 1:G:394:LEU:HD23 | 1.83                     | 0.59              |
| 1:A:53:LEU:HD12  | 1:A:326:VAL:CG2  | 2.33                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:113:ARG:CD   | 1:A:113:ARG:H    | 2.14                     | 0.59              |
| 1:G:200:ALA:HA   | 1:G:348:LEU:CD1  | 2.32                     | 0.59              |
| 1:G:348:LEU:O    | 1:G:348:LEU:HD23 | 2.03                     | 0.59              |
| 1:G:402:PHE:O    | 1:G:407:LYS:HE3  | 2.02                     | 0.59              |
| 1:A:170:ILE:O    | 1:A:313:LYS:HE2  | 2.02                     | 0.59              |
| 1:C:411:GLU:CD   | 1:C:411:GLU:H    | 2.11                     | 0.59              |
| 1:E:112:TRP:HZ3  | 1:E:124:GLN:HB2  | 1.67                     | 0.59              |
| 1:E:121:THR:N    | 1:E:151:PHE:CE2  | 2.71                     | 0.59              |
| 1:G:232:GLY:O    | 1:G:266:CYS:HB3  | 2.03                     | 0.59              |
| 1:A:113:ARG:H    | 1:A:113:ARG:NE   | 2.01                     | 0.59              |
| 1:E:120:THR:HB   | 1:E:151:PHE:CZ   | 2.37                     | 0.59              |
| 1:E:186:ASP:C    | 1:E:188:GLN:H    | 2.11                     | 0.59              |
| 1:E:267:PHE:CE2  | 1:E:300:LEU:HB2  | 2.37                     | 0.59              |
| 1:G:66:GLU:OE1   | 1:G:138:LYS:HD2  | 2.03                     | 0.59              |
| 1:A:46:PHE:HE1   | 1:A:162:THR:CB   | 2.16                     | 0.59              |
| 1:A:393:GLN:HG3  | 1:A:394:LEU:HD12 | 1.85                     | 0.59              |
| 1:C:379:LYS:HB3  | 1:C:380:PRO:CD   | 2.27                     | 0.59              |
| 1:E:84:MET:HE3   | 1:E:87:MET:CE    | 2.33                     | 0.59              |
| 1:G:84:MET:HE3   | 1:G:87:MET:CE    | 2.32                     | 0.59              |
| 1:A:335:ILE:HG23 | 1:A:342:PRO:HB3  | 1.85                     | 0.58              |
| 1:E:393:GLN:O    | 1:E:397:GLU:HG3  | 2.03                     | 0.58              |
| 1:G:67:VAL:HG12  | 1:G:320:ILE:O    | 2.03                     | 0.58              |
| 1:A:85:ASP:HB3   | 1:A:89:ARG:NH1   | 2.18                     | 0.58              |
| 1:E:196:TYR:OH   | 1:E:351:THR:HG21 | 2.02                     | 0.58              |
| 1:G:367:TYR:CD1  | 1:G:394:LEU:HB3  | 2.37                     | 0.58              |
| 1:E:204:THR:CG2  | 1:E:408:MET:HE3  | 2.33                     | 0.58              |
| 1:C:210:GLN:HE22 | 1:C:314:GLU:N    | 2.00                     | 0.58              |
| 1:E:172:SER:HB3  | 1:E:313:LYS:HB2  | 1.86                     | 0.58              |
| 1:G:197:GLY:HA3  | 1:G:260:CYS:SG   | 2.44                     | 0.58              |
| 1:E:120:THR:CA   | 1:E:151:PHE:HZ   | 2.17                     | 0.58              |
| 1:A:352:ALA:HA   | 1:A:408:MET:HB2  | 1.85                     | 0.58              |
| 1:A:396:GLU:HG3  | 1:A:397:GLU:N    | 2.17                     | 0.58              |
| 1:C:182:VAL:O    | 1:C:239:ARG:NH1  | 2.29                     | 0.58              |
| 1:E:269:LEU:CD1  | 1:E:270:PRO:HD2  | 2.31                     | 0.58              |
| 1:G:209:PHE:HB2  | 1:G:260:CYS:O    | 2.04                     | 0.58              |
| 1:A:111:SER:HA   | 1:A:113:ARG:HH12 | 1.68                     | 0.58              |
| 1:E:178:LEU:HD12 | 1:E:182:VAL:HG22 | 1.84                     | 0.58              |
| 1:A:38:LEU:C     | 1:A:38:LEU:CD2   | 2.77                     | 0.57              |
| 1:A:227:TYR:CE2  | 1:A:270:PRO:HB3  | 2.39                     | 0.57              |
| 1:A:243:SER:CB   | 1:E:401:LEU:HD13 | 2.34                     | 0.57              |
| 1:A:41:LYS:NZ    | 1:A:42:ASP:H     | 2.03                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:44:HIS:ND1   | 1:A:339:GLU:HA   | 2.19                     | 0.57              |
| 1:G:365:ASP:O    | 1:G:369:LYS:HD3  | 2.04                     | 0.57              |
| 1:G:221:PHE:N    | 1:G:222:PRO:HD3  | 2.19                     | 0.57              |
| 1:G:332:TYR:OH   | 1:G:351:THR:CG2  | 2.51                     | 0.57              |
| 1:A:316:ASN:HB3  | 1:A:406:LYS:CD   | 2.35                     | 0.57              |
| 1:E:107:LEU:HD11 | 1:E:282:PHE:HE1  | 1.68                     | 0.57              |
| 1:G:348:LEU:HD23 | 1:G:348:LEU:C    | 2.30                     | 0.57              |
| 1:G:376:GLY:HA3  | 1:G:377:GLY:C    | 2.29                     | 0.57              |
| 1:A:50:GLU:OE1   | 1:A:330:LYS:HE2  | 2.04                     | 0.57              |
| 1:A:154:GLN:HG2  | 1:A:155:SER:N    | 2.18                     | 0.57              |
| 1:A:162:THR:HG22 | 1:A:341:LEU:HD12 | 1.87                     | 0.57              |
| 1:A:165:ALA:HA   | 1:A:193:PHE:CE1  | 2.39                     | 0.57              |
| 1:E:194:THR:HA   | 1:E:260:CYS:SG   | 2.44                     | 0.57              |
| 1:A:258:HIS:CD2  | 1:A:264:ILE:HD12 | 2.40                     | 0.57              |
| 1:C:53:LEU:O     | 1:C:53:LEU:HD22  | 2.05                     | 0.57              |
| 1:E:80:LYS:HB2   | 2:E:3850:GDP:O2B | 2.04                     | 0.57              |
| 1:E:335:ILE:HD11 | 1:E:346:SER:C    | 2.30                     | 0.57              |
| 1:A:46:PHE:HE1   | 1:A:162:THR:OG1  | 1.87                     | 0.57              |
| 1:A:62:VAL:HG11  | 1:A:129:ILE:HD12 | 1.87                     | 0.57              |
| 1:A:242:VAL:HG23 | 1:A:247:HIS:NE2  | 2.20                     | 0.57              |
| 1:E:48:LEU:HD22  | 1:E:333:ILE:CG1  | 2.35                     | 0.57              |
| 1:E:121:THR:N    | 1:E:151:PHE:HE2  | 2.03                     | 0.57              |
| 1:C:367:TYR:HD1  | 1:C:394:LEU:HB3  | 1.70                     | 0.56              |
| 1:E:38:LEU:HD12  | 1:E:47:GLU:O     | 2.05                     | 0.56              |
| 1:E:72:VAL:HA    | 1:E:175:VAL:HG13 | 1.86                     | 0.56              |
| 1:C:105:GLU:HG3  | 1:C:106:PRO:HD2  | 1.87                     | 0.56              |
| 1:C:335:ILE:HG22 | 1:C:336:TYR:CD1  | 2.39                     | 0.56              |
| 1:G:286:LEU:HD22 | 1:G:294:ILE:CD1  | 2.36                     | 0.56              |
| 1:A:400:LYS:HA   | 1:A:403:ARG:CD   | 2.34                     | 0.56              |
| 1:E:52:ALA:O     | 1:E:56:ILE:HD12  | 2.05                     | 0.56              |
| 1:G:162:THR:HG23 | 1:G:341:LEU:HD21 | 1.86                     | 0.56              |
| 1:G:210:GLN:HE22 | 1:G:313:LYS:HD2  | 1.69                     | 0.56              |
| 1:A:247:HIS:ND1  | 1:A:251:GLN:HG2  | 2.20                     | 0.56              |
| 1:A:335:ILE:CD1  | 1:A:347:MET:HA   | 2.35                     | 0.56              |
| 1:C:425:ILE:C    | 1:C:427:GLU:H    | 2.12                     | 0.56              |
| 1:E:254:ARG:O    | 1:E:254:ARG:NE   | 2.38                     | 0.56              |
| 1:A:118:ARG:O    | 1:A:118:ARG:CG   | 2.52                     | 0.56              |
| 1:A:46:PHE:CE1   | 1:A:162:THR:OG1  | 2.56                     | 0.56              |
| 1:E:123:ILE:HG21 | 1:E:145:MET:HE3  | 1.88                     | 0.56              |
| 1:G:336:TYR:CE2  | 1:G:342:PRO:HG2  | 2.40                     | 0.56              |
| 1:A:258:HIS:HD2  | 1:A:264:ILE:HD12 | 1.70                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:347:MET:O    | 1:C:350:ALA:HB3  | 2.06                     | 0.56              |
| 1:E:379:LYS:HB2  | 1:E:380:PRO:CD   | 2.34                     | 0.56              |
| 1:A:343:HIS:O    | 1:A:344:PRO:C    | 2.47                     | 0.56              |
| 1:C:116:SER:OG   | 1:C:117:GLU:N    | 2.39                     | 0.56              |
| 1:E:46:PHE:CZ    | 1:E:162:THR:OG1  | 2.59                     | 0.56              |
| 1:A:53:LEU:CD1   | 1:A:326:VAL:HG23 | 2.36                     | 0.55              |
| 1:G:197:GLY:HA2  | 1:G:208:PRO:HG3  | 1.88                     | 0.55              |
| 1:A:251:GLN:HE22 | 1:E:400:LYS:CE   | 2.19                     | 0.55              |
| 1:A:243:SER:C    | 1:A:245:ASN:N    | 2.63                     | 0.55              |
| 1:C:315:ILE:HD13 | 1:C:328:TYR:CZ   | 2.41                     | 0.55              |
| 1:E:204:THR:O    | 1:E:205:PHE:HB2  | 2.05                     | 0.55              |
| 1:G:415:ARG:HG3  | 1:G:415:ARG:HH11 | 1.70                     | 0.55              |
| 1:A:111:SER:OG   | 1:A:113:ARG:HD2  | 2.07                     | 0.55              |
| 1:A:423:SER:O    | 1:A:427:GLU:HG3  | 2.07                     | 0.55              |
| 1:E:36:GLN:HG2   | 1:E:124:GLN:HE21 | 1.71                     | 0.55              |
| 1:G:319:LYS:N    | 1:G:319:LYS:HD2  | 2.21                     | 0.55              |
| 1:A:77:ARG:O     | 1:A:78:LYS:HD2   | 2.06                     | 0.55              |
| 1:C:335:ILE:HG23 | 1:C:342:PRO:HB3  | 1.89                     | 0.55              |
| 1:A:337:GLN:HE21 | 1:A:337:GLN:HA   | 1.71                     | 0.55              |
| 1:G:170:ILE:HD13 | 1:G:329:PHE:CZ   | 2.42                     | 0.55              |
| 1:E:56:ILE:CD1   | 1:E:125:ILE:HD11 | 2.29                     | 0.55              |
| 1:E:344:PRO:O    | 1:E:347:MET:HB2  | 2.06                     | 0.55              |
| 1:G:371:MET:O    | 1:G:375:CYS:HB3  | 2.07                     | 0.55              |
| 1:A:381:PHE:HD1  | 1:A:381:PHE:N    | 2.05                     | 0.55              |
| 1:E:71:SER:CB    | 1:E:174:GLN:HE22 | 2.20                     | 0.55              |
| 1:G:214:PHE:HD2  | 1:G:236:LEU:CD2  | 2.19                     | 0.55              |
| 1:G:321:THR:CG2  | 1:G:324:GLY:H    | 2.18                     | 0.55              |
| 1:G:402:PHE:CE2  | 1:G:407:LYS:HE2  | 2.42                     | 0.55              |
| 1:A:184:GLU:OE1  | 1:A:250:LEU:HD13 | 2.07                     | 0.54              |
| 1:A:249:GLU:CD   | 1:A:249:GLU:H    | 2.15                     | 0.54              |
| 1:A:375:CYS:SG   | 1:A:387:LEU:HD11 | 2.47                     | 0.54              |
| 1:E:301:ILE:HB   | 1:E:302:PRO:HD3  | 1.89                     | 0.54              |
| 1:A:153:SER:O    | 1:A:157:LEU:N    | 2.41                     | 0.54              |
| 1:C:313:LYS:HE3  | 1:C:315:ILE:HD11 | 1.90                     | 0.54              |
| 1:E:227:TYR:CE1  | 1:E:270:PRO:HB3  | 2.42                     | 0.54              |
| 1:G:191:GLN:HE21 | 1:G:191:GLN:HA   | 1.72                     | 0.54              |
| 1:A:85:ASP:CG    | 1:A:113:ARG:CZ   | 2.80                     | 0.54              |
| 1:A:318:ASN:CG   | 1:A:406:LYS:HZ3  | 2.15                     | 0.54              |
| 1:G:175:VAL:HG12 | 1:G:213:ILE:HD13 | 1.90                     | 0.54              |
| 1:E:86:PHE:CE1   | 1:E:89:ARG:NH1   | 2.76                     | 0.54              |
| 1:G:286:LEU:HD23 | 1:G:289:ILE:HD12 | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:178:LEU:HD13 | 1:A:182:VAL:HA   | 1.89                     | 0.54              |
| 1:C:382:LEU:HD11 | 1:C:386:ASP:HB2  | 1.89                     | 0.54              |
| 1:C:176:TYR:CZ   | 1:C:178:LEU:HD21 | 2.43                     | 0.54              |
| 1:E:335:ILE:HD11 | 1:E:346:SER:O    | 2.08                     | 0.54              |
| 1:G:169:MET:HE3  | 1:G:332:TYR:CZ   | 2.43                     | 0.54              |
| 1:A:337:GLN:HE21 | 1:A:337:GLN:CA   | 2.20                     | 0.54              |
| 1:E:97:VAL:O     | 1:E:98:ASP:CB    | 2.55                     | 0.54              |
| 1:A:41:LYS:HZ3   | 1:A:42:ASP:H     | 1.55                     | 0.54              |
| 1:A:247:HIS:CE1  | 1:A:251:GLN:HG2  | 2.43                     | 0.54              |
| 1:C:196:TYR:CG   | 1:C:347:MET:HE2  | 2.43                     | 0.54              |
| 1:G:73:ALA:HB2   | 1:G:147:THR:OG1  | 2.07                     | 0.54              |
| 1:G:147:THR:HG21 | 1:G:167:SER:CB   | 2.37                     | 0.54              |
| 1:G:319:LYS:C    | 1:G:320:ILE:HD12 | 2.32                     | 0.54              |
| 1:A:104:ASN:O    | 1:A:285:LYS:HE2  | 2.09                     | 0.53              |
| 1:E:332:TYR:OH   | 1:E:351:THR:HB   | 2.08                     | 0.53              |
| 1:G:344:PRO:HA   | 1:G:347:MET:HE2  | 1.89                     | 0.53              |
| 1:A:188:GLN:HE21 | 1:A:250:LEU:CD2  | 2.20                     | 0.53              |
| 1:C:335:ILE:CD1  | 1:C:347:MET:HA   | 2.35                     | 0.53              |
| 1:G:241:LYS:HA   | 1:G:241:LYS:CE   | 2.38                     | 0.53              |
| 1:C:187:LEU:HB2  | 1:C:250:LEU:HD22 | 1.90                     | 0.53              |
| 1:C:386:ASP:O    | 1:C:390:LYS:HB2  | 2.09                     | 0.53              |
| 1:G:190:LEU:HD23 | 1:G:257:ILE:CD1  | 2.34                     | 0.53              |
| 1:G:429:TYR:O    | 1:G:433:ILE:HG23 | 2.09                     | 0.53              |
| 1:A:243:SER:C    | 1:A:245:ASN:H    | 2.15                     | 0.53              |
| 1:E:270:PRO:O    | 1:E:293:PHE:HD1  | 1.90                     | 0.53              |
| 1:A:76:PHE:CE2   | 1:A:148:GLN:HB3  | 2.44                     | 0.53              |
| 1:A:279:ASN:C    | 1:A:279:ASN:ND2  | 2.67                     | 0.53              |
| 1:A:335:ILE:CG2  | 1:A:342:PRO:HG3  | 2.39                     | 0.53              |
| 1:E:164:PHE:CE1  | 1:E:176:TYR:CD2  | 2.97                     | 0.53              |
| 1:E:300:LEU:O    | 1:E:303:TRP:HB3  | 2.08                     | 0.53              |
| 1:G:313:LYS:HE3  | 1:G:315:ILE:HD11 | 1.91                     | 0.53              |
| 1:A:113:ARG:O    | 1:A:114:GLY:C    | 2.51                     | 0.53              |
| 1:A:247:HIS:CE1  | 1:A:251:GLN:CD   | 2.87                     | 0.53              |
| 1:A:381:PHE:N    | 1:A:381:PHE:CD1  | 2.76                     | 0.53              |
| 1:C:188:GLN:HG2  | 1:C:250:LEU:HD21 | 1.91                     | 0.53              |
| 1:G:222:PRO:HG3  | 1:G:227:TYR:CE2  | 2.43                     | 0.53              |
