



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 03:50 am BST

PDB ID : 1MAB  
Title : RAT LIVER F1-ATPASE  
Authors : Bianchet, M.A.; Amzel, L.M.  
Deposited on : 1998-08-06  
Resolution : 2.80 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

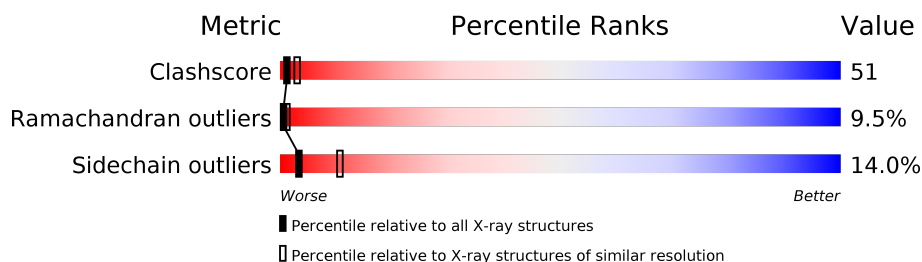
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 141614                      | 3569 (2.80-2.80)                                      |
| Ramachandran outliers | 138981                      | 3498 (2.80-2.80)                                      |
| Sidechain outliers    | 138945                      | 3500 (2.80-2.80)                                      |

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 on 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  $\leq 5\%$ .

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 510    | <div> <div>29%</div> <div>57%</div> <div>12%</div> <div>..</div> </div> |
| 2   | B     | 479    | <div> <div>25%</div> <div>58%</div> <div>14%</div> <div>.</div> </div>  |
| 3   | G     | 270    | <div> <div>24%</div> <div>20%</div> <div>.</div> <div>54%</div> </div>  |

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8489 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 PROTEIN (F1-ATPASE ALPHA CHAIN).

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 501      | Total | C    | N   | O   | S  | 0       | 13      | 0     |
|     |       |          | 3810  | 2395 | 673 | 730 | 12 |         |         |       |

- Molecule 2 is a protein called PROTEIN (F1-ATPASE BETA CHAIN).

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 477      | Total | C    | N   | O   | S  | 0       | 19      | 0     |
|     |       |          | 3598  | 2279 | 610 | 697 | 12 |         |         |       |

- Molecule 3 is a protein called PROTEIN (F1-ATPASE GAMMA CHAIN).

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | G     | 124      | Total | C   | N   | O   | S | 0       | 124     | 0     |
|     |       |          | 956   | 592 | 175 | 182 | 7 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| G     | 1       | ARG      | LYS    | CONFLICT | UNP P35435 |

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 5   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 6   | B     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 7   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |

- Molecule 8 is water.

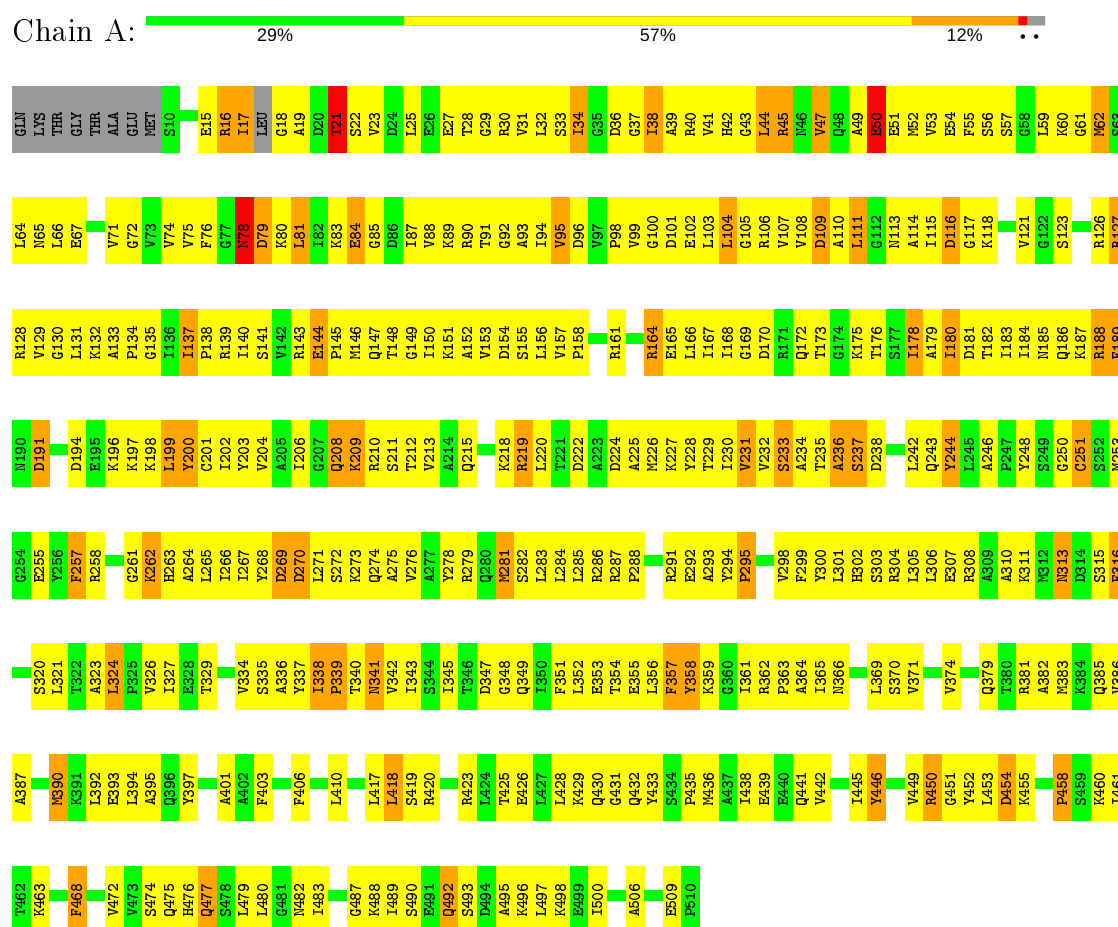
| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 8   | A     | 34       | Total O<br>34 34 | 0       | 0       |
| 8   | B     | 24       | Total O<br>24 24 | 0       | 0       |
| 8   | G     | 3        | Total O<br>3 3   | 0       | 0       |

### 3 Residue-property plots

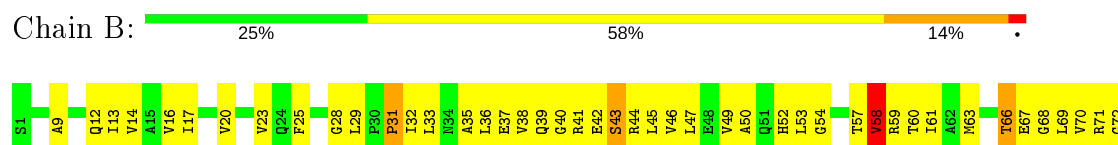
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

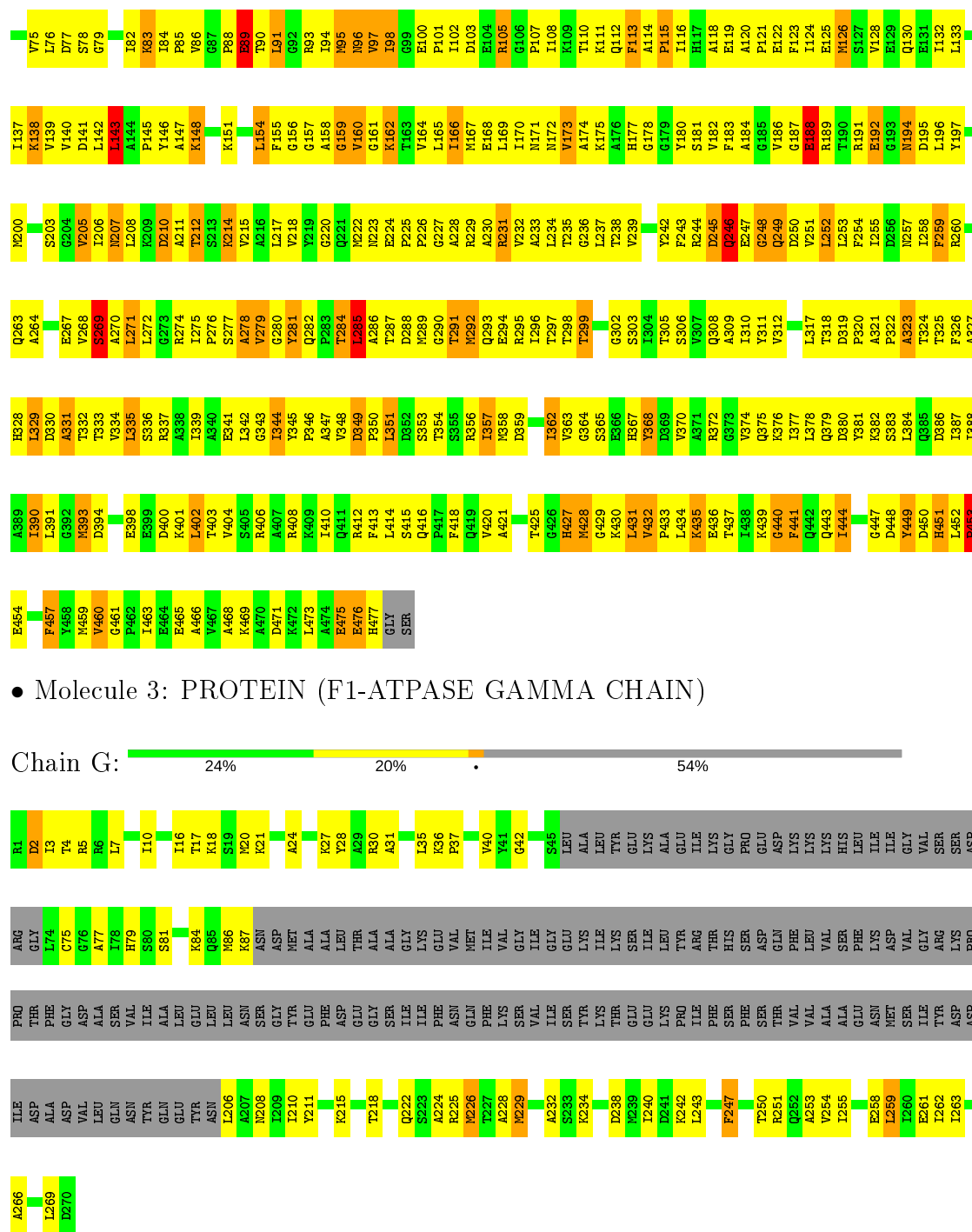
Note EDS was not executed.