| 1:G:57:LEU:HD23  | 1:G:129:ILE:HD11 | 1.89                     | 0.52              |
| 1:A:336:TYR:C    | 1:A:337:GLN:HE21 | 2.16                     | 0.52              |
| 1:C:243:SER:C    | 1:C:245:ASN:H    | 2.17                     | 0.52              |
| 1:A:112:TRP:HB2  | 1:A:113:ARG:NH2  | 2.24                     | 0.52              |
| 1:A:228:GLY:HA2  | 1:A:267:PHE:CZ   | 2.45                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:335:ILE:HG22 | 1:E:336:TYR:N    | 2.23                     | 0.52              |
| 1:G:332:TYR:HE1  | 1:G:351:THR:HG22 | 1.72                     | 0.52              |
| 1:C:187:LEU:O    | 1:C:190:LEU:HB2  | 2.10                     | 0.52              |
| 1:A:62:VAL:HG21  | 1:A:129:ILE:HG21 | 1.92                     | 0.52              |
| 1:G:194:THR:HB   | 1:G:256:HIS:HB3  | 1.90                     | 0.52              |
| 1:A:301:ILE:HB   | 1:A:302:PRO:HD3  | 1.92                     | 0.52              |
| 1:C:193:PHE:C    | 1:C:195:GLU:H    | 2.18                     | 0.52              |
| 1:C:301:ILE:N    | 1:C:302:PRO:CD   | 2.72                     | 0.52              |
| 1:E:241:LYS:HA   | 1:E:241:LYS:CE   | 2.38                     | 0.52              |
| 1:A:82:PHE:O     | 1:A:85:ASP:HB2   | 2.10                     | 0.52              |
| 1:A:368:ASN:C    | 1:A:368:ASN:ND2  | 2.59                     | 0.52              |
| 1:G:104:ASN:HD22 | 1:G:287:LYS:HZ3  | 1.55                     | 0.52              |
| 1:A:48:LEU:HB2   | 1:A:333:ILE:HG12 | 1.91                     | 0.52              |
| 1:A:356:ASN:OD1  | 1:A:407:LYS:CG   | 2.58                     | 0.52              |
| 1:A:412:GLU:CD   | 1:A:412:GLU:N    | 2.60                     | 0.52              |
| 1:G:33:GLY:O     | 1:G:127:SER:HB3  | 2.09                     | 0.52              |
| 1:G:367:TYR:CE1  | 1:G:394:LEU:HB3  | 2.45                     | 0.52              |
| 1:A:315:ILE:HD13 | 1:A:320:ILE:HG12 | 1.92                     | 0.51              |
| 1:A:393:GLN:HA   | 1:A:396:GLU:HG2  | 1.91                     | 0.51              |
| 1:E:204:THR:HG21 | 1:E:408:MET:HE3  | 1.93                     | 0.51              |
| 1:E:220:SER:C    | 1:E:222:PRO:HD3  | 2.36                     | 0.51              |
| 1:G:68:VAL:HG22  | 1:G:311:ASP:O    | 2.10                     | 0.51              |
| 1:G:382:LEU:HD23 | 1:G:386:ASP:HB3  | 1.93                     | 0.51              |
| 1:C:95:GLU:HA    | 1:C:95:GLU:OE1   | 2.09                     | 0.51              |
| 1:C:401:LEU:O    | 1:C:401:LEU:HD12 | 2.10                     | 0.51              |
| 1:A:123:ILE:HG21 | 1:A:145:MET:HE3  | 1.91                     | 0.51              |
| 1:E:120:THR:CA   | 1:E:151:PHE:CZ   | 2.93                     | 0.51              |
| 1:C:57:LEU:HD22  | 1:C:322:CYS:HB3  | 1.91                     | 0.51              |
| 1:A:38:LEU:HD11  | 1:A:166:LEU:HD13 | 1.92                     | 0.51              |
| 1:C:165:ALA:HA   | 1:C:193:PHE:CZ   | 2.46                     | 0.51              |
| 1:E:184:GLU:O    | 1:E:188:GLN:HG2  | 2.10                     | 0.51              |
| 1:G:48:LEU:HB2   | 1:G:333:ILE:HG13 | 1.93                     | 0.51              |
| 1:G:394:LEU:C    | 1:G:397:GLU:HB3  | 2.35                     | 0.51              |
| 1:A:147:THR:CG2  | 1:A:163:VAL:HG13 | 2.41                     | 0.51              |
| 1:A:157:LEU:HD23 | 1:A:189:HIS:NE2  | 2.26                     | 0.51              |
| 1:G:271:HIS:ND1  | 1:G:272:PRO:HD2  | 2.26                     | 0.51              |
| 1:G:367:TYR:CE2  | 1:G:425:ILE:HG23 | 2.46                     | 0.51              |
| 1:A:370:LYS:O    | 1:A:373:GLU:HG3  | 2.10                     | 0.51              |
| 1:A:389:THR:HA   | 1:A:392:LEU:CD1  | 2.37                     | 0.51              |
| 1:C:343:HIS:HD2  | 1:C:345:LYS:N    | 2.04                     | 0.51              |
| 1:A:315:ILE:O    | 1:A:316:ASN:HB2  | 2.09                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:196:TYR:HB2  | 1:C:347:MET:CE   | 2.38                     | 0.51              |
| 1:E:370:LYS:HB3  | 1:E:394:LEU:HD21 | 1.93                     | 0.51              |
| 1:G:253:VAL:O    | 1:G:253:VAL:HG23 | 2.10                     | 0.51              |
| 1:G:381:PHE:HD2  | 1:G:382:LEU:N    | 2.09                     | 0.51              |
| 1:G:407:LYS:NZ   | 1:G:407:LYS:HB2  | 2.26                     | 0.51              |
| 1:A:71:SER:HB2   | 1:A:145:MET:HB2  | 1.93                     | 0.51              |
| 1:C:202:GLU:HB2  | 1:G:205:PHE:CE1  | 2.46                     | 0.51              |
| 1:E:94:GLN:HE21  | 1:E:94:GLN:N     | 2.07                     | 0.51              |
| 1:A:53:LEU:HD12  | 1:A:326:VAL:HG22 | 1.92                     | 0.50              |
| 1:A:222:PRO:HG3  | 1:A:227:TYR:CE1  | 2.46                     | 0.50              |
| 1:A:393:GLN:HG3  | 1:A:394:LEU:N    | 2.25                     | 0.50              |
| 1:C:194:THR:CG2  | 1:C:257:ILE:HD13 | 2.41                     | 0.50              |
| 1:A:60:GLU:HG3   | 1:A:61:ALA:N     | 2.25                     | 0.50              |
| 1:G:428:LEU:HD23 | 1:G:431:GLN:NE2  | 2.25                     | 0.50              |
| 1:A:41:LYS:HB2   | 1:A:45:SER:O     | 2.11                     | 0.50              |
| 1:A:300:LEU:O    | 1:A:303:TRP:HB3  | 2.12                     | 0.50              |
| 1:G:257:ILE:HG13 | 1:G:264:ILE:HD13 | 1.93                     | 0.50              |
| 1:C:56:ILE:HD12  | 1:C:125:ILE:HD11 | 1.94                     | 0.50              |
| 1:C:228:GLY:HA2  | 1:C:267:PHE:CE2  | 2.45                     | 0.50              |
| 1:G:84:MET:HA    | 1:G:87:MET:HG3   | 1.93                     | 0.50              |
| 1:G:163:VAL:HG12 | 1:G:164:PHE:N    | 2.25                     | 0.50              |
| 1:A:77:ARG:C     | 1:A:78:LYS:HD2   | 2.36                     | 0.50              |
| 1:A:302:PRO:O    | 1:A:306:SER:N    | 2.36                     | 0.50              |
| 1:C:411:GLU:HG2  | 1:C:412:GLU:HG2  | 1.92                     | 0.50              |
| 1:E:124:GLN:O    | 1:E:145:MET:HA   | 2.11                     | 0.50              |
| 1:C:96:SER:C     | 1:C:98:ASP:H     | 2.18                     | 0.50              |
| 1:C:269:LEU:HD12 | 1:C:270:PRO:CD   | 2.41                     | 0.50              |
| 1:C:247:HIS:HE1  | 1:C:254:ARG:NE   | 2.06                     | 0.50              |
| 1:A:117:GLU:HB2  | 1:A:119:GLU:N    | 2.27                     | 0.50              |
| 1:A:163:VAL:HG12 | 1:A:164:PHE:N    | 2.26                     | 0.50              |
| 1:C:210:GLN:NE2  | 1:C:314:GLU:N    | 2.60                     | 0.50              |
| 1:C:367:TYR:CD1  | 1:C:394:LEU:HB3  | 2.46                     | 0.50              |
| 1:A:402:PHE:O    | 1:A:405:VAL:HG13 | 2.12                     | 0.49              |
| 1:E:326:VAL:O    | 1:E:326:VAL:CG1  | 2.59                     | 0.49              |
| 1:G:343:HIS:HD2  | 1:G:345:LYS:H    | 1.60                     | 0.49              |
| 1:A:251:GLN:HE22 | 1:E:400:LYS:HE2  | 1.76                     | 0.49              |
| 1:C:195:GLU:HB3  | 1:C:344:PRO:HG3  | 1.94                     | 0.49              |
| 1:E:71:SER:CB    | 1:E:174:GLN:NE2  | 2.74                     | 0.49              |
| 1:G:305:LEU:O    | 1:G:310:LEU:HD11 | 2.11                     | 0.49              |
| 1:C:225:PHE:CE1  | 1:C:234:LYS:HB2  | 2.47                     | 0.49              |
| 1:G:84:MET:CE    | 1:G:112:TRP:CZ2  | 2.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:372:GLU:HA   | 1:G:376:GLY:O    | 2.12                     | 0.49              |
| 1:A:248:GLU:HB2  | 1:A:249:GLU:OE2  | 2.13                     | 0.49              |
| 1:C:201:MET:HA   | 1:C:206:LEU:O    | 2.11                     | 0.49              |
| 1:E:66:GLU:OE1   | 1:E:138:LYS:HD3  | 2.11                     | 0.49              |
| 1:E:388:GLN:O    | 1:E:388:GLN:HG3  | 2.12                     | 0.49              |
| 1:A:91:MET:HE1   | 1:A:132:ILE:HD11 | 1.95                     | 0.49              |
| 1:E:71:SER:HB3   | 1:E:174:GLN:HE22 | 1.78                     | 0.49              |
| 1:G:170:ILE:HD13 | 1:G:329:PHE:CE2  | 2.47                     | 0.49              |
| 1:A:407:LYS:HG2  | 1:A:414:SER:OG   | 2.12                     | 0.49              |
| 1:A:196:TYR:HA   | 1:A:344:PRO:HB3  | 1.95                     | 0.49              |
| 1:A:337:GLN:HA   | 1:A:337:GLN:NE2  | 2.28                     | 0.49              |
| 1:A:111:SER:HB2  | 1:A:113:ARG:HD2  | 1.93                     | 0.49              |
| 1:G:395:LYS:O    | 1:G:399:VAL:HG23 | 2.12                     | 0.49              |
| 1:E:35:VAL:HG11  | 1:E:56:ILE:HD11  | 1.95                     | 0.49              |
| 1:G:68:VAL:HG22  | 1:G:312:ILE:HA   | 1.94                     | 0.48              |
| 1:A:154:GLN:C    | 1:A:156:THR:N    | 2.70                     | 0.48              |
| 1:C:71:SER:HB2   | 1:C:145:MET:HE2  | 1.95                     | 0.48              |
| 1:C:272:PRO:HG3  | 2:C:3850:GDP:C6  | 2.48                     | 0.48              |
| 1:E:46:PHE:HD2   | 1:E:336:TYR:O    | 1.96                     | 0.48              |
| 1:G:360:VAL:HG23 | 1:G:402:PHE:HE1  | 1.78                     | 0.48              |
| 1:C:117:GLU:HA   | 1:C:118:ARG:C    | 2.39                     | 0.48              |
| 1:A:71:SER:OG    | 1:A:174:GLN:NE2  | 2.42                     | 0.48              |
| 1:A:314:GLU:OE2  | 1:A:319:LYS:NZ   | 2.47                     | 0.48              |
| 1:C:85:ASP:OD1   | 1:C:111:SER:HA   | 2.12                     | 0.48              |
| 1:C:280:PRO:HA   | 2:C:3850:GDP:O3' | 2.13                     | 0.48              |
| 1:C:367:TYR:CE2  | 1:C:425:ILE:HG23 | 2.47                     | 0.48              |
| 1:G:360:VAL:HG23 | 1:G:402:PHE:CE1  | 2.49                     | 0.48              |
| 1:A:232:GLY:O    | 1:A:266:CYS:HB3  | 2.13                     | 0.48              |
| 1:A:235:PHE:CZ   | 1:A:239:ARG:HG3  | 2.48                     | 0.48              |
| 1:A:316:ASN:C    | 1:A:406:LYS:HE2  | 2.34                     | 0.48              |
| 1:E:190:LEU:HD23 | 1:E:257:ILE:HD11 | 1.94                     | 0.48              |
| 1:G:381:PHE:C    | 1:G:381:PHE:HD2  | 2.21                     | 0.48              |
| 1:A:103:TYR:HA   | 1:A:286:LEU:HB3  | 1.95                     | 0.48              |
| 1:A:255:LYS:HD2  | 1:E:404:GLY:HA2  | 1.95                     | 0.48              |
| 1:C:193:PHE:C    | 1:C:195:GLU:N    | 2.70                     | 0.48              |
| 1:C:399:VAL:O    | 1:C:403:ARG:HG3  | 2.14                     | 0.48              |
| 1:E:72:VAL:HG22  | 1:E:175:VAL:CG1  | 2.44                     | 0.48              |
| 1:A:305:LEU:HA   | 1:A:310:LEU:CD1  | 2.44                     | 0.48              |
| 1:E:197:GLY:O    | 1:E:201:MET:HB2  | 2.14                     | 0.48              |
| 1:E:368:ASN:HB2  | 1:E:428:LEU:HD13 | 1.96                     | 0.48              |
| 1:G:411:GLU:CD   | 1:G:411:GLU:H    | 2.21                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:289:ILE:HB   | 1:A:294:ILE:HD11 | 1.96                     | 0.48              |
| 1:E:38:LEU:HD23  | 1:E:123:ILE:HG13 | 1.95                     | 0.48              |
| 1:E:64:ASP:CG    | 1:E:323:ARG:HH22 | 2.22                     | 0.48              |
| 1:E:343:HIS:O    | 1:E:344:PRO:C    | 2.54                     | 0.48              |
| 1:G:335:ILE:HG22 | 1:G:336:TYR:CD1  | 2.49                     | 0.48              |
| 1:A:247:HIS:HB2  | 1:A:250:LEU:HB2  | 1.96                     | 0.47              |
| 1:A:318:ASN:ND2  | 1:A:406:LYS:HZ3  | 2.11                     | 0.47              |
| 1:C:42:ASP:C     | 1:C:44:HIS:H     | 2.21                     | 0.47              |
| 1:E:239:ARG:HG2  | 1:E:239:ARG:NH1  | 2.29                     | 0.47              |
| 1:G:102:ASP:HB3  | 1:G:105:GLU:HB2  | 1.95                     | 0.47              |
| 1:A:112:TRP:N    | 1:A:113:ARG:CZ   | 2.74                     | 0.47              |
| 1:A:117:GLU:HA   | 1:A:118:ARG:CB   | 2.45                     | 0.47              |
| 1:C:35:VAL:HG11  | 1:C:56:ILE:HD11  | 1.96                     | 0.47              |
| 1:C:247:HIS:CG   | 1:C:250:LEU:HB2  | 2.50                     | 0.47              |
| 1:E:87:MET:HA    | 1:E:301:ILE:HD13 | 1.96                     | 0.47              |
| 1:G:371:MET:HE3  | 1:G:432:TYR:HD1  | 1.78                     | 0.47              |
| 1:A:158:ARG:HG2  | 1:A:158:ARG:H    | 1.46                     | 0.47              |
| 1:G:86:PHE:CD2   | 1:G:297:LEU:HD21 | 2.49                     | 0.47              |
| 1:G:394:LEU:CA   | 1:G:397:GLU:HB3  | 2.44                     | 0.47              |
| 1:A:199:LEU:HD22 | 1:A:199:LEU:HA   | 1.73                     | 0.47              |
| 1:E:335:ILE:HG23 | 1:E:342:PRO:HB3  | 1.96                     | 0.47              |
| 1:A:401:LEU:C    | 1:A:401:LEU:CD1  | 2.81                     | 0.47              |
| 1:G:367:TYR:CD2  | 1:G:367:TYR:O    | 2.68                     | 0.47              |
| 1:A:335:ILE:HD11 | 1:A:346:SER:O    | 2.14                     | 0.47              |
| 1:C:38:LEU:HD23  | 1:C:123:ILE:HG13 | 1.95                     | 0.47              |
| 1:E:100:VAL:HG21 | 1:E:298:LYS:HZ3  | 1.80                     | 0.47              |
| 1:E:169:MET:HB3  | 1:E:169:MET:HE3  | 1.66                     | 0.47              |
| 1:G:103:TYR:C    | 1:G:105:GLU:H    | 2.23                     | 0.47              |
| 1:A:46:PHE:CE1   | 1:A:336:TYR:HB3  | 2.50                     | 0.47              |
| 1:A:56:ILE:HD13  | 1:A:127:SER:HA   | 1.97                     | 0.47              |
| 1:A:222:PRO:HG3  | 1:A:227:TYR:CZ   | 2.50                     | 0.47              |
| 1:A:299:ILE:HG12 | 1:A:300:LEU:N    | 2.28                     | 0.47              |
| 1:C:239:ARG:HA   | 1:C:239:ARG:NE   | 2.29                     | 0.47              |
| 1:C:57:LEU:HD22  | 1:C:322:CYS:SG   | 2.55                     | 0.47              |
| 1:C:242:VAL:HG23 | 1:G:401:LEU:HD13 | 1.96                     | 0.47              |
| 1:E:43:ASP:O     | 1:E:44:HIS:HB2   | 2.14                     | 0.47              |
| 1:E:216:VAL:HB   | 1:E:268:LEU:HD12 | 1.97                     | 0.47              |
| 1:E:348:LEU:HD23 | 1:E:348:LEU:HA   | 1.65                     | 0.47              |
| 1:G:62:VAL:HG11  | 1:G:129:ILE:HD13 | 1.97                     | 0.47              |
| 1:G:86:PHE:CG    | 1:G:297:LEU:HD21 | 2.49                     | 0.47              |
| 1:A:242:VAL:CG2  | 1:A:243:SER:N    | 2.77                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:196:TYR:O    | 1:E:199:LEU:HD12 | 2.14                     | 0.47              |
| 1:E:204:THR:C    | 1:E:205:PHE:CD2  | 2.93                     | 0.47              |
| 1:A:316:ASN:ND2  | 1:A:408:MET:HG2  | 2.30                     | 0.46              |
| 1:E:120:THR:CB   | 1:E:151:PHE:CZ   | 2.97                     | 0.46              |
| 1:E:338:GLY:O    | 1:E:339:GLU:C    | 2.58                     | 0.46              |
| 1:A:72:VAL:HG13  | 1:A:175:VAL:CG2  | 2.39                     | 0.46              |
| 1:C:147:THR:HG22 | 1:C:163:VAL:HG12 | 1.97                     | 0.46              |
| 1:G:335:ILE:HD11 | 1:G:346:SER:C    | 2.41                     | 0.46              |
| 1:G:371:MET:HB3  | 1:G:432:TYR:CD1  | 2.50                     | 0.46              |
| 1:G:48:LEU:HD22  | 1:G:333:ILE:HG13 | 1.97                     | 0.46              |
| 1:C:196:TYR:HB3  | 1:C:347:MET:CE   | 2.45                     | 0.46              |
| 1:E:33:GLY:HA2   | 1:E:126:TRP:CH2  | 2.50                     | 0.46              |
| 1:E:240:LEU:HB3  | 1:E:254:ARG:CG   | 2.43                     | 0.46              |
| 1:E:343:HIS:HD2  | 1:E:344:PRO:CD   | 2.27                     | 0.46              |
| 1:A:117:GLU:HB2  | 1:A:119:GLU:CA   | 2.45                     | 0.46              |
| 1:C:210:GLN:HE22 | 1:C:313:LYS:HA   | 1.79                     | 0.46              |
| 1:E:72:VAL:HG22  | 1:E:175:VAL:HG11 | 1.97                     | 0.46              |
| 1:E:186:ASP:C    | 1:E:188:GLN:N    | 2.70                     | 0.46              |
| 1:E:50:GLU:OE1   | 1:E:330:LYS:HE3  | 2.15                     | 0.46              |
| 1:A:64:ASP:OD1   | 1:A:323:ARG:NH2  | 2.45                     | 0.46              |
| 1:A:316:ASN:HB3  | 1:A:406:LYS:CE   | 2.45                     | 0.46              |
| 1:A:319:LYS:C    | 1:A:320:ILE:HD12 | 2.41                     | 0.46              |
| 1:A:385:ASN:O    | 1:A:388:GLN:HB3  | 2.14                     | 0.46              |
| 1:C:247:HIS:CE1  | 1:C:254:ARG:NH2  | 2.84                     | 0.46              |
| 1:E:123:ILE:CG2  | 1:E:145:MET:HE3  | 2.45                     | 0.46              |
| 1:E:225:PHE:CG   | 1:E:235:PHE:HB2  | 2.51                     | 0.46              |
| 1:E:349:GLN:HE22 | 1:G:102:ASP:CG   | 2.24                     | 0.46              |
| 1:C:91:MET:HB3   | 1:C:130:PHE:CE2  | 2.51                     | 0.46              |
| 1:C:335:ILE:CG2  | 1:C:342:PRO:HG3  | 2.45                     | 0.46              |
| 1:E:71:SER:O     | 1:E:175:VAL:HG12 | 2.15                     | 0.46              |
| 1:E:195:GLU:O    | 1:E:199:LEU:HG   | 2.15                     | 0.46              |
| 1:E:335:ILE:CD1  | 1:E:347:MET:HA   | 2.46                     | 0.46              |
| 1:A:348:LEU:HD23 | 1:A:348:LEU:HA   | 1.79                     | 0.46              |
| 1:C:156:THR:HA   | 1:C:159:ASP:HB3  | 1.98                     | 0.46              |
| 1:G:201:MET:HG3  | 1:G:206:LEU:O    | 2.16                     | 0.46              |
| 1:C:433:ILE:O    | 1:C:436:ASN:HB3  | 2.15                     | 0.45              |
| 1:E:62:VAL:HG22  | 1:E:322:CYS:SG   | 2.56                     | 0.45              |
| 1:E:421:LEU:O    | 1:E:425:ILE:HG13 | 2.15                     | 0.45              |
| 1:A:158:ARG:C    | 1:A:162:THR:HG23 | 2.38                     | 0.45              |
| 1:C:335:ILE:HG22 | 1:C:336:TYR:CG   | 2.51                     | 0.45              |
| 1:C:336:TYR:O    | 1:C:337:GLN:CB   | 2.63                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:396:GLU:O    | 1:C:396:GLU:HG2  | 2.16                     | 0.45              |
| 1:E:333:ILE:O    | 1:E:333:ILE:HG23 | 2.16                     | 0.45              |
| 1:G:56:ILE:HD12  | 1:G:125:ILE:HD11 | 1.98                     | 0.45              |
| 1:A:87:MET:HE2   | 1:A:87:MET:HB3   | 1.78                     | 0.45              |
| 1:A:117:GLU:HA   | 1:A:118:ARG:C    | 2.41                     | 0.45              |
| 1:G:190:LEU:HD21 | 1:G:212:LEU:HD21 | 1.98                     | 0.45              |
| 1:G:425:ILE:HA   | 1:G:428:LEU:HB2  | 1.98                     | 0.45              |
| 1:A:39:ILE:HD12  | 1:A:40:VAL:H     | 1.82                     | 0.45              |
| 1:A:133:ASN:H    | 1:A:133:ASN:ND2  | 2.13                     | 0.45              |
| 1:C:84:MET:HE2   | 1:C:84:MET:HB3   | 1.72                     | 0.45              |
| 1:C:201:MET:HE2  | 1:C:201:MET:HB3  | 1.83                     | 0.45              |
| 1:G:416:ARG:HG2  | 1:G:416:ARG:HH11 | 1.82                     | 0.45              |
| 1:A:104:ASN:ND2  | 1:A:285:LYS:HE2  | 2.28                     | 0.45              |
| 1:A:390:LYS:HD3  | 1:A:390:LYS:HA   | 1.81                     | 0.45              |
| 1:C:210:GLN:NE2  | 1:C:313:LYS:HA   | 2.32                     | 0.45              |
| 1:E:341:LEU:HD12 | 1:E:341:LEU:N    | 2.31                     | 0.45              |
| 1:A:54:ASN:O     | 1:A:58:LEU:HB2   | 2.16                     | 0.45              |
| 1:E:191:GLN:HA   | 1:E:253:VAL:HG11 | 1.99                     | 0.45              |
| 1:A:271:HIS:ND1  | 1:A:272:PRO:HD2  | 2.31                     | 0.45              |
| 1:C:227:TYR:CZ   | 1:C:270:PRO:HB3  | 2.52                     | 0.45              |
| 1:E:170:ILE:HD13 | 1:E:329:PHE:CZ   | 2.52                     | 0.45              |
| 1:C:193:PHE:O    | 1:C:195:GLU:N    | 2.49                     | 0.45              |
| 1:C:305:LEU:HA   | 1:C:310:LEU:HD11 | 1.99                     | 0.45              |
| 1:E:237:GLU:C    | 1:E:239:ARG:H    | 2.25                     | 0.45              |
| 1:G:200:ALA:CA   | 1:G:348:LEU:HD12 | 2.43                     | 0.45              |
| 1:A:243:SER:HA   | 1:A:247:HIS:CE1  | 2.52                     | 0.45              |
| 1:C:57:LEU:HD22  | 1:C:322:CYS:CB   | 2.46                     | 0.45              |
| 1:C:429:TYR:O    | 1:C:433:ILE:HG23 | 2.16                     | 0.45              |
| 1:E:367:TYR:C    | 1:E:367:TYR:CD2  | 2.94                     | 0.45              |
| 1:E:372:GLU:HB3  | 1:E:432:TYR:OH   | 2.17                     | 0.45              |
| 1:A:53:LEU:HD12  | 1:A:326:VAL:HG23 | 1.98                     | 0.44              |
| 1:A:161:ALA:HB1  | 1:A:192:LEU:HD21 | 1.99                     | 0.44              |
| 1:A:183:GLN:O    | 1:A:186:ASP:N    | 2.50                     | 0.44              |
| 1:C:173:ILE:HG12 | 1:C:211:SER:OG   | 2.16                     | 0.44              |
| 1:G:34:PRO:HB3   | 1:G:112:TRP:CE3  | 2.52                     | 0.44              |
| 1:G:217:ARG:HD2  | 1:G:217:ARG:HA   | 1.54                     | 0.44              |
| 1:A:272:PRO:CG   | 2:A:3850:GDP:C6  | 3.00                     | 0.44              |
| 1:A:394:LEU:HA   | 1:A:397:GLU:HG2  | 1.99                     | 0.44              |
| 1:E:405:VAL:O    | 1:E:406:LYS:C    | 2.59                     | 0.44              |
| 1:C:94:GLN:HE21  | 1:C:94:GLN:HB2   | 1.51                     | 0.44              |
| 1:E:386:ASP:HA   | 1:E:389:THR:OG1  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:100:VAL:CG1  | 1:A:286:LEU:HD11 | 2.48                     | 0.44              |
| 1:A:314:GLU:O    | 1:A:314:GLU:HG2  | 2.17                     | 0.44              |
| 1:C:184:GLU:C    | 1:C:186:ASP:H    | 2.24                     | 0.44              |
| 1:E:49:ASP:O     | 1:E:50:GLU:C     | 2.60                     | 0.44              |
| 1:G:178:LEU:CD1  | 1:G:182:VAL:HG13 | 2.47                     | 0.44              |
| 1:A:85:ASP:HB3   | 1:A:89:ARG:HH12  | 1.82                     | 0.44              |
| 1:A:150:THR:C    | 1:A:151:PHE:CD1  | 2.89                     | 0.44              |
| 1:A:221:PHE:N    | 1:A:222:PRO:HD3  | 2.32                     | 0.44              |
| 1:A:241:LYS:HD3  | 1:A:241:LYS:C    | 2.37                     | 0.44              |
| 1:G:57:LEU:HB2   | 1:G:326:VAL:CG2  | 2.47                     | 0.44              |
| 1:A:154:GLN:HG3  | 1:C:105:GLU:OE1  | 2.17                     | 0.44              |
| 1:C:62:VAL:HG21  | 1:C:129:ILE:HG21 | 1.99                     | 0.44              |
| 1:E:76:PHE:CD2   | 1:E:77:ARG:HG3   | 2.53                     | 0.44              |
| 1:E:405:VAL:O    | 1:E:407:LYS:HG3  | 2.17                     | 0.44              |
| 1:A:146:ASP:OD2  | 1:A:146:ASP:C    | 2.60                     | 0.44              |
| 1:E:66:GLU:HB3   | 1:E:312:ILE:HG21 | 2.00                     | 0.44              |
| 1:E:84:MET:HE2   | 1:E:84:MET:HB3   | 1.70                     | 0.44              |
| 1:E:231:GLY:HA2  | 1:E:234:LYS:HG3  | 2.00                     | 0.44              |
| 1:G:112:TRP:CD1  | 1:G:112:TRP:N    | 2.86                     | 0.44              |
| 1:A:165:ALA:O    | 1:A:169:MET:HG2  | 2.18                     | 0.44              |
| 1:A:188:GLN:HE21 | 1:A:250:LEU:HD23 | 1.83                     | 0.44              |
| 1:A:279:ASN:ND2  | 1:A:280:PRO:N    | 2.66                     | 0.44              |
| 1:C:430:ILE:HA   | 1:C:433:ILE:HG12 | 2.00                     | 0.44              |
| 1:A:38:LEU:CD1   | 1:A:166:LEU:HD13 | 2.47                     | 0.44              |
| 1:A:244:GLY:C    | 1:A:246:GLN:N    | 2.70                     | 0.44              |
| 1:A:316:ASN:HD21 | 1:A:408:MET:HG2  | 1.82                     | 0.44              |
| 1:C:379:LYS:CB   | 1:C:380:PRO:CD   | 2.94                     | 0.44              |
| 1:A:433:ILE:HG22 | 1:A:437:ASP:OD1  | 2.18                     | 0.43              |
| 1:C:338:GLY:O    | 1:C:340:GLU:HA   | 2.18                     | 0.43              |
| 1:E:187:LEU:O    | 1:E:253:VAL:HG21 | 2.17                     | 0.43              |
| 1:G:185:ASP:O    | 1:G:188:GLN:HB2  | 2.18                     | 0.43              |
| 1:A:35:VAL:HG11  | 1:A:56:ILE:HD11  | 1.99                     | 0.43              |
| 1:A:46:PHE:HE1   | 1:A:162:THR:HB   | 1.83                     | 0.43              |
| 1:A:154:GLN:HA   | 1:A:157:LEU:CD1  | 2.49                     | 0.43              |
| 1:A:181:ASN:OD1  | 1:A:235:PHE:HZ   | 2.02                     | 0.43              |
| 1:A:185:ASP:OD2  | 1:A:185:ASP:N    | 2.42                     | 0.43              |
| 1:A:202:GLU:HA   | 1:E:205:PHE:CD1  | 2.53                     | 0.43              |
| 1:C:58:LEU:HD22  | 1:C:323:ARG:HG3  | 1.98                     | 0.43              |
| 1:E:40:VAL:HG13  | 1:E:46:PHE:CD1   | 2.53                     | 0.43              |
| 1:E:143:LEU:O    | 1:E:144:LEU:HD23 | 2.18                     | 0.43              |
| 1:E:170:ILE:HD13 | 1:E:329:PHE:CE2  | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:390:LYS:HD3  | 1:E:390:LYS:HA   | 1.86                     | 0.43              |
| 1:G:341:LEU:HA   | 1:G:342:PRO:HD3  | 1.73                     | 0.43              |
| 1:A:318:ASN:HD21 | 1:A:406:LYS:NZ   | 2.16                     | 0.43              |
| 1:C:326:VAL:CG1  | 1:C:330:LYS:HE3  | 2.48                     | 0.43              |
| 1:E:129:ILE:HG21 | 1:E:141:ALA:HB1  | 1.99                     | 0.43              |
| 1:G:124:GLN:HG3  | 1:G:146:ASP:HB3  | 1.99                     | 0.43              |
| 1:A:393:GLN:CG   | 1:A:394:LEU:HD12 | 2.47                     | 0.43              |
| 1:E:433:ILE:HA   | 1:E:436:ASN:CB   | 2.48                     | 0.43              |
| 1:G:102:ASP:HB3  | 1:G:105:GLU:CB   | 2.48                     | 0.43              |
| 1:G:134:LYS:HE2  | 1:G:134:LYS:HB3  | 1.76                     | 0.43              |
| 1:G:225:PHE:CD2  | 1:G:235:PHE:HD1  | 2.37                     | 0.43              |
| 1:A:49:ASP:OD1   | 1:A:49:ASP:C     | 2.62                     | 0.43              |
| 1:C:236:LEU:HG   | 1:C:240:LEU:HD12 | 2.00                     | 0.43              |
| 1:E:210:GLN:NE2  | 1:E:313:LYS:HA   | 2.33                     | 0.43              |
| 1:G:257:ILE:HG13 | 1:G:264:ILE:CD1  | 2.48                     | 0.43              |
| 1:A:81:SER:O     | 1:A:113:ARG:NH2  | 2.52                     | 0.43              |
| 1:A:337:GLN:CA   | 1:A:337:GLN:NE2  | 2.81                     | 0.43              |
| 1:C:86:PHE:CG    | 1:C:297:LEU:HD21 | 2.54                     | 0.43              |
| 1:C:95:GLU:O     | 1:C:96:SER:C     | 2.61                     | 0.43              |
| 1:E:240:LEU:C    | 1:E:254:ARG:HG3  | 2.44                     | 0.43              |
| 1:A:154:GLN:HA   | 1:A:157:LEU:HD12 | 2.01                     | 0.43              |
| 1:A:197:GLY:O    | 1:A:198:ARG:C    | 2.62                     | 0.43              |
| 1:A:323:ARG:CZ   | 1:A:323:ARG:HB3  | 2.48                     | 0.43              |
| 1:E:341:LEU:HB3  | 1:E:342:PRO:HD2  | 2.01                     | 0.43              |
| 1:E:393:GLN:CG   | 1:E:394:LEU:N    | 2.82                     | 0.43              |
| 1:A:315:ILE:N    | 1:A:315:ILE:CD1  | 2.81                     | 0.43              |
| 1:C:59:SER:O     | 1:C:63:ARG:HB2   | 2.19                     | 0.43              |
| 1:C:152:ASP:O    | 1:C:153:SER:HB2  | 2.19                     | 0.43              |
| 1:C:302:PRO:O    | 1:C:306:SER:N    | 2.41                     | 0.43              |
| 1:G:286:LEU:C    | 1:G:288:GLU:N    | 2.76                     | 0.43              |
| 1:A:76:PHE:CE2   | 1:A:119:GLU:HB2  | 2.54                     | 0.43              |