#### • Molecule 1: PROTEIN (F1-ATPASE ALPHA CHAIN)



#### • Molecule 2: PROTEIN (F1-ATPASE BETA CHAIN)





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property   | Value  | Source    |
|--|--|-----------|
| Space group  | H 3 2  | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 143.67Å 143.67Å 361.15Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å)   | 6.00 – 2.80                                      | Depositor |
| % Data completeness<br>(in resolution range)             | 65.0 (6.00-2.80)                                 | Depositor |
| $R_{merge}$  | (Not available)                                  | Depositor |
| $R_{sym}$  | 0.10   | Depositor |
| Refinement program                                       | X-PLOR 3.851                                     | Depositor |
| R, $R_{free}$  | 0.217 , 0.290                                    | Depositor |
| Estimated twinning fraction                              | No twinning to report.                           | Xtriage   |
| Total number of atoms                                    | 8489   | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 52.0   | wwPDB-VP  |



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, PO4, ADP

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     | 0.47         | 0/3862  | 0.78        | 1/5212 (0.0%)  |
| 2   | B     | 0.51         | 0/3657  | 0.81        | 1/4961 (0.0%)  |
| 3   | G     | 0.31         | 0/960   | 0.53        | 0/1279         |
| All | All   | 0.47         | 0/8479  | 0.77        | 2/11452 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | B     | 115 | PRO  | N-CA-CB | 5.50 | 109.90      | 103.30   |
| 1   | A     | 79  | ASP  | N-CA-C  | 5.45 | 125.71      | 111.00   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3810  | 0        | 3884     | 406     | 0            |
| 2   | B     | 3598  | 0        | 3640     | 449     | 0            |
| 3   | G     | 956   | 0        | 1016     | 39      | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 31    | 0        | 12       | 6       | 0            |
| 6   | B     | 5     | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | B     | 27    | 0        | 12       | 7       | 0            |
| 8   | A     | 34    | 0        | 0        | 12      | 0            |
| 8   | B     | 24    | 0        | 0        | 5       | 0            |
| 8   | G     | 3     | 0        | 0        | 0       | 0            |
| All | All   | 8489  | 0        | 8564     | 866     | 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 51.