| 1:A:154:GLN:O    | 1:A:157:LEU:N    | 2.52                     | 0.43              |
| 1:C:177:ASN:OD1  | 1:C:217:ARG:NH1  | 2.48                     | 0.43              |
| 1:C:325:LEU:HD12 | 1:C:325:LEU:HA   | 1.78                     | 0.43              |
| 1:C:337:GLN:O    | 1:C:337:GLN:HG2  | 2.11                     | 0.43              |
| 1:E:254:ARG:O    | 1:E:257:ILE:HG22 | 2.18                     | 0.43              |
| 1:E:367:TYR:HD2  | 1:E:368:ASN:N    | 2.16                     | 0.43              |
| 1:E:433:ILE:HA   | 1:E:436:ASN:HB3  | 2.00                     | 0.43              |
| 1:G:310:LEU:HD12 | 1:G:310:LEU:H    | 1.83                     | 0.43              |
| 1:E:30:LYS:O     | 1:E:31:LYS:O     | 2.36                     | 0.43              |
| 1:E:369:LYS:HD2  | 1:E:369:LYS:HA   | 1.75                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:70:VAL:HB    | 1:G:144:LEU:HD23 | 2.01                     | 0.43              |
| 1:G:343:HIS:HD2  | 1:G:345:LYS:N    | 2.17                     | 0.43              |
| 1:A:241:LYS:HA   | 1:A:241:LYS:CE   | 2.40                     | 0.42              |
| 1:E:204:THR:O    | 1:E:205:PHE:CB   | 2.64                     | 0.42              |
| 1:E:222:PRO:HG3  | 1:E:227:TYR:CZ   | 2.54                     | 0.42              |
| 1:G:136:ASP:OD1  | 1:G:136:ASP:C    | 2.62                     | 0.42              |
| 1:A:62:VAL:HG21  | 1:A:129:ILE:CG2  | 2.49                     | 0.42              |
| 1:A:183:GLN:HG3  | 1:A:186:ASP:OD2  | 2.19                     | 0.42              |
| 1:A:393:GLN:O    | 1:A:396:GLU:HG2  | 2.20                     | 0.42              |
| 1:A:395:LYS:O    | 1:A:399:VAL:HG23 | 2.20                     | 0.42              |
| 2:C:3850:GDP:H8  | 2:C:3850:GDP:H2' | 1.76                     | 0.42              |
| 1:E:42:ASP:C     | 1:E:44:HIS:N     | 2.71                     | 0.42              |
| 1:E:120:THR:HB   | 1:E:151:PHE:HE2  | 1.78                     | 0.42              |
| 1:E:257:ILE:HD12 | 1:E:257:ILE:HA   | 1.83                     | 0.42              |
| 1:G:57:LEU:O     | 1:G:58:LEU:HD23  | 2.19                     | 0.42              |
| 1:G:191:GLN:O    | 1:G:192:LEU:C    | 2.63                     | 0.42              |
| 1:A:35:VAL:O     | 1:A:35:VAL:HG22  | 2.19                     | 0.42              |
| 1:C:46:PHE:HD2   | 1:C:337:GLN:HA   | 1.83                     | 0.42              |
| 1:E:34:PRO:HD3   | 1:E:126:TRP:HZ3  | 1.83                     | 0.42              |
| 1:G:286:LEU:O    | 1:G:288:GLU:N    | 2.52                     | 0.42              |
| 1:G:307:PRO:HA   | 1:G:310:LEU:HD13 | 2.01                     | 0.42              |
| 1:A:76:PHE:CE2   | 1:A:148:GLN:NE2  | 2.81                     | 0.42              |
| 1:A:162:THR:OG1  | 1:A:163:VAL:N    | 2.52                     | 0.42              |
| 1:A:166:LEU:O    | 1:A:167:SER:C    | 2.61                     | 0.42              |
| 1:C:196:TYR:HE2  | 1:C:348:LEU:HA   | 1.84                     | 0.42              |
| 1:C:196:TYR:OH   | 1:C:351:THR:HG21 | 2.19                     | 0.42              |
| 1:C:227:TYR:CE2  | 1:C:270:PRO:HB3  | 2.53                     | 0.42              |
| 1:C:235:PHE:O    | 1:C:239:ARG:HG2  | 2.20                     | 0.42              |
| 1:C:425:ILE:C    | 1:C:427:GLU:N    | 2.76                     | 0.42              |
| 1:E:89:ARG:NH2   | 1:E:107:LEU:HB3  | 2.33                     | 0.42              |
| 1:E:192:LEU:HD22 | 1:E:341:LEU:CD2  | 2.49                     | 0.42              |
| 1:E:293:PHE:O    | 1:E:297:LEU:HB2  | 2.19                     | 0.42              |
| 1:E:367:TYR:CD2  | 1:E:368:ASN:N    | 2.87                     | 0.42              |
| 1:G:272:PRO:HG3  | 2:G:3850:GDP:C6  | 2.54                     | 0.42              |
| 1:A:129:ILE:CG2  | 1:A:141:ALA:HB1  | 2.49                     | 0.42              |
| 1:A:242:VAL:HA   | 1:A:254:ARG:HD2  | 2.00                     | 0.42              |
| 1:A:257:ILE:HD12 | 1:A:257:ILE:HA   | 1.78                     | 0.42              |
| 1:E:143:LEU:HD12 | 1:E:144:LEU:N    | 2.34                     | 0.42              |
| 1:G:83:LEU:O     | 1:G:87:MET:HG3   | 2.18                     | 0.42              |
| 1:G:210:GLN:HE22 | 1:G:313:LYS:CD   | 2.31                     | 0.42              |
| 1:A:367:TYR:CD2  | 1:A:367:TYR:C    | 2.98                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:77:ARG:C     | 1:C:78:LYS:HD2   | 2.45                     | 0.42              |
| 1:C:181:ASN:OD1  | 1:C:182:VAL:N    | 2.52                     | 0.42              |
| 1:C:247:HIS:CD2  | 1:C:250:LEU:HD13 | 2.55                     | 0.42              |
| 1:C:393:GLN:O    | 1:C:397:GLU:HG3  | 2.20                     | 0.42              |
| 1:E:121:THR:H    | 1:E:151:PHE:HE2  | 1.66                     | 0.42              |
| 1:G:327:GLU:OE2  | 1:G:357:LEU:HB3  | 2.19                     | 0.42              |
| 1:A:245:ASN:HD21 | 1:E:397:GLU:HB3  | 1.85                     | 0.42              |
| 1:C:217:ARG:HH11 | 1:C:217:ARG:CG   | 2.33                     | 0.42              |
| 1:C:376:GLY:HA3  | 1:C:377:GLY:C    | 2.43                     | 0.42              |
| 1:E:57:LEU:HD23  | 1:E:57:LEU:HA    | 1.79                     | 0.42              |
| 1:E:195:GLU:HA   | 1:E:198:ARG:HB3  | 2.01                     | 0.42              |
| 1:E:217:ARG:HD2  | 1:E:217:ARG:HA   | 1.76                     | 0.42              |
| 1:G:281:ASN:O    | 1:G:281:ASN:CG   | 2.63                     | 0.42              |
| 1:A:315:ILE:O    | 1:A:316:ASN:CB   | 2.68                     | 0.42              |
| 1:E:35:VAL:HG12  | 1:E:125:ILE:O    | 2.20                     | 0.42              |
| 1:E:48:LEU:HB2   | 1:E:333:ILE:HG13 | 2.01                     | 0.42              |
| 1:A:76:PHE:CZ    | 1:A:119:GLU:HG2  | 2.55                     | 0.42              |
| 1:G:38:LEU:HB3   | 1:G:123:ILE:HB   | 2.02                     | 0.42              |
| 1:G:166:LEU:O    | 1:G:167:SER:C    | 2.62                     | 0.42              |
| 1:G:188:GLN:C    | 1:G:190:LEU:N    | 2.77                     | 0.42              |
| 1:A:41:LYS:HB3   | 1:A:43:ASP:OD1   | 2.19                     | 0.41              |
| 1:A:337:GLN:HE21 | 1:A:337:GLN:N    | 2.18                     | 0.41              |
| 1:C:181:ASN:OD1  | 1:C:239:ARG:NH1  | 2.53                     | 0.41              |
| 1:C:367:TYR:CZ   | 1:C:425:ILE:HG23 | 2.55                     | 0.41              |
| 1:G:162:THR:O    | 1:G:163:VAL:C    | 2.63                     | 0.41              |
| 1:G:187:LEU:N    | 1:G:187:LEU:HD23 | 2.35                     | 0.41              |
| 1:G:339:GLU:H    | 1:G:339:GLU:HG3  | 1.37                     | 0.41              |
| 1:A:147:THR:HG23 | 1:A:163:VAL:HG13 | 2.02                     | 0.41              |
| 1:A:162:THR:HG22 | 1:A:341:LEU:CD1  | 2.48                     | 0.41              |
| 1:E:272:PRO:HG3  | 2:E:3850:GDP:C6  | 2.56                     | 0.41              |
| 1:E:375:CYS:SG   | 1:E:375:CYS:O    | 2.78                     | 0.41              |
| 1:G:228:GLY:HA2  | 1:G:267:PHE:CZ   | 2.55                     | 0.41              |
| 1:G:270:PRO:CG   | 1:G:293:PHE:HA   | 2.48                     | 0.41              |
| 1:A:129:ILE:HG21 | 1:A:141:ALA:HB1  | 2.01                     | 0.41              |
| 1:A:133:ASN:ND2  | 1:A:133:ASN:N    | 2.67                     | 0.41              |
| 1:A:175:VAL:HG22 | 1:A:175:VAL:O    | 2.19                     | 0.41              |
| 1:C:97:VAL:O     | 1:C:97:VAL:CG1   | 2.67                     | 0.41              |
| 1:G:335:ILE:HD11 | 1:G:346:SER:O    | 2.21                     | 0.41              |
| 1:A:330:LYS:O    | 1:A:333:ILE:HG22 | 2.21                     | 0.41              |
| 1:C:107:LEU:CD2  | 1:C:286:LEU:HD12 | 2.51                     | 0.41              |
| 1:C:217:ARG:NH1  | 1:C:217:ARG:HG3  | 2.34                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:34:PRO:HB3   | 1:E:112:TRP:CE3  | 2.54                     | 0.41              |
| 1:E:50:GLU:CD    | 1:E:330:LYS:HE3  | 2.45                     | 0.41              |
| 1:E:353:GLU:HG2  | 1:E:417:TYR:OH   | 2.21                     | 0.41              |
| 1:G:42:ASP:C     | 1:G:44:HIS:H     | 2.27                     | 0.41              |
| 1:G:415:ARG:HH11 | 1:G:415:ARG:CG   | 2.33                     | 0.41              |
| 1:C:107:LEU:HD21 | 1:C:286:LEU:HB2  | 2.02                     | 0.41              |
| 1:C:314:GLU:HA   | 1:C:318:ASN:O    | 2.21                     | 0.41              |
| 1:C:391:HIS:CG   | 1:C:429:TYR:CD2  | 3.08                     | 0.41              |
| 1:G:196:TYR:HE2  | 1:G:348:LEU:HA   | 1.86                     | 0.41              |
| 1:A:85:ASP:CG    | 1:A:113:ARG:NH1  | 2.78                     | 0.41              |
| 1:E:402:PHE:CZ   | 1:E:407:LYS:HE3  | 2.55                     | 0.41              |
| 1:C:243:SER:OG   | 1:C:244:GLY:N    | 2.53                     | 0.41              |
| 1:C:243:SER:OG   | 1:C:245:ASN:OD1  | 2.39                     | 0.41              |
| 1:C:314:GLU:OE2  | 1:C:319:LYS:HE2  | 2.20                     | 0.41              |
| 1:G:386:ASP:C    | 1:G:388:GLN:H    | 2.28                     | 0.41              |
| 1:G:398:SER:HA   | 1:G:401:LEU:HB3  | 2.03                     | 0.41              |
| 1:A:121:THR:HA   | 1:A:148:GLN:O    | 2.21                     | 0.41              |
| 1:C:178:LEU:HD12 | 1:C:182:VAL:HG22 | 2.03                     | 0.41              |
| 1:E:183:GLN:O    | 1:E:184:GLU:C    | 2.64                     | 0.41              |
| 1:A:117:GLU:CA   | 1:A:118:ARG:C    | 2.94                     | 0.41              |
| 1:A:242:VAL:HG22 | 1:A:243:SER:N    | 2.34                     | 0.41              |
| 1:A:249:GLU:CD   | 1:A:249:GLU:N    | 2.78                     | 0.41              |
| 1:A:365:ASP:O    | 1:A:369:LYS:HD3  | 2.21                     | 0.41              |
| 1:C:70:VAL:HB    | 1:C:144:LEU:HD23 | 2.03                     | 0.41              |
| 1:C:96:SER:C     | 1:C:98:ASP:N     | 2.79                     | 0.41              |
| 1:C:228:GLY:HA2  | 1:C:267:PHE:CZ   | 2.56                     | 0.41              |
| 1:C:429:TYR:O    | 1:C:429:TYR:CG   | 2.74                     | 0.41              |
| 1:E:188:GLN:C    | 1:E:190:LEU:N    | 2.77                     | 0.41              |
| 1:G:417:TYR:HA   | 1:G:420:GLN:HG2  | 2.01                     | 0.41              |
| 1:C:68:VAL:HB    | 1:C:142:VAL:HG22 | 2.03                     | 0.41              |
| 1:C:94:GLN:OE1   | 1:C:132:ILE:HD11 | 2.21                     | 0.41              |
| 1:C:165:ALA:HA   | 1:C:193:PHE:CE1  | 2.56                     | 0.41              |
| 1:C:176:TYR:CE1  | 1:C:178:LEU:HD21 | 2.56                     | 0.41              |
| 1:C:356:ASN:C    | 1:C:358:ALA:N    | 2.79                     | 0.41              |
| 1:E:99:TRP:CE3   | 1:E:99:TRP:C     | 2.99                     | 0.41              |
| 1:E:355:ASN:CG   | 1:E:408:MET:HG3  | 2.46                     | 0.41              |
| 1:A:154:GLN:CG   | 1:A:155:SER:N    | 2.82                     | 0.40              |
| 1:A:399:VAL:HG13 | 1:A:418:LEU:HD21 | 2.02                     | 0.40              |
| 1:C:339:GLU:HA   | 1:C:340:GLU:HA   | 1.92                     | 0.40              |
| 1:C:355:ASN:HB3  | 1:C:408:MET:HG3  | 2.03                     | 0.40              |
| 1:C:418:LEU:HD23 | 1:C:418:LEU:O    | 2.20                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:241:LYS:CE   | 1:E:254:ARG:HD2  | 2.51                     | 0.40              |
| 1:G:160:SER:C    | 1:G:162:THR:N    | 2.77                     | 0.40              |
| 1:G:269:LEU:CD1  | 1:G:270:PRO:HD2  | 2.49                     | 0.40              |
| 1:C:225:PHE:HE1  | 1:C:234:LYS:HB2  | 1.86                     | 0.40              |
| 1:E:76:PHE:HB3   | 1:E:152:ASP:O    | 2.21                     | 0.40              |
| 1:A:111:SER:HB2  | 1:A:113:ARG:CD   | 2.51                     | 0.40              |
| 1:A:227:TYR:CD2  | 1:A:270:PRO:HG3  | 2.56                     | 0.40              |
| 1:C:320:ILE:N    | 1:C:320:ILE:HD12 | 2.36                     | 0.40              |
| 1:C:411:GLU:O    | 1:C:415:ARG:HG3  | 2.21                     | 0.40              |
| 1:G:63:ARG:HG2   | 1:G:64:ASP:OD2   | 2.20                     | 0.40              |
| 1:A:81:SER:OG    | 2:A:3850:GDP:O2B | 2.38                     | 0.40              |
| 1:A:247:HIS:HD2  | 1:A:254:ARG:HH11 | 1.67                     | 0.40              |
| 1:C:375:CYS:O    | 1:C:376:GLY:C    | 2.64                     | 0.40              |
| 1:G:34:PRO:HD3   | 1:G:126:TRP:CZ3  | 2.57                     | 0.40              |
| 1:G:236:LEU:CD2  | 1:G:266:CYS:HB2  | 2.49                     | 0.40              |
| 1:G:399:VAL:C    | 1:G:401:LEU:N    | 2.80                     | 0.40              |
| 1:C:46:PHE:CD2   | 1:C:46:PHE:N     | 2.88                     | 0.40              |
| 1:C:323:ARG:NH2  | 1:C:365:ASP:CG   | 2.80                     | 0.40              |
| 1:E:347:MET:O    | 1:E:351:THR:HG22 | 2.22                     | 0.40              |
| 1:G:144:LEU:HD23 | 1:G:144:LEU:HA   | 1.83                     | 0.40              |
| 1:G:178:LEU:HD22 | 1:G:186:ASP:OD2  | 2.20                     | 0.40              |
| 1:G:368:ASN:O    | 1:G:372:GLU:HG2  | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | A     | 409/447 (92%) | 371 (91%) | 36 (9%)  | 2 (0%)   | 24          | 59 |
| 1   | C     | 407/447 (91%) | 344 (84%) | 52 (13%) | 11 (3%)  | 4           | 20 |
| 1   | E     | 378/447 (85%) | 330 (87%) | 41 (11%) | 7 (2%)   | 6           | 28 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | G     | 376/447 (84%)   | 332 (88%)  | 35 (9%)   | 9 (2%)   | 4           | 23 |
| All | All   | 1570/1788 (88%) | 1377 (88%) | 164 (10%) | 29 (2%)  | 6           | 29 |

All (29) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 75  | ALA  |
| 1   | C     | 97  | VAL  |
| 1   | E     | 31  | LYS  |
| 1   | E     | 150 | THR  |
| 1   | C     | 63  | ARG  |
| 1   | C     | 380 | PRO  |
| 1   | C     | 381 | PHE  |
| 1   | E     | 284 | GLY  |
| 1   | E     | 380 | PRO  |
| 1   | G     | 63  | ARG  |
| 1   | G     | 197 | GLY  |
| 1   | G     | 380 | PRO  |
| 1   | A     | 243 | SER  |
| 1   | C     | 153 | SER  |
| 1   | C     | 194 | THR  |
| 1   | C     | 426 | ASP  |
| 1   | E     | 76  | PHE  |
| 1   | G     | 287 | LYS  |
| 1   | G     | 163 | VAL  |
| 1   | G     | 196 | TYR  |
| 1   | G     | 210 | GLN  |
| 1   | A     | 210 | GLN  |
| 1   | C     | 210 | GLN  |
| 1   | C     | 96  | SER  |
| 1   | C     | 437 | ASP  |
| 1   | E     | 43  | ASP  |
| 1   | E     | 238 | LYS  |
| 1   | G     | 104 | ASN  |
| 1   | G     | 379 | LYS  |