All (866) 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:62:MET:SD    | 1:A:95:VAL:HG21  | 1.95                     | 1.07              |
| 2:B:38:VAL:HG21  | 2:B:45:LEU:HD23  | 1.38                     | 1.05              |
| 2:B:37:GLU:HB2   | 2:B:76:LEU:HB3   | 1.32                     | 1.05              |
| 2:B:133:LEU:HD13 | 2:B:148:LYS:HE3  | 1.40                     | 1.04              |
| 1:A:151:LYS:HE3  | 1:A:436:MET:HG3  | 1.39                     | 1.02              |
| 2:B:186:VAL:HG21 | 2:B:233:ALA:HB2  | 1.40                     | 1.01              |
| 1:A:270:ASP:HB3  | 1:A:273:LYS:HB2  | 1.45                     | 0.99              |
| 2:B:189:ARG:HB2  | 2:B:192:GLU:HG2  | 1.44                     | 0.97              |
| 2:B:377:ILE:HG12 | 2:B:403:THR:HG23 | 1.49                     | 0.95              |
| 1:A:257:PHE:HD2  | 1:A:264:ALA:HB2  | 1.33                     | 0.94              |
| 1:A:108:VAL:HG12 | 1:A:114:ALA:HA   | 1.49                     | 0.94              |
| 2:B:154:LEU:HD12 | 2:B:162:LYS:HA   | 1.50                     | 0.94              |
| 1:A:506:ALA:HA   | 1:A:509:GLU:HB3  | 1.49                     | 0.93              |
| 1:A:137:ILE:HG12 | 1:A:138:PRO:HD3  | 1.47                     | 0.92              |
| 2:B:94:ILE:HB    | 2:B:103:ASP:HB3  | 1.52                     | 0.90              |
| 1:A:150:ILE:HD11 | 1:A:181:ASP:HB2  | 1.53                     | 0.90              |
| 2:B:243:PHE:HB3  | 2:B:249:GLN:HE21 | 1.36                     | 0.90              |
| 1:A:32:LEU:HG    | 1:A:42:HIS:HB2   | 1.53                     | 0.90              |
| 2:B:339:ILE:HD13 | 2:B:342:LEU:HD12 | 1.51                     | 0.90              |
| 2:B:94:ILE:HG22  | 2:B:102:ILE:HG13 | 1.55                     | 0.88              |
| 1:A:358:TYR:HE2  | 2:B:351:LEU:HD12 | 1.38                     | 0.87              |
| 2:B:465:GLU:HA   | 2:B:468:ALA:HB3  | 1.54                     | 0.87              |
| 1:A:301:LEU:HA   | 1:A:304:ARG:HH21 | 1.40                     | 0.85              |
| 1:A:203:TYR:HB3  | 1:A:231:VAL:HG13 | 1.58                     | 0.84              |
| 2:B:105:ARG:HE   | 2:B:208:LEU:HD22 | 1.41                     | 0.84              |
| 1:A:431:GLY:HA2  | 5:A:603:ATP:HN62 | 1.42                     | 0.84              |
| 1:A:211:SER:OG   | 2:B:126:MET:HG3  | 1.77                     | 0.84              |
| 1:A:158:PRO:HG2  | 1:A:379:GLN:HB3  | 1.60                     | 0.83              |
| 1:A:49:ALA:O     | 1:A:50:GLU:HB2   | 1.78                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:225:ALA:HA   | 1:A:228:TYR:CE1  | 2.14                     | 0.82              |
| 1:A:271:LEU:HB3  | 1:A:302:HIS:CE1  | 2.13                     | 0.82              |
| 1:A:140:ILE:HG23 | 1:A:141:SER:H    | 1.42                     | 0.82              |
| 2:B:88:PRO:HA    | 2:B:91:LEU:HD12  | 1.62                     | 0.82              |
| 2:B:298:THR:HG22 | 2:B:299:THR:H    | 1.43                     | 0.82              |
| 1:A:137:ILE:HD13 | 1:A:137:ILE:H    | 1.42                     | 0.82              |
| 1:A:302:HIS:O    | 1:A:306:LEU:HD23 | 1.79                     | 0.81              |
| 2:B:289:MET:SD   | 2:B:293:GLN:NE2  | 2.53                     | 0.81              |
| 1:A:426:GLU:HB2  | 1:A:461:ILE:HD12 | 1.63                     | 0.81              |
| 1:A:96:ASP:HA    | 1:A:128:ARG:HA   | 1.61                     | 0.81              |
| 2:B:335:LEU:HB3  | 2:B:347:ALA:HB3  | 1.60                     | 0.81              |
| 2:B:200:MET:HB3  | 2:B:206:ILE:HG13 | 1.64                     | 0.80              |
| 1:A:183:ILE:HD11 | 1:A:267:ILE:HG13 | 1.62                     | 0.80              |
| 1:A:267:ILE:HD13 | 1:A:324:LEU:HD13 | 1.60                     | 0.80              |
| 1:A:103:LEU:O    | 1:A:230:ILE:HG12 | 1.83                     | 0.79              |
| 1:A:156:LEU:O    | 1:A:158:PRO:HD3  | 1.81                     | 0.79              |
| 2:B:184:ALA:HB2  | 2:B:236:GLY:HA3  | 1.64                     | 0.79              |
| 1:A:141:SER:HB3  | 1:A:143:ARG:NH2  | 1.98                     | 0.79              |
| 2:B:257:ASN:HA   | 2:B:309:ALA:O    | 1.83                     | 0.78              |
| 1:A:156:LEU:HD11 | 1:A:428:LEU:HD21 | 1.64                     | 0.78              |
| 2:B:243:PHE:HB3  | 2:B:249:GLN:NE2  | 1.97                     | 0.78              |
| 2:B:120:ALA:HB1  | 2:B:121:PRO:HD2  | 1.66                     | 0.77              |
| 2:B:82:ILE:O     | 2:B:116:ILE:HG12 | 1.85                     | 0.77              |
| 1:A:152:ALA:O    | 1:A:156:LEU:HB2  | 1.85                     | 0.77              |
| 1:A:183:ILE:HG23 | 1:A:201:CYS:SG   | 2.25                     | 0.77              |
| 1:A:52:MET:O     | 1:A:91:THR:HB    | 1.86                     | 0.76              |
| 1:A:479:LEU:HD23 | 1:A:497:LEU:HG   | 1.68                     | 0.76              |
| 2:B:155:PHE:HE1  | 2:B:310:ILE:HB   | 1.51                     | 0.76              |
| 1:A:44:LEU:HD12  | 1:A:47:VAL:HG23  | 1.68                     | 0.75              |
| 2:B:38:VAL:HG21  | 2:B:45:LEU:CD2   | 2.15                     | 0.75              |
| 2:B:93:ARG:NH2   | 2:B:101:PRO:HB3  | 2.02                     | 0.75              |
| 2:B:155:PHE:CE1  | 2:B:310:ILE:HB   | 2.22                     | 0.75              |
| 1:A:105:GLY:HA2  | 1:A:226:MET:O    | 1.87                     | 0.74              |
| 2:B:151:LYS:H    | 2:B:330:ASP:HB3  | 1.51                     | 0.74              |
| 2:B:166:ILE:HG12 | 2:B:254:PHE:HD2  | 1.52                     | 0.74              |
| 2:B:200:MET:SD   | 2:B:215:VAL:HG21 | 2.28                     | 0.74              |
| 2:B:86:VAL:HG21  | 2:B:114:ALA:HB2  | 1.69                     | 0.73              |
| 1:A:133:ALA:HB1  | 1:A:139:ARG:HH22 | 1.53                     | 0.73              |
| 2:B:63:MET:SD    | 2:B:227:GLY:O    | 2.46                     | 0.73              |
| 2:B:271:LEU:H    | 2:B:271:LEU:HD23 | 1.52                     | 0.73              |
| 2:B:268:VAL:O    | 2:B:272:LEU:HG   | 1.89                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:259:PHE:CE1  | 2:B:311:TYR:HB3  | 2.24                     | 0.73              |
| 2:B:335:LEU:HA   | 2:B:347:ALA:O    | 1.89                     | 0.73              |
| 2:B:339:ILE:HG23 | 2:B:344:ILE:HB   | 1.71                     | 0.72              |
| 1:A:476:HIS:HB3  | 1:A:479:LEU:HD13 | 1.72                     | 0.72              |
| 2:B:187:GLY:O    | 2:B:222:MET:HG3  | 1.88                     | 0.72              |
| 1:A:299:PHE:HA   | 1:A:341:ASN:HD21 | 1.54                     | 0.72              |
| 1:A:359:LYS:HA   | 2:B:376:LYS:HB2  | 1.70                     | 0.72              |
| 1:A:386:VAL:HG11 | 1:A:446:TYR:HB2  | 1.69                     | 0.72              |
| 2:B:253:LEU:HG   | 2:B:255:ILE:HD11 | 1.72                     | 0.72              |
| 1:A:98:PRO:HA    | 1:A:126:ARG:HD3  | 1.71                     | 0.72              |
| 1:A:425:THR:O    | 1:A:429:LYS:HG3  | 1.90                     | 0.72              |
| 1:A:386:VAL:HG12 | 1:A:450:ARG:NH2  | 2.05                     | 0.71              |
| 2:B:323:ALA:HA   | 2:B:326:PHE:HD2  | 1.55                     | 0.71              |
| 1:A:303:SER:HA   | 1:A:345:ILE:HD13 | 1.72                     | 0.71              |
| 1:A:479:LEU:HD12 | 1:A:479:LEU:H    | 1.54                     | 0.71              |
| 8:A:607:HOH:O    | 2:B:123:PHE:HB3  | 1.90                     | 0.71              |
| 2:B:137:ILE:HG23 | 2:B:416:GLN:NE2  | 2.05                     | 0.71              |
| 2:B:326:PHE:HA   | 2:B:329:LEU:HD21 | 1.73                     | 0.71              |
| 2:B:32:ILE:HG22  | 2:B:33:LEU:HG    | 1.73                     | 0.71              |
| 2:B:269:SER:OG   | 2:B:282:GLN:HB3  | 1.91                     | 0.71              |
| 2:B:181:SER:HB3  | 2:B:215:VAL:HG12 | 1.73                     | 0.70              |
| 1:A:257:PHE:CD2  | 1:A:264:ALA:HB2  | 2.23                     | 0.70              |
| 2:B:452:LEU:HD22 | 2:B:466:ALA:HB1  | 1.72                     | 0.70              |
| 1:A:441:GLN:O    | 1:A:445:ILE:HG22 | 1.91                     | 0.70              |
| 2:B:38:VAL:HB    | 2:B:45:LEU:HB3   | 1.73                     | 0.70              |
| 2:B:374:VAL:HG13 | 2:B:410:ILE:HG21 | 1.74                     | 0.70              |
| 2:B:259:PHE:HB3  | 2:B:310:ILE:HG23 | 1.73                     | 0.70              |
| 1:A:272:SER:O    | 1:A:275:ALA:HB3  | 1.92                     | 0.70              |
| 1:A:265:LEU:HD11 | 1:A:324:LEU:HD11 | 1.73                     | 0.70              |
| 2:B:368:TYR:O    | 2:B:372:ARG:HG2  | 1.92                     | 0.70              |
| 1:A:397:TYR:HE1  | 1:A:418:LEU:HA   | 1.56                     | 0.70              |
| 2:B:323:ALA:HA   | 2:B:326:PHE:CD2  | 2.26                     | 0.69              |
| 1:A:40:ARG:HH21  | 1:A:285:LEU:HD23 | 1.58                     | 0.69              |
| 1:A:351:PHE:O    | 1:A:365:ILE:HA   | 1.92                     | 0.69              |
| 2:B:310:ILE:HG12 | 2:B:325:THR:HG21 | 1.75                     | 0.69              |
| 2:B:9:ALA:HB1    | 2:B:77:ASP:HB3   | 1.73                     | 0.69              |
| 2:B:226:PRO:N    | 2:B:229:ARG:HH21 | 1.91                     | 0.68              |
| 2:B:439:LYS:O    | 2:B:443:GLN:HG2  | 1.92                     | 0.68              |
| 2:B:252:LEU:HG   | 2:B:305:THR:HB   | 1.76                     | 0.68              |
| 2:B:49:VAL:HA    | 2:B:60:THR:HG22  | 1.76                     | 0.68              |
| 2:B:44:ARG:HH11  | 2:B:44:ARG:HG2   | 1.58                     | 0.68              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B:184:ALA:HA    | 2:B:218:VAL:O      | 1.94                     | 0.68              |
| 1:A:279:ARG:O     | 1:A:283:LEU:HG     | 1.94                     | 0.67              |
| 2:B:292:MET:HE1   | 2:B:293:GLN:HG2    | 1.75                     | 0.67              |
| 2:B:255:ILE:HD13  | 2:B:308:GLN:HG2    | 1.75                     | 0.67              |
| 1:A:40:ARG:NH2    | 1:A:285:LEU:HD23   | 2.10                     | 0.67              |
| 1:A:139:ARG:HG2   | 1:A:310:ALA:HB1    | 1.77                     | 0.67              |
| 1:A:106:ARG:O     | 1:A:231:VAL:HG23   | 1.94                     | 0.67              |
| 1:A:151:LYS:CE    | 1:A:436:MET:HG3    | 2.22                     | 0.67              |
| 2:B:105:ARG:NE    | 2:B:208:LEU:HD22   | 2.10                     | 0.67              |
| 2:B:317:LEU:HD11  | 2:B:334:VAL:HG11   | 1.77                     | 0.66              |
| 1:A:358:TYR:CE2   | 2:B:351:LEU:HD12   | 2.28                     | 0.66              |