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

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 364/395 (92%)   | 268 (74%)  | 96 (26%)  | 0           | 2  |
| 1   | C     | 362/395 (92%)   | 310 (86%)  | 52 (14%)  | 3           | 14 |
| 1   | E     | 342/395 (87%)   | 281 (82%)  | 61 (18%)  | 2           | 9  |
| 1   | G     | 340/395 (86%)   | 290 (85%)  | 50 (15%)  | 3           | 14 |
| All | All   | 1408/1580 (89%) | 1149 (82%) | 259 (18%) | 1           | 8  |

All (259) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 35  | VAL  |
| 1   | A     | 36  | GLN  |
| 1   | A     | 38  | LEU  |
| 1   | A     | 39  | ILE  |
| 1   | A     | 40  | VAL  |
| 1   | A     | 41  | LYS  |
| 1   | A     | 44  | HIS  |
| 1   | A     | 46  | PHE  |
| 1   | A     | 51  | THR  |
| 1   | A     | 53  | LEU  |
| 1   | A     | 56  | ILE  |
| 1   | A     | 59  | SER  |
| 1   | A     | 60  | GLU  |
| 1   | A     | 62  | VAL  |
| 1   | A     | 71  | SER  |
| 1   | A     | 72  | VAL  |
| 1   | A     | 78  | LYS  |
| 1   | A     | 81  | SER  |
| 1   | A     | 93  | ASN  |
| 1   | A     | 94  | GLN  |
| 1   | A     | 95  | GLU  |
| 1   | A     | 96  | SER  |
| 1   | A     | 100 | VAL  |
| 1   | A     | 104 | ASN  |
| 1   | A     | 111 | SER  |
| 1   | A     | 113 | ARG  |
| 1   | A     | 117 | GLU  |
| 1   | A     | 118 | ARG  |
| 1   | A     | 131 | LEU  |
| 1   | A     | 133 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 150 | THR  |
| 1   | A     | 154 | GLN  |
| 1   | A     | 157 | LEU  |
| 1   | A     | 158 | ARG  |
| 1   | A     | 159 | ASP  |
| 1   | A     | 163 | VAL  |
| 1   | A     | 170 | ILE  |
| 1   | A     | 175 | VAL  |
| 1   | A     | 180 | GLN  |
| 1   | A     | 183 | GLN  |
| 1   | A     | 185 | ASP  |
| 1   | A     | 190 | LEU  |
| 1   | A     | 192 | LEU  |
| 1   | A     | 199 | LEU  |
| 1   | A     | 203 | GLU  |
| 1   | A     | 204 | THR  |
| 1   | A     | 210 | GLN  |
| 1   | A     | 241 | LYS  |
| 1   | A     | 242 | VAL  |
| 1   | A     | 247 | HIS  |
| 1   | A     | 248 | GLU  |
| 1   | A     | 249 | GLU  |
| 1   | A     | 257 | ILE  |
| 1   | A     | 262 | THR  |
| 1   | A     | 265 | SER  |
| 1   | A     | 268 | LEU  |
| 1   | A     | 276 | VAL  |
| 1   | A     | 279 | ASN  |
| 1   | A     | 286 | LEU  |
| 1   | A     | 287 | LYS  |
| 1   | A     | 288 | GLU  |
| 1   | A     | 299 | ILE  |
| 1   | A     | 305 | LEU  |
| 1   | A     | 308 | GLU  |
| 1   | A     | 310 | LEU  |
| 1   | A     | 314 | GLU  |
| 1   | A     | 315 | ILE  |
| 1   | A     | 319 | LYS  |
| 1   | A     | 321 | THR  |
| 1   | A     | 326 | VAL  |
| 1   | A     | 335 | ILE  |
| 1   | A     | 337 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 340 | GLU  |
| 1   | A     | 341 | LEU  |
| 1   | A     | 346 | SER  |
| 1   | A     | 348 | LEU  |
| 1   | A     | 368 | ASN  |
| 1   | A     | 371 | MET  |
| 1   | A     | 373 | GLU  |
| 1   | A     | 381 | PHE  |
| 1   | A     | 382 | LEU  |
| 1   | A     | 392 | LEU  |
| 1   | A     | 393 | GLN  |
| 1   | A     | 401 | LEU  |
| 1   | A     | 403 | ARG  |
| 1   | A     | 405 | VAL  |
| 1   | A     | 406 | LYS  |
| 1   | A     | 408 | MET  |
| 1   | A     | 411 | GLU  |
| 1   | A     | 412 | GLU  |
| 1   | A     | 414 | SER  |
| 1   | A     | 416 | ARG  |
| 1   | A     | 418 | LEU  |
| 1   | A     | 428 | LEU  |
| 1   | A     | 431 | GLN  |
| 1   | A     | 433 | ILE  |
| 1   | C     | 35  | VAL  |
| 1   | C     | 37  | VAL  |
| 1   | C     | 53  | LEU  |
| 1   | C     | 65  | LYS  |
| 1   | C     | 72  | VAL  |
| 1   | C     | 84  | MET  |
| 1   | C     | 89  | ARG  |
| 1   | C     | 94  | GLN  |
| 1   | C     | 97  | VAL  |
| 1   | C     | 98  | ASP  |
| 1   | C     | 100 | VAL  |
| 1   | C     | 102 | ASP  |
| 1   | C     | 113 | ARG  |
| 1   | C     | 121 | THR  |
| 1   | C     | 140 | VAL  |
| 1   | C     | 154 | GLN  |
| 1   | C     | 162 | THR  |
| 1   | C     | 166 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 170 | ILE  |
| 1   | C     | 175 | VAL  |
| 1   | C     | 183 | GLN  |
| 1   | C     | 190 | LEU  |
| 1   | C     | 192 | LEU  |
| 1   | C     | 195 | GLU  |
| 1   | C     | 198 | ARG  |
| 1   | C     | 217 | ARG  |
| 1   | C     | 226 | SER  |
| 1   | C     | 247 | HIS  |
| 1   | C     | 249 | GLU  |
| 1   | C     | 253 | VAL  |
| 1   | C     | 257 | ILE  |
| 1   | C     | 268 | LEU  |
| 1   | C     | 294 | ILE  |
| 1   | C     | 305 | LEU  |
| 1   | C     | 333 | ILE  |
| 1   | C     | 335 | ILE  |
| 1   | C     | 337 | GLN  |
| 1   | C     | 346 | SER  |
| 1   | C     | 348 | LEU  |
| 1   | C     | 351 | THR  |
| 1   | C     | 357 | LEU  |
| 1   | C     | 360 | VAL  |
| 1   | C     | 366 | THR  |
| 1   | C     | 371 | MET  |
| 1   | C     | 381 | PHE  |
| 1   | C     | 391 | HIS  |
| 1   | C     | 392 | LEU  |
| 1   | C     | 405 | VAL  |
| 1   | C     | 407 | LYS  |
| 1   | C     | 408 | MET  |
| 1   | C     | 411 | GLU  |
| 1   | C     | 437 | ASP  |
| 1   | E     | 35  | VAL  |
| 1   | E     | 37  | VAL  |
| 1   | E     | 43  | ASP  |
| 1   | E     | 44  | HIS  |
| 1   | E     | 47  | GLU  |
| 1   | E     | 51  | THR  |
| 1   | E     | 55  | ARG  |
| 1   | E     | 56  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 65  | LYS  |
| 1   | E     | 78  | LYS  |
| 1   | E     | 94  | GLN  |
| 1   | E     | 99  | TRP  |
| 1   | E     | 100 | VAL  |
| 1   | E     | 107 | LEU  |
| 1   | E     | 108 | THR  |
| 1   | E     | 121 | THR  |
| 1   | E     | 123 | ILE  |
| 1   | E     | 125 | ILE  |
| 1   | E     | 132 | ILE  |
| 1   | E     | 143 | LEU  |
| 1   | E     | 162 | THR  |
| 1   | E     | 163 | VAL  |
| 1   | E     | 192 | LEU  |
| 1   | E     | 199 | LEU  |
| 1   | E     | 201 | MET  |
| 1   | E     | 203 | GLU  |
| 1   | E     | 230 | ASP  |
| 1   | E     | 241 | LYS  |
| 1   | E     | 254 | ARG  |
| 1   | E     | 265 | SER  |
| 1   | E     | 268 | LEU  |
| 1   | E     | 279 | ASN  |
| 1   | E     | 299 | ILE  |
| 1   | E     | 312 | ILE  |
| 1   | E     | 320 | ILE  |
| 1   | E     | 326 | VAL  |
| 1   | E     | 333 | ILE  |
| 1   | E     | 335 | ILE  |
| 1   | E     | 346 | SER  |
| 1   | E     | 348 | LEU  |
| 1   | E     | 351 | THR  |
| 1   | E     | 357 | LEU  |
| 1   | E     | 362 | THR  |
| 1   | E     | 369 | LYS  |
| 1   | E     | 374 | ILE  |
| 1   | E     | 385 | ASN  |
| 1   | E     | 387 | LEU  |
| 1   | E     | 388 | GLN  |
| 1   | E     | 389 | THR  |
| 1   | E     | 390 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 394 | LEU  |
| 1   | E     | 396 | GLU  |
| 1   | E     | 400 | LYS  |
| 1   | E     | 401 | LEU  |
| 1   | E     | 405 | VAL  |
| 1   | E     | 406 | LYS  |
| 1   | E     | 412 | GLU  |
| 1   | E     | 416 | ARG  |
| 1   | E     | 423 | SER  |
| 1   | E     | 430 | ILE  |
| 1   | E     | 431 | GLN  |
| 1   | G     | 35  | VAL  |
| 1   | G     | 39  | ILE  |
| 1   | G     | 43  | ASP  |
| 1   | G     | 48  | LEU  |
| 1   | G     | 65  | LYS  |
| 1   | G     | 96  | SER  |
| 1   | G     | 97  | VAL  |
| 1   | G     | 121 | THR  |
| 1   | G     | 124 | GLN  |
| 1   | G     | 125 | ILE  |
| 1   | G     | 127 | SER  |
| 1   | G     | 147 | THR  |
| 1   | G     | 148 | GLN  |
| 1   | G     | 160 | SER  |
| 1   | G     | 175 | VAL  |
| 1   | G     | 181 | ASN  |
| 1   | G     | 182 | VAL  |
| 1   | G     | 183 | GLN  |
| 1   | G     | 185 | ASP  |
| 1   | G     | 191 | GLN  |
| 1   | G     | 199 | LEU  |
| 1   | G     | 203 | GLU  |
| 1   | G     | 213 | ILE  |
| 1   | G     | 226 | SER  |
| 1   | G     | 241 | LYS  |
| 1   | G     | 254 | ARG  |
| 1   | G     | 268 | LEU  |
| 1   | G     | 279 | ASN  |
| 1   | G     | 287 | LYS  |
| 1   | G     | 299 | ILE  |
| 1   | G     | 333 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 335 | ILE  |
| 1   | G     | 339 | GLU  |
| 1   | G     | 341 | LEU  |
| 1   | G     | 349 | GLN  |
| 1   | G     | 360 | VAL  |
| 1   | G     | 366 | THR  |
| 1   | G     | 382 | LEU  |
| 1   | G     | 386 | ASP  |
| 1   | G     | 394 | LEU  |
| 1   | G     | 397 | GLU  |
| 1   | G     | 401 | LEU  |
| 1   | G     | 405 | VAL  |
| 1   | G     | 407 | LYS  |
| 1   | G     | 415 | ARG  |
| 1   | G     | 416 | ARG  |
| 1   | G     | 418 | LEU  |
| 1   | G     | 420 | GLN  |
| 1   | G     | 428 | LEU  |
| 1   | G     | 431 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 104 | ASN  |
| 1   | A     | 148 | GLN  |
| 1   | A     | 154 | GLN  |
| 1   | A     | 174 | GLN  |
| 1   | A     | 188 | GLN  |
| 1   | A     | 251 | GLN  |
| 1   | A     | 252 | ASN  |
| 1   | A     | 256 | HIS  |
| 1   | A     | 258 | HIS  |
| 1   | A     | 279 | ASN  |
| 1   | A     | 318 | ASN  |
| 1   | A     | 337 | GLN  |
| 1   | A     | 368 | ASN  |
| 1   | A     | 419 | GLN  |
| 1   | A     | 436 | ASN  |
| 1   | C     | 124 | GLN  |
| 1   | C     | 183 | GLN  |
| 1   | C     | 188 | GLN  |
| 1   | C     | 191 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 210 | GLN  |
| 1   | C     | 245 | ASN  |
| 1   | C     | 247 | HIS  |
| 1   | C     | 343 | HIS  |
| 1   | C     | 368 | ASN  |
| 1   | C     | 388 | GLN  |
| 1   | C     | 393 | GLN  |
| 1   | C     | 419 | GLN  |
| 1   | C     | 436 | ASN  |
| 1   | E     | 93  | ASN  |
| 1   | E     | 94  | GLN  |
| 1   | E     | 124 | GLN  |
| 1   | E     | 133 | ASN  |
| 1   | E     | 174 | GLN  |
| 1   | E     | 189 | HIS  |
| 1   | E     | 210 | GLN  |
| 1   | E     | 256 | HIS  |
| 1   | E     | 263 | ASN  |
| 1   | E     | 318 | ASN  |
| 1   | E     | 343 | HIS  |
| 1   | E     | 349 | GLN  |
| 1   | E     | 419 | GLN  |
| 1   | E     | 420 | GLN  |
| 1   | E     | 436 | ASN  |
| 1   | G     | 94  | GLN  |
| 1   | G     | 104 | ASN  |
| 1   | G     | 124 | GLN  |
| 1   | G     | 133 | ASN  |
| 1   | G     | 174 | GLN  |
| 1   | G     | 191 | GLN  |
| 1   | G     | 210 | GLN  |
| 1   | G     | 258 | HIS  |
| 1   | G     | 263 | ASN  |
| 1   | G     | 279 | ASN  |
| 1   | G     | 318 | ASN  |
| 1   | G     | 343 | HIS  |
| 1   | G     | 419 | GLN  |
| 1   | G     | 431 | 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 ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | GDP  | C     | 3850 | -    | 29,30,30     | 1.15 | 3 (10%)  | 45,47,47    | 1.83 | 9 (20%)  |
| 2   | GDP  | A     | 3850 | 3    | 29,30,30     | 1.19 | 3 (10%)  | 45,47,47    | 1.81 | 6 (13%)  |
| 2   | GDP  | G     | 3850 | -    | 29,30,30     | 1.25 | 3 (10%)  | 45,47,47    | 1.75 | 6 (13%)  |
| 2   | GDP  | E     | 3850 | -    | 29,30,30     | 1.26 | 3 (10%)  | 45,47,47    | 1.78 | 7 (15%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | GDP  | C     | 3850 | -    | -       | 6/16/32/32 | 0/3/3/3 |
| 2   | GDP  | A     | 3850 | 3    | -       | 1/16/32/32 | 0/3/3/3 |
| 2   | GDP  | G     | 3850 | -    | -       | 3/16/32/32 | 0/3/3/3 |
| 2   | GDP  | E     | 3850 | -    | -       | 6/16/32/32 | 0/3/3/3 |

All (12) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2   | A     | 3850 | GDP  | C5-C4 | 3.52 | 1.48        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2   | E     | 3850 | GDP  | C5-C4  | 3.42  | 1.48        | 1.38     |
| 2   | C     | 3850 | GDP  | C5-C4  | 3.27  | 1.47        | 1.38     |
| 2   | G     | 3850 | GDP  | C6-N1  | -3.17 | 1.32        | 1.38     |
| 2   | E     | 3850 | GDP  | C6-N1  | -2.96 | 1.33        | 1.38     |
| 2   | G     | 3850 | GDP  | C5-C4  | 2.93  | 1.46        | 1.38     |
| 2   | C     | 3850 | GDP  | C6-N1  | -2.79 | 1.33        | 1.38     |
| 2   | A     | 3850 | GDP  | C6-N1  | -2.45 | 1.34        | 1.38     |
| 2   | G     | 3850 | GDP  | C5-N7  | -2.41 | 1.34        | 1.39     |
| 2   | A     | 3850 | GDP  | C5-N7  | -2.41 | 1.34        | 1.39     |
| 2   | C     | 3850 | GDP  | C5-N7  | -2.24 | 1.34        | 1.39     |
| 2   | E     | 3850 | GDP  | PA-O3A | 2.09  | 1.61        | 1.59     |

All (28) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | C     | 3850 | GDP  | C5-C4-N3    | -6.46 | 118.12      | 128.39   |
| 2   | A     | 3850 | GDP  | C5-C4-N3    | -6.44 | 118.15      | 128.39   |
| 2   | G     | 3850 | GDP  | C5-C4-N3    | -6.21 | 118.51      | 128.39   |
| 2   | E     | 3850 | GDP  | C5-C4-N3    | -6.08 | 118.71      | 128.39   |
| 2   | A     | 3850 | GDP  | C2-N3-C4    | 4.85  | 120.65      | 112.30   |
| 2   | C     | 3850 | GDP  | N9-C4-N3    | 4.76  | 135.47      | 125.95   |
| 2   | C     | 3850 | GDP  | C2-N3-C4    | 4.70  | 120.40      | 112.30   |
| 2   | A     | 3850 | GDP  | N9-C4-N3    | 4.52  | 134.98      | 125.95   |
| 2   | G     | 3850 | GDP  | C2-N3-C4    | 4.49  | 120.04      | 112.30   |
| 2   | G     | 3850 | GDP  | N9-C4-N3    | 4.47  | 134.90      | 125.95   |
| 2   | E     | 3850 | GDP  | C2-N3-C4    | 4.39  | 119.85      | 112.30   |
| 2   | E     | 3850 | GDP  | N9-C4-N3    | 4.30  | 134.54      | 125.95   |
| 2   | E     | 3850 | GDP  | C6-C5-N7    | 3.54  | 136.73      | 130.29   |
| 2   | C     | 3850 | GDP  | C6-C5-N7    | 3.08  | 135.89      | 130.29   |
| 2   | E     | 3850 | GDP  | C4-C5-N7    | -3.06 | 105.83      | 110.67   |
| 2   | A     | 3850 | GDP  | C6-C5-N7    | 3.01  | 135.77      | 130.29   |
| 2   | G     | 3850 | GDP  | C6-C5-N7    | 2.95  | 135.66      | 130.29   |
| 2   | G     | 3850 | GDP  | C4-C5-N7    | -2.80 | 106.23      | 110.67   |
| 2   | C     | 3850 | GDP  | C4-C5-N7    | -2.78 | 106.27      | 110.67   |
| 2   | A     | 3850 | GDP  | C4-C5-N7    | -2.74 | 106.33      | 110.67   |
| 2   | E     | 3850 | GDP  | O3B-PB-O3A  | 2.56  | 113.21      | 104.64   |
| 2   | C     | 3850 | GDP  | O3B-PB-O3A  | 2.29  | 112.31      | 104.64   |
| 2   | C     | 3850 | GDP  | C2-N1-C6    | -2.25 | 121.03      | 125.11   |
| 2   | G     | 3850 | GDP  | O3B-PB-O3A  | 2.24  | 112.16      | 104.64   |
| 2   | E     | 3850 | GDP  | C8-N7-C5    | 2.09  | 107.99      | 104.26   |
| 2   | A     | 3850 | GDP  | C5'-C4'-C3' | -2.09 | 107.71      | 115.21   |
| 2   | C     | 3850 | GDP  | C8-N7-C5    | 2.06  | 107.94      | 104.26   |

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| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 2   | C     | 3850 | GDP  | C5-C6-N1 | 2.05 | 118.46      | 113.25   |

There are no chirality outliers.

All (16) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 2   | C     | 3850 | GDP  | C5'-O5'-PA-O1A |
| 2   | E     | 3850 | GDP  | PA-O3A-PB-O3B  |
| 2   | E     | 3850 | GDP  | C5'-O5'-PA-O3A |
| 2   | E     | 3850 | GDP  | C5'-O5'-PA-O1A |
| 2   | E     | 3850 | GDP  | C5'-O5'-PA-O2A |
| 2   | G     | 3850 | GDP  | C5'-O5'-PA-O3A |
| 2   | G     | 3850 | GDP  | C5'-O5'-PA-O1A |
| 2   | C     | 3850 | GDP  | C5'-O5'-PA-O3A |
| 2   | C     | 3850 | GDP  | C5'-O5'-PA-O2A |
| 2   | G     | 3850 | GDP  | C5'-O5'-PA-O2A |
| 2   | C     | 3850 | GDP  | PA-O3A-PB-O1B  |
| 2   | E     | 3850 | GDP  | PA-O3A-PB-O2B  |
| 2   | C     | 3850 | GDP  | PB-O3A-PA-O1A  |
| 2   | C     | 3850 | GDP  | PB-O3A-PA-O2A  |
| 2   | E     | 3850 | GDP  | PB-O3A-PA-O2A  |
| 2   | A     | 3850 | GDP  | PB-O3A-PA-O2A  |

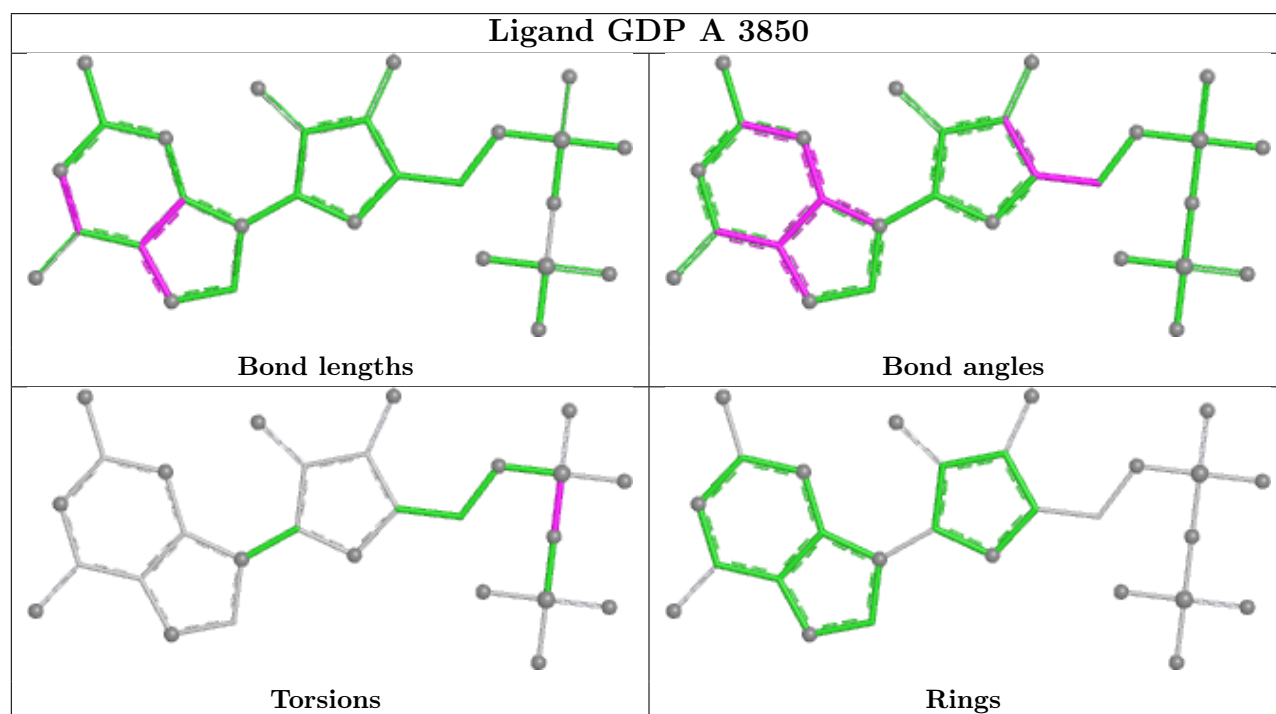
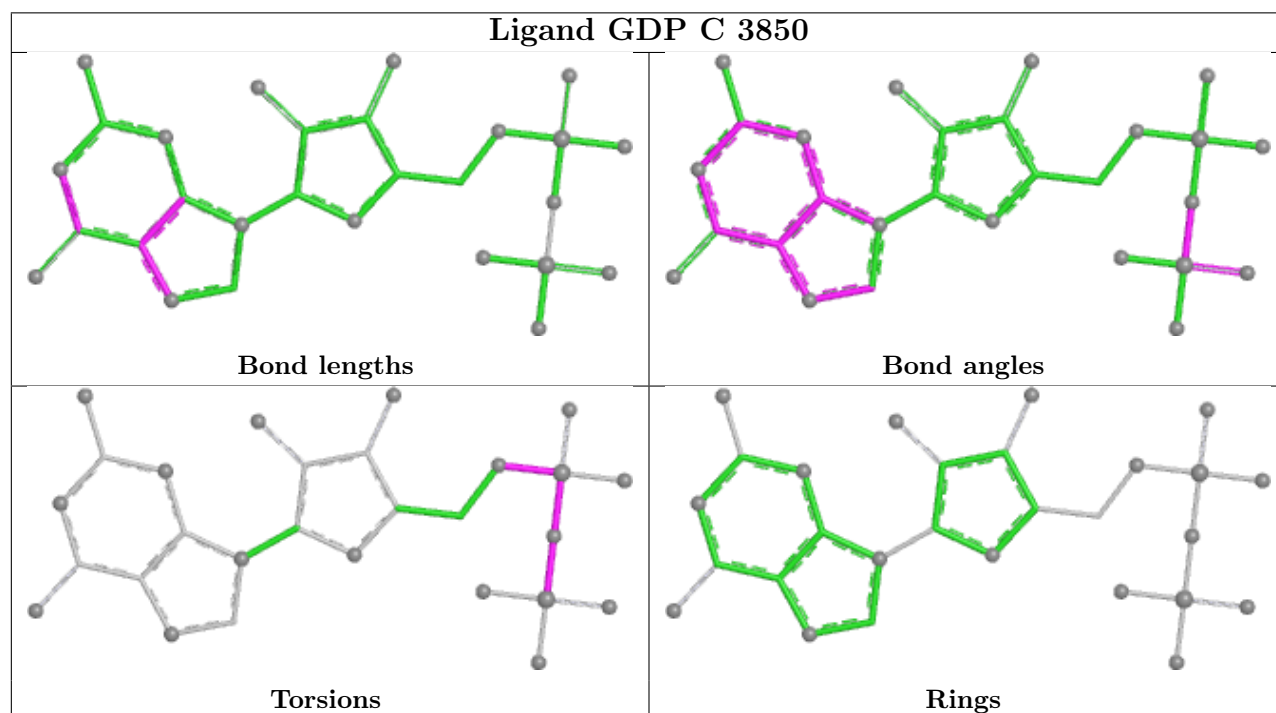
There are no ring outliers.