| 1:A:155:SER:HA    | 1:A:383:MET:SD     | 2.35                     | 0.66              |
| 1:A:59:LEU:HD11   | 1:A:76:PHE:O       | 1.96                     | 0.66              |
| 2:B:335:LEU:HD11  | 8:B:612:HOH:O      | 1.95                     | 0.66              |
| 2:B:351:LEU:HB3   | 8:B:628:HOH:O      | 1.95                     | 0.66              |
| 1:A:287:ARG:HG2   | 8:A:631:HOH:O      | 1.95                     | 0.66              |
| 1:A:182:THR:HG22  | 1:A:265:LEU:HD21   | 1.78                     | 0.66              |
| 1:A:361:ILE:O     | 1:A:364:ALA:HB2    | 1.96                     | 0.66              |
| 2:B:378:LEU:O     | 2:B:381[B]:TYR:HB3 | 1.96                     | 0.66              |
| 1:A:446:TYR:CD2   | 1:A:489:ILE:HD13   | 2.30                     | 0.66              |
| 2:B:138:LYS:HZ1   | 2:B:441:PHE:HD2    | 1.42                     | 0.66              |
| 2:B:469:LYS:HE3   | 2:B:473:LEU:HD13   | 1.76                     | 0.66              |
| 1:A:379:GLN:HB2   | 1:A:383:MET:HB2    | 1.77                     | 0.66              |
| 2:B:259:PHE:CZ    | 2:B:311:TYR:HB3    | 2.31                     | 0.66              |
| 1:A:38:ILE:HG13   | 1:A:284:LEU:HB3    | 1.78                     | 0.65              |
| 2:B:345:TYR:HA    | 2:B:346:PRO:C      | 2.16                     | 0.65              |
| 1:A:34:ILE:HG23   | 2:B:52:HIS:HB2     | 1.77                     | 0.65              |
| 1:A:301:LEU:HA    | 1:A:304:ARG:NH2    | 2.12                     | 0.65              |
| 1:A:141:SER:O     | 1:A:311:LYS:HG2    | 1.96                     | 0.65              |
| 1:A:203:TYR:HB3   | 1:A:231:VAL:CG1    | 2.26                     | 0.65              |
| 1:A:167:ILE:HD11  | 1:A:326:VAL:HG22   | 1.79                     | 0.65              |
| 2:B:121:PRO:HG3   | 2:B:297:THR:CG2    | 2.27                     | 0.65              |
| 1:A:154:ASP:O     | 1:A:158:PRO:HG3    | 1.97                     | 0.65              |
| 1:A:175:LYS:HD2   | 1:A:326:VAL:HG13   | 1.78                     | 0.65              |
| 1:A:246:ALA:HA    | 8:A:606:HOH:O      | 1.95                     | 0.65              |
| 2:B:105:ARG:HH21  | 2:B:208:LEU:HB3    | 1.61                     | 0.64              |
| 2:B:189:ARG:HD2   | 2:B:189:ARG:H      | 1.60                     | 0.64              |
| 2:B:84:ILE:HG21   | 2:B:235:THR:HG22   | 1.80                     | 0.64              |
| 1:A:110:ALA:HB1   | 8:A:606:HOH:O      | 1.96                     | 0.64              |
| 3:G:4[A]:THR:HG23 | 3:G:247[A]:PHE:HE2 | 1.62                     | 0.64              |
| 1:A:32:LEU:CG     | 1:A:42:HIS:HB2     | 2.27                     | 0.64              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:B:97:VAL:O        | 2:B:98:ILE:HG12     | 1.97                     | 0.64              |
| 1:A:108:VAL:HG12    | 1:A:114:ALA:CA      | 2.26                     | 0.64              |
| 2:B:188:GLU:HA      | 2:B:222:MET:CE      | 2.28                     | 0.64              |
| 2:B:387[B]:ILE:HG22 | 2:B:388[B]:ILE:HG13 | 1.80                     | 0.64              |
| 1:A:168:ILE:HG12    | 1:A:329:THR:OG1     | 1.97                     | 0.64              |
| 1:A:215:GLN:O       | 1:A:219:ARG:HB2     | 1.98                     | 0.64              |
| 1:A:386:VAL:HG23    | 1:A:387:ALA:H       | 1.63                     | 0.64              |
| 1:A:442:VAL:O       | 1:A:446:TYR:HB3     | 1.98                     | 0.64              |
| 1:A:27:GLU:O        | 1:A:90:ARG:HG3      | 1.97                     | 0.64              |
| 2:B:200:MET:HB3     | 2:B:206:ILE:CG1     | 2.27                     | 0.64              |
| 3:G:37[A]:PRO:O     | 3:G:42[A]:GLY:HA3   | 1.97                     | 0.64              |
| 2:B:122:GLU:O       | 2:B:126:MET:SD      | 2.56                     | 0.64              |
| 2:B:155:PHE:HB2     | 2:B:334:VAL:HG22    | 1.80                     | 0.64              |
| 1:A:359:LYS:HA      | 2:B:376:LYS:CB      | 2.27                     | 0.64              |
| 2:B:96:ASN:HB3      | 2:B:102:ILE:CG2     | 2.28                     | 0.63              |
| 2:B:167:MET:SD      | 2:B:196:LEU:HD13    | 2.39                     | 0.63              |
| 1:A:189:PHE:N       | 1:A:189:PHE:HD1     | 1.96                     | 0.63              |
| 2:B:61:ILE:HG23     | 2:B:268:VAL:HG21    | 1.79                     | 0.63              |
| 2:B:32:ILE:O        | 2:B:33:LEU:HB2      | 1.99                     | 0.63              |
| 2:B:36:LEU:HD23     | 2:B:77:ASP:HA       | 1.81                     | 0.63              |
| 1:A:189:PHE:CD1     | 1:A:189:PHE:N       | 2.67                     | 0.63              |
| 2:B:36:LEU:O        | 2:B:46:VAL:HA       | 1.98                     | 0.63              |
| 2:B:172:ASN:HD21    | 2:B:431:LEU:HD22    | 1.63                     | 0.63              |
| 1:A:218:LYS:HD3     | 1:A:219:ARG:N       | 2.13                     | 0.63              |
| 2:B:289:MET:SD      | 2:B:293:GLN:HG3     | 2.38                     | 0.63              |
| 2:B:91:LEU:HD11     | 2:B:180:TYR:CE2     | 2.33                     | 0.63              |
| 1:A:16:ARG:HG2      | 1:A:17:ILE:HG12     | 1.81                     | 0.63              |
| 2:B:378:LEU:O       | 2:B:382[B]:LYS:HG2  | 1.98                     | 0.63              |
| 2:B:234:LEU:O       | 2:B:237:LEU:HB3     | 1.99                     | 0.62              |
| 2:B:237:LEU:HD21    | 2:B:295:ARG:HB3     | 1.81                     | 0.62              |
| 2:B:139:VAL:CG2     | 2:B:414:LEU:HB3     | 2.29                     | 0.62              |
| 1:A:52:MET:HA       | 1:A:62:MET:HA       | 1.81                     | 0.62              |
| 2:B:242:TYR:HA      | 2:B:246:GLN:NE2     | 2.15                     | 0.62              |
| 2:B:259:PHE:CD2     | 2:B:321:ALA:HB1     | 2.34                     | 0.62              |
| 2:B:402:LEU:O       | 2:B:406:ARG:HG2     | 1.99                     | 0.62              |
| 2:B:186:VAL:CG2     | 2:B:233:ALA:HB2     | 2.24                     | 0.62              |
| 2:B:212:THR:HG22    | 2:B:214:LYS:NZ      | 2.15                     | 0.62              |
| 2:B:440:GLY:HA2     | 2:B:463:ILE:HG21    | 1.80                     | 0.62              |
| 2:B:251:VAL:HG12    | 2:B:252:LEU:H       | 1.65                     | 0.61              |
| 1:A:267:ILE:CD1     | 1:A:324:LEU:HD13    | 2.31                     | 0.61              |
| 2:B:226:PRO:HB3     | 2:B:267:GLU:OE1     | 2.00                     | 0.61              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:B:181:SER:O    | 2:B:215:VAL:HA     | 2.00                     | 0.61              |
| 2:B:253:LEU:HG   | 2:B:255:ILE:CD1    | 2.29                     | 0.61              |
| 2:B:138:LYS:HD2  | 2:B:414:LEU:HD23   | 1.82                     | 0.61              |
| 2:B:475:GLU:O    | 2:B:476:GLU:HB2    | 1.99                     | 0.61              |
| 1:A:168:ILE:HG23 | 1:A:351:PHE:HD1    | 1.64                     | 0.61              |
| 2:B:267:GLU:O    | 2:B:271:LEU:HD21   | 2.00                     | 0.61              |
| 2:B:59:ARG:NH1   | 2:B:272:LEU:HA     | 2.15                     | 0.61              |
| 2:B:86:VAL:HG22  | 2:B:114:ALA:H      | 1.66                     | 0.61              |
| 2:B:169:LEU:O    | 2:B:173:VAL:HB     | 2.01                     | 0.61              |
| 1:A:218:LYS:HD2  | 2:B:128:VAL:HG11   | 1.83                     | 0.61              |
| 2:B:94:ILE:HG12  | 2:B:217:LEU:HD12   | 1.81                     | 0.61              |
| 1:A:362:ARG:HD3  | 5:A:603:ATP:C2     | 2.35                     | 0.61              |
| 2:B:66:THR:HG22  | 2:B:69:LEU:HD12    | 1.81                     | 0.61              |
| 2:B:85:PRO:O     | 2:B:90:THR:HG21    | 2.01                     | 0.61              |
| 1:A:164:ARG:HA   | 1:A:323:ALA:O      | 2.01                     | 0.61              |
| 1:A:337:TYR:O    | 1:A:338:ILE:HB     | 1.99                     | 0.61              |
| 1:A:366:ASN:ND2  | 1:A:369:LEU:HD23   | 2.16                     | 0.61              |
| 2:B:36:LEU:HD12  | 2:B:60:THR:HG21    | 1.82                     | 0.61              |
| 1:A:45:ARG:O     | 1:A:45:ARG:HD3     | 2.01                     | 0.60              |
| 2:B:244:ARG:O    | 2:B:248:GLY:HA2    | 2.01                     | 0.60              |
| 1:A:144:GLU:HG2  | 1:A:144:GLU:O      | 2.01                     | 0.60              |
| 1:A:107:VAL:HG13 | 1:A:231:VAL:HB     | 1.82                     | 0.60              |
| 2:B:375:GLN:HA   | 2:B:378:LEU:HB2    | 1.83                     | 0.60              |
| 3:G:238[A]:ASP:O | 3:G:242[A]:LYS:HG2 | 2.01                     | 0.60              |
| 1:A:426:GLU:HA   | 1:A:429:LYS:HZ2    | 1.65                     | 0.60              |
| 2:B:164:VAL:HG11 | 7:B:604:ADP:N7     | 2.16                     | 0.60              |
| 2:B:459:MET:O    | 2:B:460:VAL:HG13   | 2.00                     | 0.60              |
| 1:A:151:LYS:HG2  | 8:A:609:HOH:O      | 2.00                     | 0.60              |
| 1:A:387:ALA:HA   | 1:A:390:MET:SD     | 2.41                     | 0.60              |
| 2:B:93:ARG:HH22  | 2:B:101:PRO:HB3    | 1.65                     | 0.60              |
| 1:A:172:GLN:HG2  | 2:B:354:THR:HB     | 1.84                     | 0.60              |
| 2:B:410:ILE:HG12 | 2:B:441:PHE:HE1    | 1.65                     | 0.60              |
| 1:A:446:TYR:CE1  | 1:A:497:LEU:HD13   | 2.37                     | 0.60              |
| 2:B:406:ARG:HD2  | 2:B:444:ILE:O      | 2.01                     | 0.60              |
| 1:A:168:ILE:HG23 | 1:A:351:PHE:CD1    | 2.37                     | 0.60              |
| 2:B:225:PRO:C    | 2:B:229:ARG:HH21   | 2.05                     | 0.60              |
| 2:B:404:VAL:O    | 2:B:408:ARG:HG3    | 2.02                     | 0.59              |
| 2:B:413:PHE:HA   | 2:B:461:GLY:HA2    | 1.83                     | 0.59              |
| 1:A:135:GLY:N    | 1:A:139:ARG:HH21   | 1.99                     | 0.59              |
| 1:A:279:ARG:HD2  | 1:A:293:ALA:CB     | 2.31                     | 0.59              |
| 2:B:410:ILE:HG23 | 2:B:441:PHE:HZ     | 1.66                     | 0.59              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:108:VAL:HG22 | 1:A:232:VAL:HG12   | 1.83                     | 0.59              |
| 1:A:137:ILE:HD13 | 1:A:137:ILE:N      | 2.17                     | 0.59              |
| 1:A:135:GLY:H    | 1:A:139:ARG:HE     | 1.49                     | 0.59              |
| 1:A:176:THR:O    | 1:A:180:ILE:HB     | 2.03                     | 0.59              |
| 2:B:449:TYR:HB3  | 2:B:463:ILE:HD11   | 1.84                     | 0.59              |
| 1:A:426:GLU:HA   | 1:A:429:LYS:NZ     | 2.16                     | 0.59              |
| 1:A:64:LEU:CD2   | 1:A:281:MET:SD     | 2.90                     | 0.59              |
| 2:B:140:VAL:HG13 | 2:B:146:TYR:OH     | 2.01                     | 0.59              |
| 2:B:332:THR:HB   | 2:B:353:SER:HA     | 1.84                     | 0.59              |
| 2:B:342:LEU:HB2  | 2:B:344:ILE:HG12   | 1.84                     | 0.59              |
| 1:A:386:VAL:HG12 | 1:A:450:ARG:HH22   | 1.68                     | 0.59              |
| 1:A:431:GLY:CA   | 5:A:603:ATP:HN62   | 2.15                     | 0.59              |
| 2:B:321:ALA:HB3  | 2:B:322:PRO:HD3    | 1.83                     | 0.59              |
| 2:B:160:VAL:HA   | 2:B:345:TYR:OH     | 2.02                     | 0.59              |
| 1:A:49:ALA:O     | 1:A:50:GLU:CB      | 2.50                     | 0.58              |
| 1:A:78:ASN:H     | 1:A:78:ASN:ND2     | 2.01                     | 0.58              |
| 1:A:172:GLN:CD   | 5:A:603:ATP:H4'    | 2.22                     | 0.58              |
| 1:A:243:GLN:O    | 1:A:274:GLN:HG3    | 2.03                     | 0.58              |
| 1:A:497:LEU:O    | 1:A:500:ILE:HG22   | 2.04                     | 0.58              |
| 2:B:267:GLU:O    | 2:B:271:LEU:HD11   | 2.02                     | 0.58              |
| 1:A:99:VAL:HG23  | 1:A:253:MET:HA     | 1.85                     | 0.58              |
| 2:B:156:GLY:HA3  | 2:B:160:VAL:HG21   | 1.85                     | 0.58              |
| 2:B:118:ALA:HB3  | 2:B:295:ARG:NH2    | 2.19                     | 0.58              |
| 2:B:121:PRO:HG3  | 2:B:297:THR:HG22   | 1.86                     | 0.58              |
| 2:B:133:LEU:HB2  | 2:B:148:LYS:HD2    | 1.85                     | 0.58              |
| 2:B:252:LEU:HG   | 2:B:305:THR:O      | 2.04                     | 0.58              |
| 1:A:362:ARG:HH22 | 2:B:372:ARG:NH1    | 2.02                     | 0.58              |
| 1:A:385:GLN:OE1  | 1:A:488:LYS:HG2    | 2.04                     | 0.58              |
| 2:B:212:THR:HG22 | 2:B:214:LYS:HZ3    | 1.69                     | 0.58              |
| 2:B:118:ALA:HB3  | 2:B:295:ARG:HH21   | 1.68                     | 0.58              |
| 2:B:52:HIS:O     | 2:B:54:GLY:N       | 2.36                     | 0.58              |
| 2:B:94:ILE:CG2   | 2:B:102:ILE:HG13   | 2.33                     | 0.58              |
| 2:B:133:LEU:HB2  | 2:B:148:LYS:CD     | 2.34                     | 0.58              |
| 1:A:57:SER:HB2   | 1:A:81:LEU:HD22    | 1.86                     | 0.57              |
| 2:B:151:LYS:HB2  | 2:B:330:ASP:H      | 1.67                     | 0.57              |
| 1:A:472:VAL:HA   | 1:A:476:HIS:HB2    | 1.85                     | 0.57              |
| 2:B:450:ASP:O    | 2:B:451:HIS:HB3    | 2.04                     | 0.57              |
| 1:A:101:ASP:O    | 1:A:104:LEU:HB2    | 2.04                     | 0.57              |
| 1:A:107:VAL:HA   | 1:A:231:VAL:O      | 2.02                     | 0.57              |
| 2:B:23:VAL:O     | 2:B:57:THR:HG23    | 2.03                     | 0.57              |
| 1:A:291:ARG:HA   | 3:G:261[A]:GLU:OE1 | 2.04                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:457:PHE:CE2  | 2:B:466:ALA:HB2  | 2.39                     | 0.57              |
| 1:A:172:GLN:HB3  | 2:B:354:THR:HG21 | 1.86                     | 0.57              |
| 1:A:419:SER:O    | 1:A:423:ARG:HD3  | 2.04                     | 0.57              |
| 1:A:55:PHE:CE2   | 1:A:75:VAL:HG22  | 2.39                     | 0.57              |
| 2:B:138:LYS:NZ   | 2:B:441:PHE:HD2  | 2.03                     | 0.57              |
| 2:B:96:ASN:HD22  | 2:B:96:ASN:C     | 2.07                     | 0.57              |
| 2:B:188:GLU:HA   | 2:B:222:MET:HE1  | 1.86                     | 0.57              |
| 2:B:231:ARG:O    | 2:B:234:LEU:HB2  | 2.05                     | 0.57              |
| 1:A:279:ARG:HD2  | 1:A:293:ALA:HB3  | 1.85                     | 0.57              |
| 2:B:39:GLN:O     | 2:B:41:ARG:N     | 2.38                     | 0.57              |
| 2:B:94:ILE:HG22  | 2:B:102:ILE:CG1  | 2.31                     | 0.57              |
| 1:A:99:VAL:HG22  | 1:A:100:GLY:H    | 1.70                     | 0.57              |
| 2:B:220:GLY:N    | 2:B:232:VAL:HG21 | 2.20                     | 0.57              |
| 2:B:264:ALA:O    | 2:B:268:VAL:HG12 | 2.04                     | 0.57              |
| 1:A:164:ARG:HG2  | 1:A:306:LEU:HB3  | 1.86                     | 0.57              |
| 1:A:200:TYR:CD1  | 1:A:200:TYR:N    | 2.72                     | 0.57              |
| 1:A:362:ARG:HH11 | 5:A:603:ATP:H2   | 1.51                     | 0.57              |
| 1:A:78:ASN:N     | 1:A:78:ASN:HD22  | 2.03                     | 0.57              |
| 2:B:281:TYR:HD1  | 2:B:281:TYR:H    | 1.53                     | 0.57              |
| 1:A:362:ARG:HH12 | 2:B:372:ARG:HH11 | 1.51                     | 0.56              |
| 1:A:22:SER:HA    | 1:A:28:THR:HG21  | 1.87                     | 0.56              |
| 1:A:446:TYR:HD2  | 1:A:489:ILE:HD13 | 1.69                     | 0.56              |
| 1:A:22:SER:HB3   | 1:A:87:ILE:HD12  | 1.87                     | 0.56              |
| 1:A:166:LEU:O    | 1:A:349:GLN:HA   | 2.05                     | 0.56              |
| 1:A:146:MET:SD   | 1:A:265:LEU:HD13 | 2.45                     | 0.56              |
| 1:A:52:MET:SD    | 1:A:60:LYS:HD2   | 2.46                     | 0.56              |
| 1:A:358:TYR:HB2  | 2:B:375:GLN:HB2  | 1.87                     | 0.56              |
| 1:A:62:MET:SD    | 1:A:95:VAL:CG2   | 2.84                     | 0.56              |
| 1:A:338:ILE:HB   | 1:A:339:PRO:HD3  | 1.87                     | 0.56              |
| 2:B:118:ALA:H    | 2:B:295:ARG:NH2  | 2.04                     | 0.56              |
| 2:B:132:ILE:HG13 | 2:B:133:LEU:N    | 2.20                     | 0.56              |
| 2:B:218:VAL:HG11 | 2:B:235:THR:OG1  | 2.06                     | 0.56              |
| 2:B:311:TYR:O    | 2:B:322:PRO:HG3  | 2.04                     | 0.56              |
| 2:B:155:PHE:HB2  | 2:B:334:VAL:HA   | 1.87                     | 0.56              |
| 2:B:230:ALA:HB2  | 2:B:264:ALA:HB1  | 1.87                     | 0.55              |
| 1:A:438:ILE:O    | 1:A:442:VAL:HG23 | 2.06                     | 0.55              |
| 2:B:88:PRO:HA    | 2:B:91:LEU:CD1   | 2.35                     | 0.55              |
| 1:A:209:LYS:HE3  | 2:B:356:ARG:NH2  | 2.20                     | 0.55              |
| 1:A:139:ARG:HA   | 1:A:311:LYS:O    | 2.06                     | 0.55              |
| 1:A:345:ILE:HD12 | 8:A:605:HOH:O    | 2.06                     | 0.55              |
| 1:A:52:MET:HG3   | 1:A:61:GLY:O     | 2.07                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B:370:VAL:O     | 2:B:374:VAL:HG23   | 2.07                     | 0.55              |
| 2:B:410:ILE:HG12  | 2:B:441:PHE:CE1    | 2.40                     | 0.55              |
| 2:B:36:LEU:HD13   | 2:B:75:VAL:HG11    | 1.89                     | 0.55              |
| 1:A:178:ILE:HG23  | 1:A:179:ALA:N      | 2.22                     | 0.55              |
| 1:A:299:PHE:HA    | 1:A:341:ASN:ND2    | 2.22                     | 0.55              |
| 2:B:298:THR:HG22  | 2:B:299:THR:N      | 2.15                     | 0.55              |
| 3:G:20[A]:MET:SD  | 3:G:225[A]:ARG:HG3 | 2.46                     | 0.55              |
| 1:A:165:GLU:O     | 1:A:324:LEU:HA     | 2.05                     | 0.55              |
| 1:A:34:ILE:HD13   | 1:A:39:ALA:HB2     | 1.88                     | 0.55              |
| 1:A:41:VAL:HG12   | 1:A:42:HIS:O       | 2.06                     | 0.55              |
| 1:A:60:LYS:O      | 1:A:76:PHE:HB2     | 2.06                     | 0.55              |
| 2:B:154:LEU:HB3   | 8:B:612:HOH:O      | 2.05                     | 0.55              |
| 2:B:189:ARG:HB2   | 2:B:192:GLU:CG     | 2.28                     | 0.55              |
| 1:A:32:LEU:O      | 1:A:84:GLU:HG3     | 2.06                     | 0.55              |
| 1:A:496:LYS:HA    | 1:A:496:LYS:HE2    | 1.89                     | 0.55              |
| 2:B:85:PRO:HD2    | 2:B:95:MET:SD      | 2.47                     | 0.55              |
| 1:A:238:ASP:HB3   | 1:A:242:LEU:HB2    | 1.88                     | 0.55              |
| 1:A:394:LEU:HA    | 1:A:397:TYR:HB3    | 1.89                     | 0.55              |
| 2:B:207:ASN:HD21  | 2:B:210:ASP:N      | 2.05                     | 0.55              |
| 1:A:164:ARG:HD3   | 1:A:164:ARG:N      | 2.22                     | 0.54              |
| 1:A:403[B]:PHE:HA | 1:A:406[B]:PHE:CE1 | 2.42                     | 0.54              |
| 2:B:89:GLU:HB3    | 8:B:622:HOH:O      | 2.07                     | 0.54              |
| 1:A:148:THR:HG22  | 1:A:182:THR:HG23   | 1.89                     | 0.54              |
| 1:A:21:THR:HB     | 1:A:89:LYS:NZ      | 2.22                     | 0.54              |
| 2:B:96:ASN:HB3    | 2:B:102:ILE:HG23   | 1.89                     | 0.54              |
| 1:A:224:ASP:O     | 1:A:227:LYS:HB3    | 2.06                     | 0.54              |
| 1:A:204:VAL:O     | 1:A:269:ASP:HB2    | 2.08                     | 0.54              |
| 1:A:313:ASN:HD22  | 1:A:316:PHE:HB2    | 1.71                     | 0.54              |
| 2:B:410:ILE:HG23  | 2:B:441:PHE:CZ     | 2.43                     | 0.54              |
| 3:G:250[A]:THR:HA | 3:G:253[A]:ALA:HB3 | 1.90                     | 0.54              |
| 1:A:213:VAL:HB    | 2:B:123:PHE:HE1    | 1.73                     | 0.54              |
| 1:A:102:GLU:OE1   | 1:A:123:SER:HA     | 2.07                     | 0.54              |
| 1:A:166:LEU:HD12  | 1:A:342:VAL:HG12   | 1.89                     | 0.54              |
| 1:A:269:ASP:O     | 1:A:270:ASP:HB2    | 2.08                     | 0.54              |
| 1:A:248:TYR:CD1   | 1:A:305:LEU:HD13   | 2.43                     | 0.54              |
| 1:A:52:MET:HG2    | 1:A:60:LYS:HD2     | 1.89                     | 0.54              |
| 2:B:406:ARG:CZ    | 2:B:447:GLY:HA2    | 2.37                     | 0.54              |
| 2:B:435:LYS:HG2   | 2:B:436:GLU:HG2    | 1.90                     | 0.54              |
| 1:A:294:TYR:HB3   | 1:A:298:VAL:CG2    | 2.38                     | 0.54              |
| 1:A:152:ALA:HB2   | 1:A:428:LEU:O      | 2.08                     | 0.54              |
| 2:B:364:GLY:O     | 2:B:368:TYR:HB3    | 2.07                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:36:LEU:CD2     | 2:B:77:ASP:HA      | 2.38                     | 0.54              |
| 1:A:186:GLN:HB2    | 1:A:228:TYR:CE2    | 2.43                     | 0.54              |
| 1:A:264:ALA:HB3    | 1:A:321:LEU:CD1    | 2.38                     | 0.54              |
| 2:B:269:SER:HA     | 2:B:274:ARG:HD2    | 1.90                     | 0.54              |