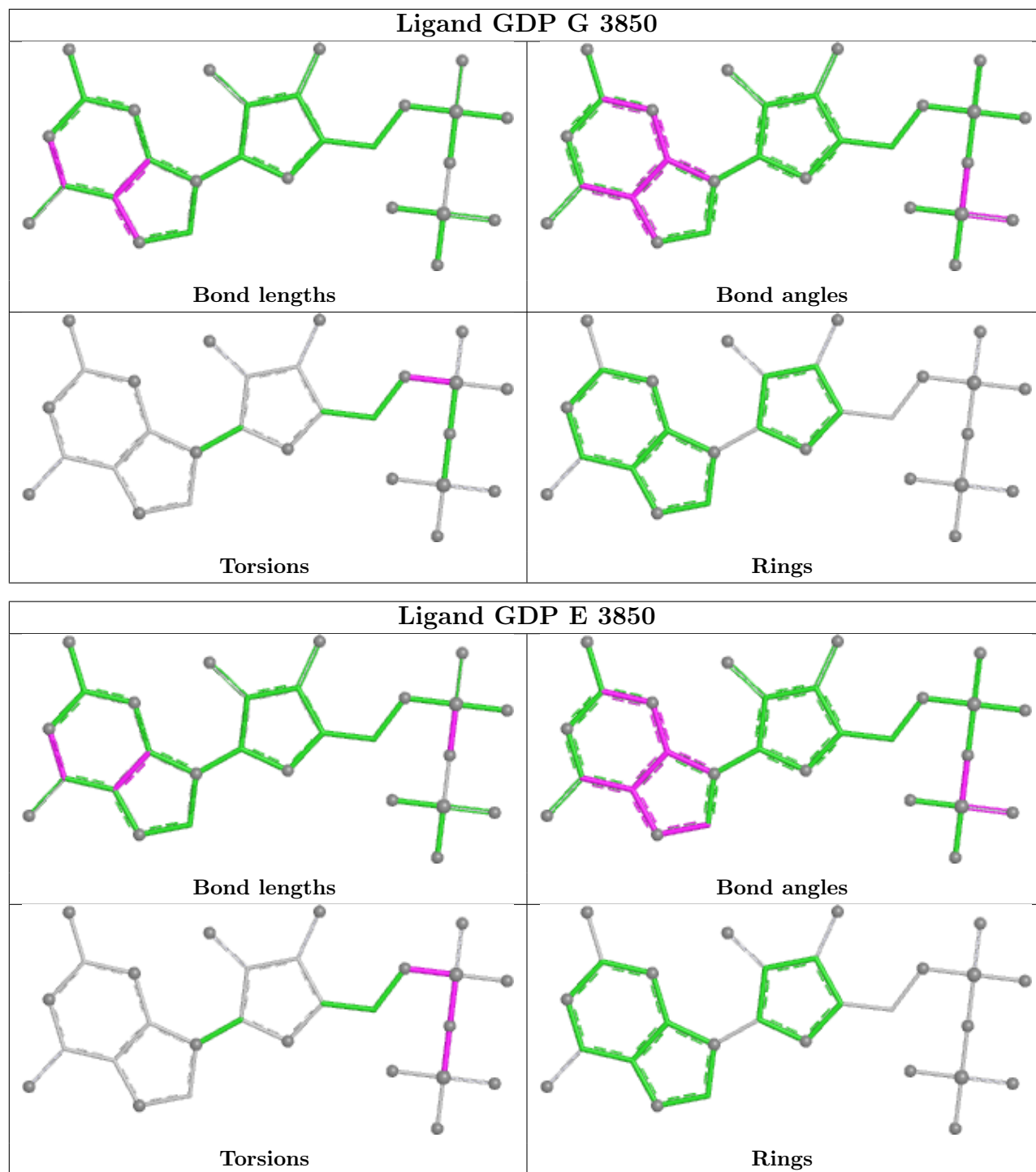
4 monomers are involved in 8 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | C     | 3850 | GDP  | 3       | 0            |
| 2   | A     | 3850 | GDP  | 2       | 0            |
| 2   | G     | 3850 | GDP  | 1       | 0            |
| 2   | E     | 3850 | GDP  | 2       | 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

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 411/447 (91%)   | -0.23  | 5 (1%) 76 55  | 19, 70, 145, 214      | 0     |
| 1   | C     | 409/447 (91%)   | -0.10  | 6 (1%) 72 49  | 28, 70, 169, 234      | 0     |
| 1   | E     | 386/447 (86%)   | -0.31  | 5 (1%) 75 53  | 18, 52, 119, 178      | 0     |
| 1   | G     | 384/447 (85%)   | -0.14  | 11 (2%) 53 31 | 24, 63, 190, 291      | 0     |
| All | All   | 1590/1788 (88%) | -0.20  | 27 (1%) 69 46 | 18, 63, 155, 291      | 0     |

All (27) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 374 | ILE  | 4.0  |
| 1   | G     | 436 | ASN  | 3.2  |
| 1   | C     | 247 | HIS  | 3.2  |
| 1   | G     | 380 | PRO  | 3.1  |
| 1   | C     | 46  | PHE  | 3.0  |
| 1   | G     | 113 | ARG  | 3.0  |
| 1   | E     | 189 | HIS  | 2.8  |
| 1   | A     | 156 | THR  | 2.8  |
| 1   | E     | 438 | SER  | 2.6  |
| 1   | G     | 189 | HIS  | 2.5  |
| 1   | C     | 157 | LEU  | 2.5  |
| 1   | A     | 243 | SER  | 2.4  |
| 1   | C     | 433 | ILE  | 2.4  |
| 1   | E     | 379 | LYS  | 2.4  |
| 1   | A     | 247 | HIS  | 2.4  |
| 1   | C     | 39  | ILE  | 2.3  |
| 1   | G     | 438 | SER  | 2.3  |
| 1   | E     | 176 | TYR  | 2.3  |
| 1   | G     | 379 | LYS  | 2.2  |
| 1   | A     | 157 | LEU  | 2.2  |
| 1   | G     | 389 | THR  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 153 | SER  | 2.1  |
| 1   | E     | 377 | GLY  | 2.1  |
| 1   | G     | 338 | GLY  | 2.1  |
| 1   | G     | 382 | LEU  | 2.1  |
| 1   | G     | 158 | ARG  | 2.1  |
| 1   | C     | 154 | GLN  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no 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.

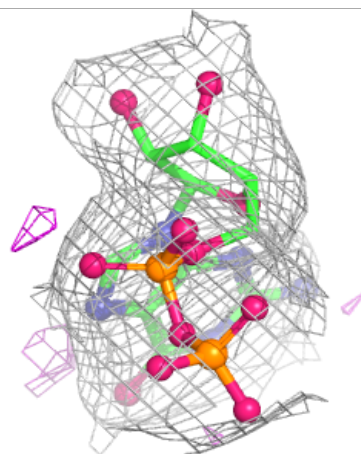
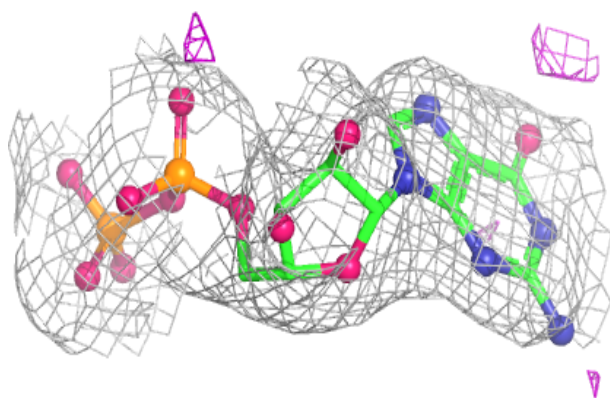
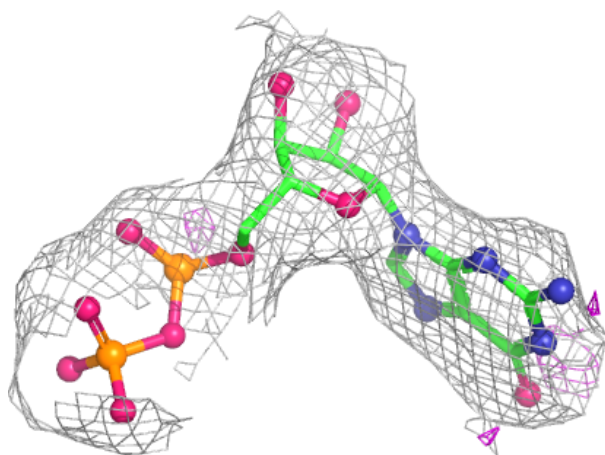
| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 3   | MG   | G     | 448  | 1/1   | 0.87 | 0.08 | 70,70,70,70                | 0     |
| 3   | MG   | C     | 448  | 1/1   | 0.88 | 0.16 | 71,71,71,71                | 0     |
| 3   | MG   | E     | 448  | 1/1   | 0.91 | 0.09 | 68,68,68,68                | 0     |
| 3   | MG   | A     | 448  | 1/1   | 0.96 | 0.16 | 72,72,72,72                | 0     |
| 2   | GDP  | A     | 3850 | 28/28 | 0.96 | 0.07 | 32,46,73,88                | 0     |
| 2   | GDP  | C     | 3850 | 28/28 | 0.96 | 0.07 | 29,45,63,69                | 0     |
| 2   | GDP  | G     | 3850 | 28/28 | 0.96 | 0.07 | 22,41,58,69                | 0     |
| 2   | GDP  | E     | 3850 | 28/28 | 0.97 | 0.06 | 22,34,48,57                | 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.



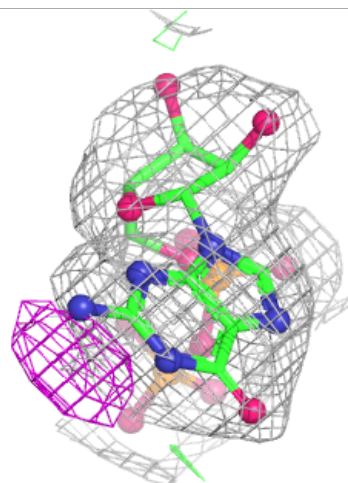
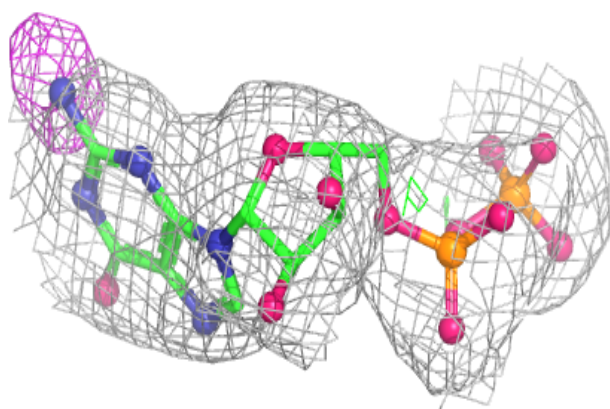
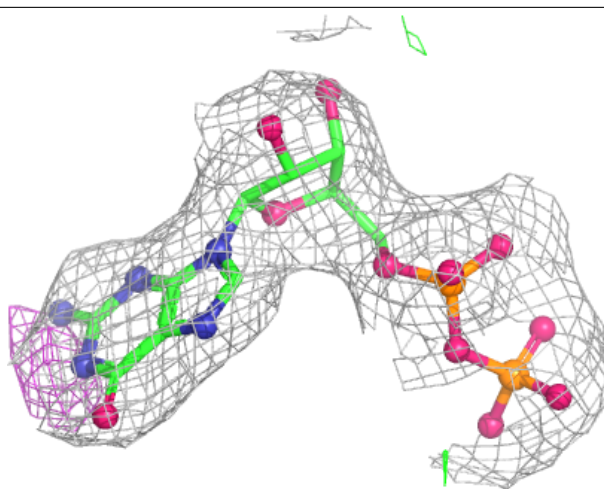
**Electron density around GDP A 3850:**

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



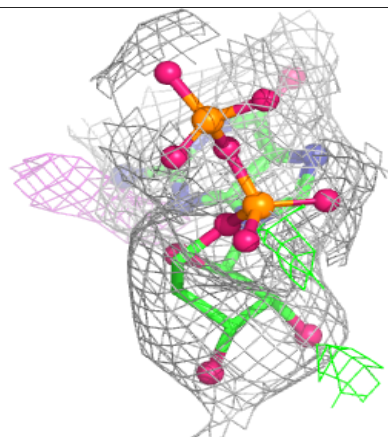
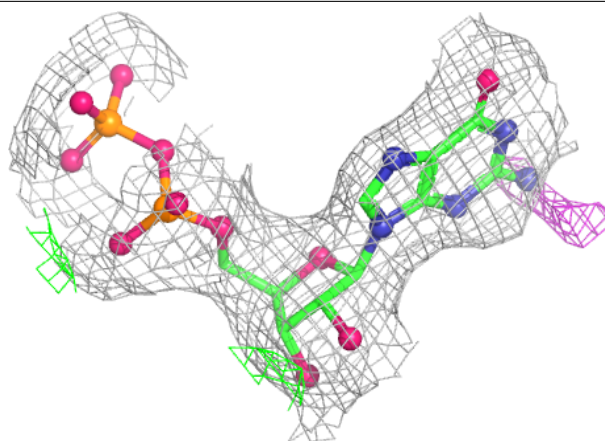
**Electron density around GDP C 3850:**

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



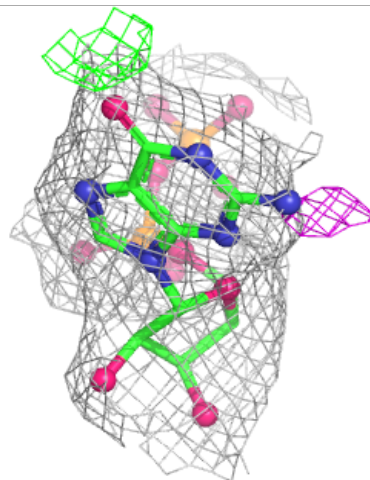
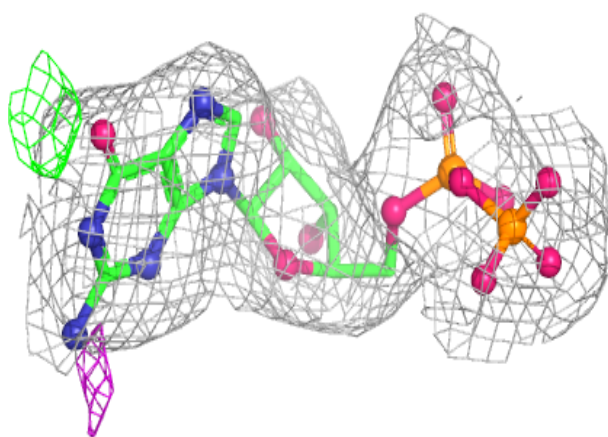
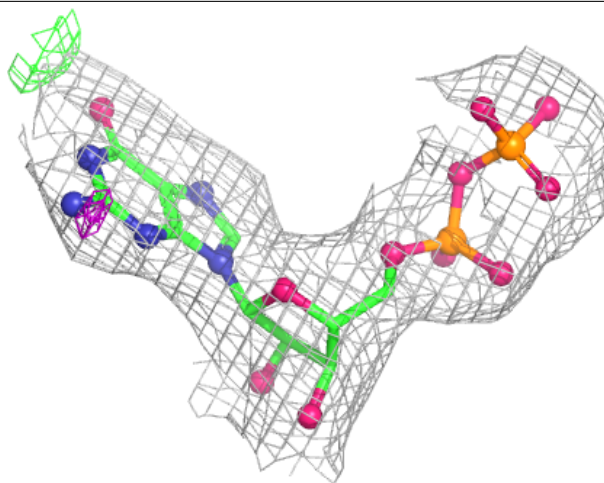
**Electron density around GDP G 3850:**

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



**Electron density around GDP E 3850:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.