| 1:A:141:SER:HB3    | 1:A:143:ARG:HH21   | 1.71                     | 0.54              |
| 2:B:50:ALA:HB2     | 2:B:61:ILE:CD1     | 2.38                     | 0.54              |
| 3:G:18[A]:LYS:O    | 3:G:21[A]:LYS:HB3  | 2.08                     | 0.54              |
| 2:B:151:LYS:HD2    | 2:B:328:HIS:O      | 2.09                     | 0.53              |
| 2:B:377:ILE:O      | 2:B:381[B]:TYR:HB2 | 2.07                     | 0.53              |
| 2:B:84:ILE:C       | 2:B:113:PHE:HB3    | 2.29                     | 0.53              |
| 2:B:140:VAL:HG13   | 2:B:146:TYR:CZ     | 2.42                     | 0.53              |
| 2:B:259:PHE:CE2    | 2:B:321:ALA:HB1    | 2.42                     | 0.53              |
| 3:G:228[A]:ALA:O   | 3:G:232[A]:ALA:HB3 | 2.08                     | 0.53              |
| 2:B:237:LEU:HD21   | 2:B:295:ARG:CB     | 2.38                     | 0.53              |
| 1:A:115:ILE:HG13   | 1:A:116:ASP:N      | 2.24                     | 0.53              |
| 1:A:336:ALA:O      | 1:A:339:PRO:HD2    | 2.09                     | 0.53              |
| 1:A:348:GLY:HA2    | 1:A:371:VAL:O      | 2.07                     | 0.53              |
| 1:A:393:GLU:O      | 1:A:397:TYR:HB2    | 2.08                     | 0.53              |
| 1:A:64:LEU:HD11    | 8:A:633:HOH:O      | 2.09                     | 0.53              |
| 1:A:148:THR:O      | 1:A:185:ASN:HB2    | 2.09                     | 0.53              |
| 1:A:44:LEU:O       | 1:A:47:VAL:HB      | 2.09                     | 0.53              |
| 2:B:89:GLU:HB2     | 2:B:110:THR:HG22   | 1.90                     | 0.53              |
| 2:B:230:ALA:HB3    | 2:B:231:ARG:HD3    | 1.91                     | 0.53              |
| 2:B:277:SER:O      | 2:B:280:GLY:N      | 2.38                     | 0.53              |
| 2:B:50:ALA:HB2     | 2:B:61:ILE:HD11    | 1.91                     | 0.53              |
| 1:A:52:MET:CG      | 1:A:60:LYS:HD2     | 2.39                     | 0.53              |
| 2:B:113:PHE:N      | 2:B:113:PHE:CD1    | 2.76                     | 0.53              |
| 2:B:378:LEU:HD23   | 2:B:381[B]:TYR:CD2 | 2.44                     | 0.53              |
| 1:A:279:ARG:CD     | 1:A:293:ALA:HB3    | 2.39                     | 0.53              |
| 2:B:94:ILE:HG12    | 2:B:217:LEU:HB2    | 1.90                     | 0.53              |
| 2:B:443:GLN:HB3    | 2:B:448:ASP:O      | 2.09                     | 0.53              |
| 2:B:66:THR:HG22    | 2:B:69:LEU:CD1     | 2.39                     | 0.53              |
| 1:A:235:THR:O      | 1:A:237:SER:N      | 2.41                     | 0.53              |
| 1:A:172:GLN:HG3    | 1:A:172:GLN:O      | 2.09                     | 0.52              |
| 2:B:119:GLU:OE1    | 2:B:119:GLU:HA     | 2.09                     | 0.52              |
| 3:G:247[A]:PHE:CE1 | 3:G:251[A]:ARG:HD2 | 2.43                     | 0.52              |
| 1:A:179:ALA:HB1    | 1:A:267:ILE:HD12   | 1.90                     | 0.52              |
| 1:A:383:MET:HB3    | 1:A:387:ALA:HB3    | 1.90                     | 0.52              |
| 2:B:394[B]:ASP:O   | 2:B:401:LYS:HE2    | 2.09                     | 0.52              |
| 1:A:450:ARG:HB3    | 1:A:452:TYR:CE2    | 2.44                     | 0.52              |
| 2:B:182:VAL:HG21   | 2:B:239:VAL:HG12   | 1.90                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B:159:GLY:HA2   | 7:B:604:ADP:O3A    | 2.09                     | 0.52              |
| 2:B:84:ILE:O      | 2:B:113:PHE:HB3    | 2.09                     | 0.52              |
| 3:G:229[A]:MET:SD | 3:G:229[A]:MET:N   | 2.82                     | 0.52              |
| 1:A:78:ASN:H      | 1:A:78:ASN:HD22    | 1.57                     | 0.52              |
| 2:B:94:ILE:CB     | 2:B:103:ASP:HB3    | 2.33                     | 0.52              |
| 2:B:242:TYR:HA    | 2:B:246:GLN:HE22   | 1.74                     | 0.52              |
| 2:B:83:LYS:HB3    | 2:B:115:PRO:HA     | 1.91                     | 0.52              |
| 1:A:278:TYR:CD2   | 1:A:301:LEU:HD22   | 2.45                     | 0.52              |
| 1:A:31:VAL:HG12   | 1:A:84:GLU:HA      | 1.91                     | 0.52              |
| 1:A:47:VAL:HG11   | 1:A:71:VAL:HG11    | 1.91                     | 0.52              |
| 2:B:96:ASN:HB3    | 2:B:102:ILE:HG21   | 1.91                     | 0.52              |
| 2:B:457:PHE:CZ    | 2:B:463:ILE:HA     | 2.44                     | 0.52              |
| 2:B:86:VAL:HG22   | 2:B:114:ALA:N      | 2.25                     | 0.52              |
| 2:B:165:LEU:HD12  | 2:B:165:LEU:O      | 2.10                     | 0.52              |
| 3:G:75[A]:CYS:SG  | 3:G:224[A]:ALA:HB1 | 2.49                     | 0.52              |
| 1:A:140:ILE:HB    | 1:A:313:ASN:HB2    | 1.90                     | 0.51              |
| 3:G:218[A]:THR:O  | 3:G:222[A]:GLN:HG2 | 2.10                     | 0.51              |
| 1:A:403[B]:PHE:HA | 1:A:406[B]:PHE:CZ  | 2.45                     | 0.51              |
| 1:A:282:SER:O     | 1:A:285:LEU:N      | 2.43                     | 0.51              |
| 2:B:156:GLY:HA3   | 2:B:160:VAL:CG2    | 2.41                     | 0.51              |
| 2:B:285:LEU:HD11  | 2:B:320:PRO:O      | 2.10                     | 0.51              |
| 1:A:131:LEU:HD12  | 1:A:132:LYS:H      | 1.75                     | 0.51              |
| 1:A:173:THR:HG21  | 1:A:352:LEU:C      | 2.31                     | 0.51              |
| 2:B:271:LEU:N     | 2:B:271:LEU:HD23   | 2.25                     | 0.51              |
| 1:A:116:ASP:O     | 1:A:118:LYS:N      | 2.44                     | 0.51              |
| 1:A:343:ILE:HD11  | 1:A:349:GLN:NE2    | 2.26                     | 0.51              |
| 2:B:330:ASP:HB2   | 2:B:356:ARG:HH21   | 1.76                     | 0.51              |
| 1:A:34:ILE:CG2    | 2:B:52:HIS:HB2     | 2.41                     | 0.51              |
| 2:B:32:ILE:HA     | 2:B:49:VAL:HG12    | 1.92                     | 0.51              |
| 1:A:300:TYR:O     | 1:A:304:ARG:HB3    | 2.11                     | 0.51              |
| 2:B:357:ILE:O     | 2:B:357:ILE:HG13   | 2.09                     | 0.51              |
| 2:B:457:PHE:CE2   | 2:B:463:ILE:HA     | 2.46                     | 0.51              |
| 1:A:116:ASP:OD2   | 1:A:118:LYS:HD2    | 2.11                     | 0.51              |
| 1:A:156:LEU:C     | 1:A:158:PRO:HD3    | 2.30                     | 0.51              |
| 1:A:436:MET:HB2   | 8:A:609:HOH:O      | 2.10                     | 0.51              |
| 1:A:84:GLU:HB2    | 2:B:52:HIS:HB3     | 1.93                     | 0.51              |
| 2:B:431:LEU:O     | 2:B:432:VAL:HB     | 2.11                     | 0.51              |
| 2:B:120:ALA:HB1   | 2:B:294:GLU:O      | 2.11                     | 0.51              |
| 2:B:142:LEU:HD23  | 2:B:143:LEU:N      | 2.26                     | 0.51              |
| 2:B:186:VAL:HG13  | 2:B:232:VAL:HG13   | 1.92                     | 0.51              |
| 3:G:255[A]:ILE:O  | 3:G:259[A]:LEU:HB2 | 2.10                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:386:VAL:HG23   | 1:A:387:ALA:N      | 2.26                     | 0.51              |
| 3:G:24[A]:ALA:HB1  | 3:G:226[A]:MET:HA  | 1.93                     | 0.51              |
| 3:G:35[A]:LEU:HD13 | 3:G:215[A]:LYS:HB3 | 1.93                     | 0.51              |
| 1:A:234:ALA:HB1    | 1:A:243:GLN:HA     | 1.93                     | 0.50              |
| 2:B:287:THR:O      | 2:B:291:THR:N      | 2.44                     | 0.50              |
| 2:B:44:ARG:NH1     | 2:B:44:ARG:HG2     | 2.24                     | 0.50              |
| 1:A:108:VAL:CG2    | 1:A:232:VAL:HG12   | 2.41                     | 0.50              |
| 1:A:189:PHE:HB3    | 1:A:197:LYS:O      | 2.11                     | 0.50              |
| 2:B:161:GLY:O      | 7:B:604:ADP:PB     | 2.70                     | 0.50              |
| 2:B:398[B]:GLU:HA  | 2:B:401:LYS:CB     | 2.40                     | 0.50              |
| 1:A:480:LEU:O      | 1:A:483:ILE:HB     | 2.12                     | 0.50              |
| 2:B:184:ALA:O      | 2:B:255:ILE:HA     | 2.11                     | 0.50              |
| 2:B:186:VAL:HG13   | 2:B:232:VAL:CG1    | 2.41                     | 0.50              |
| 2:B:96:ASN:ND2     | 2:B:96:ASN:C       | 2.65                     | 0.50              |
| 1:A:300:TYR:O      | 1:A:304:ARG:NE     | 2.45                     | 0.50              |
| 2:B:288:ASP:C      | 2:B:290:GLY:N      | 2.65                     | 0.50              |
| 2:B:290:GLY:O      | 2:B:292:MET:N      | 2.45                     | 0.50              |
| 2:B:427:HIS:HE1    | 2:B:459:MET:SD     | 2.34                     | 0.50              |
| 3:G:24[A]:ALA:O    | 3:G:226[A]:MET:SD  | 2.69                     | 0.50              |
| 1:A:452:TYR:HE1    | 8:A:610:HOH:O      | 1.94                     | 0.50              |
| 2:B:336:SER:O      | 2:B:339:ILE:HB     | 2.11                     | 0.50              |
| 2:B:137:ILE:HG23   | 2:B:416:GLN:HE22   | 1.74                     | 0.50              |
| 3:G:75[A]:CYS:SG   | 3:G:75[A]:CYS:O    | 2.69                     | 0.50              |
| 1:A:474:SER:O      | 1:A:475:GLN:HG3    | 2.12                     | 0.50              |
| 1:A:53:VAL:N       | 1:A:61:GLY:O       | 2.44                     | 0.50              |
| 2:B:91:LEU:HD21    | 2:B:180:TYR:CD2    | 2.46                     | 0.49              |
| 2:B:139:VAL:HG23   | 2:B:414:LEU:HB3    | 1.93                     | 0.49              |
| 1:A:204:VAL:HG13   | 1:A:232:VAL:CG2    | 2.41                     | 0.49              |
| 1:A:370:SER:O      | 1:A:371:VAL:HG13   | 2.13                     | 0.49              |
| 2:B:449:TYR:CB     | 2:B:463:ILE:HD11   | 2.42                     | 0.49              |
| 1:A:482:ASN:OD1    | 1:A:490:SER:HB2    | 2.12                     | 0.49              |
| 2:B:231:ARG:CD     | 2:B:231:ARG:N      | 2.74                     | 0.49              |
| 3:G:20[A]:MET:HB3  | 3:G:229[A]:MET:HG2 | 1.95                     | 0.49              |
| 1:A:198:LYS:O      | 1:A:199:LEU:HB2    | 2.13                     | 0.49              |
| 1:A:31:VAL:HB      | 1:A:85:GLY:H       | 1.77                     | 0.49              |
| 2:B:257:ASN:HB3    | 2:B:260:ARG:HG2    | 1.94                     | 0.49              |
| 1:A:156:LEU:CD2    | 1:A:390:MET:HB3    | 2.42                     | 0.49              |
| 2:B:377:ILE:HD11   | 2:B:403:THR:HA     | 1.94                     | 0.49              |
| 1:A:153:VAL:O      | 1:A:157:VAL:N      | 2.45                     | 0.49              |
| 1:A:313:ASN:ND2    | 1:A:316:PHE:HB2    | 2.27                     | 0.49              |
| 1:A:29:GLY:HA3     | 1:A:42:HIS:O       | 2.13                     | 0.49              |

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| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 2:B:259:PHE:CD1     | 2:B:259:PHE:C    | 2.84                     | 0.49              |
| 2:B:332:THR:HB      | 2:B:354:THR:N    | 2.28                     | 0.49              |
| 2:B:381[B]:TYR:CD1  | 2:B:403:THR:HG22 | 2.47                     | 0.49              |
| 1:A:181:ASP:O       | 1:A:184:ILE:HG22 | 2.13                     | 0.49              |
| 1:A:57:SER:CB       | 1:A:81:LEU:HB2   | 2.42                     | 0.49              |
| 1:A:153:VAL:HG13    | 1:A:157:VAL:HG23 | 1.95                     | 0.49              |
| 1:A:180:ILE:O       | 1:A:184:ILE:HB   | 2.13                     | 0.49              |
| 1:A:91:THR:O        | 1:A:93:ALA:N     | 2.46                     | 0.49              |
| 2:B:41:ARG:HG3      | 2:B:42:GLU:H     | 1.78                     | 0.49              |
| 2:B:166:ILE:HG12    | 2:B:254:PHE:CD2  | 2.40                     | 0.49              |
| 2:B:284:THR:O       | 2:B:286:ALA:N    | 2.45                     | 0.49              |
| 2:B:330:ASP:O       | 2:B:331:ALA:HB2  | 2.12                     | 0.49              |
| 1:A:175:LYS:HG2     | 1:A:352:LEU:HD12 | 1.95                     | 0.48              |
| 1:A:139:ARG:NH1     | 1:A:310:ALA:HB2  | 2.28                     | 0.48              |
| 2:B:374:VAL:O       | 2:B:377:ILE:HG22 | 2.12                     | 0.48              |
| 1:A:167:ILE:HG13    | 1:A:167:ILE:O    | 2.13                     | 0.48              |
| 1:A:203:TYR:O       | 1:A:231:VAL:HA   | 2.13                     | 0.48              |
| 1:A:28:THR:HG21     | 1:A:89:LYS:HZ3   | 1.77                     | 0.48              |
| 2:B:13:ILE:HD13     | 2:B:69:LEU:HD13  | 1.95                     | 0.48              |
| 2:B:191:ARG:HH21    | 2:B:192:GLU:HB3  | 1.78                     | 0.48              |
| 2:B:97:VAL:HG21     | 2:B:228:ALA:HB1  | 1.96                     | 0.48              |
| 1:A:204:VAL:HG13    | 1:A:232:VAL:HG23 | 1.95                     | 0.48              |
| 1:A:472:VAL:O       | 1:A:476:HIS:N    | 2.44                     | 0.48              |
| 2:B:381[B]:TYR:OH   | 2:B:408:ARG:HG2  | 2.13                     | 0.48              |
| 1:A:128:ARG:HG2     | 1:A:130:GLY:H    | 1.77                     | 0.48              |
| 2:B:469:LYS:CE      | 2:B:473:LEU:HD13 | 2.43                     | 0.48              |
| 2:B:476:GLU:O       | 2:B:477:HIS:HB2  | 2.13                     | 0.48              |
| 3:G:250[A]:THR:HG22 | 3:G:250[A]:THR:O | 2.13                     | 0.48              |
| 1:A:219:ARG:HA      | 1:A:222:ASP:OD2  | 2.13                     | 0.48              |
| 1:A:362:ARG:HD3     | 5:A:603:ATP:H2   | 1.78                     | 0.48              |
| 1:A:225:ALA:HA      | 1:A:228:TYR:HE1  | 1.74                     | 0.48              |
| 1:A:158:PRO:CG      | 1:A:379:GLN:HB3  | 2.38                     | 0.48              |
| 1:A:28:THR:HG21     | 1:A:89:LYS:NZ    | 2.29                     | 0.48              |
| 2:B:188:GLU:HA      | 2:B:222:MET:HE3  | 1.95                     | 0.48              |
| 2:B:312:VAL:O       | 2:B:312:VAL:HG12 | 2.13                     | 0.48              |
| 1:A:37:GLY:O        | 1:A:38:ILE:HD13  | 2.14                     | 0.48              |
| 2:B:255:ILE:HG21    | 2:B:258:ILE:HD13 | 1.96                     | 0.48              |
| 2:B:277:SER:OG      | 2:B:278:ALA:N    | 2.46                     | 0.48              |
| 1:A:135:GLY:N       | 1:A:139:ARG:HE   | 2.11                     | 0.48              |
| 2:B:298:THR:HG23    | 2:B:303:SER:HA   | 1.95                     | 0.48              |
| 2:B:36:LEU:HB2      | 2:B:47:LEU:O     | 2.14                     | 0.48              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:G:79[A]:HIS:CD2   | 3:G:79[A]:HIS:H    | 2.30                     | 0.48              |
| 1:A:99:VAL:HG22     | 1:A:100:GLY:N      | 2.29                     | 0.47              |
| 1:A:127:ARG:HH11    | 1:A:127:ARG:HG2    | 1.79                     | 0.47              |
| 1:A:495:ALA:O       | 1:A:498:LYS:HB3    | 2.13                     | 0.47              |
| 2:B:167:MET:SD      | 2:B:196:LEU:CD1    | 3.02                     | 0.47              |
| 2:B:142:LEU:HG      | 2:B:367:HIS:NE2    | 2.29                     | 0.47              |
| 1:A:211:SER:O       | 1:A:215:GLN:HG2    | 2.14                     | 0.47              |
| 1:A:397:TYR:CE1     | 1:A:418:LEU:HA     | 2.43                     | 0.47              |
| 2:B:332:THR:O       | 2:B:333:THR:HG23   | 2.13                     | 0.47              |
| 1:A:25:LEU:HA       | 1:A:28:THR:O       | 2.14                     | 0.47              |
| 1:A:446:TYR:CE2     | 1:A:489:ILE:HG21   | 2.50                     | 0.47              |
| 1:A:262:LYS:C       | 1:A:263:HIS:HD1    | 2.17                     | 0.47              |
| 1:A:356:LEU:HD12    | 1:A:364:ALA:HB1    | 1.96                     | 0.47              |
| 1:A:150:ILE:HD11    | 1:A:181:ASP:CB     | 2.37                     | 0.47              |
| 1:A:356:LEU:O       | 1:A:359:LYS:HG3    | 2.14                     | 0.47              |
| 2:B:139:VAL:HG13    | 2:B:143:LEU:HG     | 1.96                     | 0.47              |
| 1:A:172:GLN:CG      | 2:B:354:THR:HB     | 2.45                     | 0.47              |
| 1:A:140:ILE:HG13    | 1:A:143:ARG:HH22   | 1.79                     | 0.47              |
| 1:A:349:GLN:CD      | 1:A:370:SER:HA     | 2.35                     | 0.47              |
| 2:B:143:LEU:O       | 2:B:145:PRO:HD3    | 2.14                     | 0.47              |
| 2:B:39:GLN:C        | 2:B:41:ARG:H       | 2.17                     | 0.47              |
| 1:A:149:GLY:HA3     | 1:A:435:PRO:HB2    | 1.97                     | 0.47              |
| 2:B:165:LEU:HA      | 2:B:168:GLU:HB3    | 1.96                     | 0.47              |
| 2:B:187:GLY:O       | 2:B:188:GLU:O      | 2.33                     | 0.47              |
| 2:B:319:ASP:C       | 2:B:321:ALA:H      | 2.18                     | 0.47              |
| 2:B:164:VAL:HG23    | 7:B:604:ADP:O2A    | 2.15                     | 0.47              |
| 1:A:99:VAL:HG11     | 1:A:127:ARG:HB2    | 1.97                     | 0.47              |
| 2:B:384[B]:LEU:HD22 | 2:B:400:ASP:HB3    | 1.96                     | 0.47              |
| 2:B:164:VAL:HG21    | 7:B:604:ADP:C8     | 2.50                     | 0.47              |
| 1:A:137:ILE:H       | 1:A:137:ILE:CD1    | 2.16                     | 0.47              |
| 1:A:36:ASP:O        | 1:A:38:ILE:HG12    | 2.15                     | 0.47              |
| 2:B:344:ILE:HG23    | 2:B:415:SER:OG     | 2.15                     | 0.47              |
| 2:B:381[B]:TYR:HA   | 2:B:384[B]:LEU:CD2 | 2.44                     | 0.47              |
| 2:B:374:VAL:HG22    | 2:B:410:ILE:HD13   | 1.97                     | 0.47              |
| 2:B:469:LYS:HE2     | 2:B:473:LEU:HD22   | 1.96                     | 0.47              |
| 2:B:350:PRO:CB      | 2:B:378:LEU:HD13   | 2.45                     | 0.46              |
| 1:A:164:ARG:H       | 1:A:164:ARG:HD3    | 1.79                     | 0.46              |
| 1:A:178:ILE:HG23    | 1:A:179:ALA:H      | 1.81                     | 0.46              |
| 2:B:378:LEU:HD23    | 2:B:381[B]:TYR:HD2 | 1.78                     | 0.46              |
| 1:A:363:PRO:O       | 1:A:364:ALA:HB3    | 2.15                     | 0.46              |
| 2:B:84:ILE:HG21     | 2:B:235:THR:CG2    | 2.44                     | 0.46              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 3:G:2[A]:ASP:HA   | 3:G:5[A]:ARG:HH12   | 1.80                     | 0.46              |
| 1:A:382:ALA:O     | 1:A:386:VAL:HG22    | 2.16                     | 0.46              |
| 1:A:397:TYR:CE2   | 1:A:401[B]:ALA:HB2  | 2.50                     | 0.46              |
| 1:A:45:ARG:C      | 1:A:45:ARG:HD3      | 2.36                     | 0.46              |
| 2:B:137:ILE:O     | 2:B:141:ASP:N       | 2.49                     | 0.46              |
| 1:A:31:VAL:HG13   | 1:A:33:SER:O        | 2.15                     | 0.46              |
| 1:A:66:LEU:HB3    | 8:A:618:HOH:O       | 2.16                     | 0.46              |
| 2:B:186:VAL:CG1   | 2:B:260:ARG:HB2     | 2.46                     | 0.46              |
| 2:B:237:LEU:CD2   | 2:B:295:ARG:HD3     | 2.44                     | 0.46              |
| 2:B:154:LEU:HA    | 2:B:333:THR:OG1     | 2.16                     | 0.46              |
| 2:B:349:ASP:OD1   | 2:B:350:PRO:HD2     | 2.16                     | 0.46              |
| 2:B:428:MET:HB3   | 2:B:430:LYS:HE2     | 1.97                     | 0.46              |
| 2:B:160:VAL:O     | 2:B:345:TYR:CE2     | 2.69                     | 0.46              |
| 2:B:257:ASN:H     | 2:B:309:ALA:HB3     | 1.80                     | 0.46              |
| 2:B:323:ALA:O     | 2:B:325:THR:N       | 2.49                     | 0.46              |
| 2:B:145:PRO:C     | 2:B:146:TYR:HD1     | 2.19                     | 0.46              |
| 2:B:151:LYS:NZ    | 2:B:293:GLN:O       | 2.47                     | 0.46              |
| 2:B:251:VAL:HG12  | 2:B:252:LEU:O       | 2.16                     | 0.46              |
| 2:B:330:ASP:HB2   | 2:B:356:ARG:NH2     | 2.31                     | 0.46              |
| 2:B:78:SER:OG     | 2:B:79:GLY:N        | 2.49                     | 0.46              |
| 1:A:184:ILE:HD12  | 1:A:225:ALA:HB2     | 1.98                     | 0.46              |
| 1:A:208:GLN:O     | 1:A:235:THR:HG22    | 2.15                     | 0.46              |
| 1:A:54:GLU:HB3    | 1:A:89:LYS:HB2      | 1.97                     | 0.46              |
| 2:B:398[B]:GLU:HA | 2:B:401:LYS:HB2     | 1.97                     | 0.46              |
| 2:B:44:ARG:CG     | 2:B:44:ARG:NH1      | 2.79                     | 0.46              |
| 1:A:150:ILE:CG2   | 1:A:153:VAL:HG23    | 2.46                     | 0.45              |
| 2:B:222:MET:C     | 2:B:224:GLU:H       | 2.18                     | 0.45              |
| 2:B:298:THR:O     | 2:B:299:THR:HB      | 2.16                     | 0.45              |
| 1:A:104:LEU:HD22  | 1:A:230:ILE:HD11    | 1.97                     | 0.45              |
| 1:A:219:ARG:NH1   | 1:A:433:TYR:CE2     | 2.83                     | 0.45              |
| 2:B:194:ASN:O     | 2:B:197:TYR:HB3     | 2.16                     | 0.45              |
| 2:B:155:PHE:O     | 2:B:335:LEU:N       | 2.49                     | 0.45              |
| 2:B:145:PRO:HG3   | 2:B:363:VAL:HG11    | 1.97                     | 0.45              |
| 1:A:453:LEU:HD12  | 1:A:453:LEU:H       | 1.81                     | 0.45              |
| 2:B:383[B]:SER:O  | 2:B:387[B]:ILE:N    | 2.49                     | 0.45              |
| 1:A:477:GLN:HE21  | 1:A:477:GLN:HA      | 1.81                     | 0.45              |
| 2:B:96:ASN:HB3    | 2:B:102:ILE:HD13    | 1.97                     | 0.45              |
| 2:B:278:ALA:O     | 2:B:279:VAL:HB      | 2.15                     | 0.45              |
| 2:B:374:VAL:HG12  | 2:B:378:LEU:HD12    | 1.98                     | 0.45              |
| 3:G:3[A]:ILE:HG23 | 3:G:243[A]:LEU:HD12 | 1.98                     | 0.45              |
| 1:A:446:TYR:O     | 1:A:449:VAL:HG12    | 2.17                     | 0.45              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 1:A:55:PHE:CE2   | 1:A:75:VAL:CG2      | 2.99                     | 0.45              |
| 1:A:144:GLU:O    | 1:A:161:ARG:HB2     | 2.17                     | 0.45              |
| 1:A:175:LYS:CG   | 1:A:352:LEU:HD12    | 2.47                     | 0.45              |
| 2:B:400:ASP:O    | 2:B:403:THR:HB      | 2.17                     | 0.45              |
| 2:B:96:ASN:ND2   | 2:B:100:GLU:H       | 2.15                     | 0.45              |
| 1:A:166:LEU:HD23 | 1:A:167:ILE:N       | 2.32                     | 0.45              |
| 2:B:36:LEU:HD13  | 2:B:75:VAL:CG1      | 2.46                     | 0.45              |
| 3:G:258[A]:GLU:O | 3:G:262[A]:ILE:HG13 | 2.16                     | 0.45              |
| 1:A:106:ARG:CZ   | 1:A:118:LYS:HB2     | 2.47                     | 0.45              |
| 1:A:183:ILE:HD11 | 1:A:267:ILE:CG1     | 2.40                     | 0.45              |
| 1:A:326:VAL:O    | 1:A:327:ILE:HD13    | 2.16                     | 0.45              |
| 1:A:71:VAL:O     | 1:A:71:VAL:HG12     | 2.16                     | 0.45              |
| 2:B:180:TYR:CD2  | 2:B:249:GLN:NE2     | 2.80                     | 0.45              |
| 1:A:147:GLN:OE1  | 1:A:438:ILE:HB      | 2.16                     | 0.45              |
| 2:B:171:ASN:HA   | 2:B:175:LYS:HE3     | 1.98                     | 0.45              |
| 1:A:157:VAL:HG23 | 1:A:157:VAL:O       | 2.17                     | 0.45              |
| 1:A:270:ASP:CB   | 1:A:273:LYS:HB2     | 2.32                     | 0.45              |
| 1:A:106:ARG:NH2  | 1:A:118:LYS:HB2     | 2.32                     | 0.44              |
| 1:A:250:GLY:HA2  | 1:A:253:MET:CG      | 2.47                     | 0.44              |
| 2:B:128:VAL:O    | 2:B:130:GLN:HG3     | 2.18                     | 0.44              |
| 2:B:16:VAL:HG21  | 2:B:69:LEU:HB3      | 1.99                     | 0.44              |
| 2:B:38:VAL:HG12  | 2:B:39:GLN:O        | 2.17                     | 0.44              |
| 2:B:386[B]:ASP:O | 2:B:390[B]:ILE:HA   | 2.17                     | 0.44              |
| 3:G:254[A]:VAL:O | 3:G:258[A]:GLU:HG2  | 2.17                     | 0.44              |
| 1:A:209:LYS:HB2  | 1:A:209:LYS:NZ      | 2.33                     | 0.44              |
| 1:A:306:LEU:H    | 1:A:306:LEU:CD2     | 2.30                     | 0.44              |
| 1:A:460:LYS:O    | 1:A:463:LYS:HB2     | 2.18                     | 0.44              |
| 2:B:94:ILE:CG1   | 2:B:217:LEU:HD12    | 2.47                     | 0.44              |
| 2:B:365:SER:HA   | 2:B:368:TYR:CD1     | 2.52                     | 0.44              |
| 1:A:359:LYS:HG2  | 2:B:376:LYS:HA      | 1.98                     | 0.44              |
| 2:B:244:ARG:HE   | 2:B:245:ASP:CG      | 2.20                     | 0.44              |
| 2:B:296:ILE:HG13 | 2:B:296:ILE:O       | 2.17                     | 0.44              |
| 2:B:94:ILE:HG12  | 2:B:217:LEU:CB      | 2.47                     | 0.44              |
| 1:A:169:GLY:HA2  | 1:A:352:LEU:O       | 2.16                     | 0.44              |
| 1:A:51:GLU:O     | 1:A:51:GLU:HG3      | 2.17                     | 0.44              |
| 2:B:20:VAL:CG1   | 2:B:59:ARG:HD2      | 2.48                     | 0.44              |
| 2:B:251:VAL:HG12 | 2:B:252:LEU:N       | 2.32                     | 0.44              |
| 2:B:57:THR:HG22  | 2:B:58:VAL:O        | 2.18                     | 0.44              |
| 1:A:298:VAL:HG11 | 1:A:337:TYR:HE1     | 1.83                     | 0.44              |
| 1:A:306:LEU:H    | 1:A:306:LEU:HD22    | 1.82                     | 0.44              |
| 1:A:65:ASN:HB3   | 1:A:67:GLU:OE2      | 2.16                     | 0.44              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:B:146:TYR:O      | 2:B:147:ALA:HB2     | 2.18                     | 0.44              |
| 2:B:336:SER:HB3    | 2:B:339:ILE:CG1     | 2.47                     | 0.44              |
| 1:A:106:ARG:HD3    | 1:A:121:VAL:HG21    | 2.00                     | 0.44              |
| 1:A:140:ILE:HG23   | 1:A:141:SER:N       | 2.20                     | 0.44              |
| 1:A:169:GLY:N      | 1:A:175:LYS:HD3     | 2.33                     | 0.44              |
| 1:A:189:PHE:CD2    | 1:A:197:LYS:O       | 2.70                     | 0.44              |
| 2:B:133:LEU:CD1    | 2:B:148:LYS:HE3     | 2.29                     | 0.44              |
| 1:A:188:ARG:HG3    | 1:A:189:PHE:CD1     | 2.53                     | 0.44              |
| 1:A:62:MET:HG3     | 1:A:64:LEU:HD13     | 2.00                     | 0.44              |
| 2:B:214:LYS:HD3    | 2:B:214:LYS:N       | 2.33                     | 0.44              |
| 1:A:219:ARG:HH11   | 1:A:433:TYR:HE2     | 1.66                     | 0.44              |
| 1:A:27:GLU:OE1     | 1:A:90:ARG:NH1      | 2.51                     | 0.44              |
| 2:B:230:ALA:CB     | 2:B:231:ARG:HD3     | 2.47                     | 0.44              |
| 2:B:246:GLN:HE21   | 2:B:246:GLN:H       | 1.66                     | 0.44              |
| 2:B:269:SER:O      | 2:B:272:LEU:N       | 2.43                     | 0.44              |
| 2:B:33:LEU:HD23    | 2:B:33:LEU:HA       | 1.60                     | 0.44              |
| 1:A:170:ASP:HA     | 1:A:329:THR:O       | 2.18                     | 0.44              |
| 1:A:261:GLY:O      | 1:A:263:HIS:CE1     | 2.70                     | 0.44              |
| 1:A:313:ASN:ND2    | 1:A:316:PHE:N       | 2.66                     | 0.44              |
| 1:A:458:PRO:HB3    | 1:A:461:ILE:HD11    | 1.99                     | 0.44              |
| 2:B:200:MET:SD     | 2:B:205:VAL:HG11    | 2.58                     | 0.44              |
| 2:B:157:GLY:C      | 2:B:311:TYR:HE1     | 2.21                     | 0.44              |
| 2:B:259:PHE:HD2    | 2:B:321:ALA:HB1     | 1.78                     | 0.44              |
| 2:B:367:HIS:CD2    | 2:B:367:HIS:C       | 2.91                     | 0.44              |
| 2:B:89:GLU:H       | 2:B:89:GLU:HG2      | 1.57                     | 0.44              |
| 1:A:209:LYS:HE3    | 2:B:356:ARG:HH22    | 1.83                     | 0.43              |
| 1:A:99:VAL:CG2     | 1:A:253:MET:HA      | 2.46                     | 0.43              |
| 1:A:29:GLY:N       | 1:A:44:LEU:HD22     | 2.32                     | 0.43              |
| 1:A:29:GLY:O       | 1:A:88:VAL:N        | 2.51                     | 0.43              |
| 2:B:83:LYS:NZ      | 2:B:113:PHE:O       | 2.51                     | 0.43              |
| 1:A:483:ILE:O      | 1:A:487:GLY:HA2     | 2.18                     | 0.43              |
| 2:B:70:VAL:O       | 2:B:72:GLY:N        | 2.51                     | 0.43              |
| 2:B:86:VAL:HG21    | 2:B:114:ALA:CB      | 2.41                     | 0.43              |
| 3:G:206[A]:LEU:O   | 3:G:210[A]:ILE:HG22 | 2.17                     | 0.43              |
| 1:A:248:TYR:OH     | 1:A:301:LEU:HD12    | 2.18                     | 0.43              |
| 2:B:154:LEU:HD12   | 2:B:162:LYS:CA      | 2.34                     | 0.43              |
| 2:B:98:ILE:HG22    | 2:B:98:ILE:O        | 2.17                     | 0.43              |
| 3:G:16[A]:ILE:N    | 3:G:16[A]:ILE:HD12  | 2.33                     | 0.43              |
| 3:G:228[A]:ALA:HB3 | 3:G:229[A]:MET:SD   | 2.58                     | 0.43              |
| 1:A:155:SER:N      | 1:A:441:GLN:OE1     | 2.51                     | 0.43              |
| 2:B:177:HIS:CE1    | 2:B:178:GLY:O       | 2.72                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:177:HIS:CD2   | 2:B:178:GLY:O    | 2.72                     | 0.43              |
| 2:B:393[B]:MET:SD | 2:B:404:VAL:HG11 | 2.58                     | 0.43              |
| 1:A:200:TYR:HD1   | 1:A:200:TYR:N    | 2.15                     | 0.43              |
| 1:A:426:GLU:CD    | 1:A:429:LYS:HZ1  | 2.22                     | 0.43              |
| 1:A:79:ASP:O      | 1:A:81:LEU:N     | 2.51                     | 0.43              |
| 1:A:94:ILE:HG22   | 1:A:95:VAL:N     | 2.33                     | 0.43              |
| 2:B:222:MET:O     | 2:B:224:GLU:N    | 2.52                     | 0.43              |
| 2:B:326:PHE:C     | 2:B:328:HIS:H    | 2.21                     | 0.43              |
| 2:B:130:GLN:HB3   | 2:B:357:ILE:HD13 | 2.01                     | 0.43              |
| 2:B:42:GLU:O      | 2:B:43:SER:HB2   | 2.19                     | 0.43              |
| 1:A:286:ARG:HA    | 2:B:275:ILE:HD12 | 2.00                     | 0.43              |
| 1:A:429:LYS:HB2   | 1:A:429:LYS:NZ   | 2.34                     | 0.43              |
| 1:A:59:LEU:HD21   | 1:A:76:PHE:O     | 2.18                     | 0.43              |
| 2:B:90:THR:HG22   | 2:B:108:ILE:CG2  | 2.49                     | 0.43              |
| 2:B:118:ALA:N     | 2:B:295:ARG:NH2  | 2.66                     | 0.43              |
| 2:B:296:ILE:HD12  | 2:B:306:SER:OG   | 2.19                     | 0.43              |
| 1:A:355:GLU:HG2   | 2:B:379:GLN:NE2  | 2.33                     | 0.43              |
| 1:A:180:ILE:HA    | 1:A:180:ILE:HD12 | 1.80                     | 0.43              |
| 1:A:196:LYS:HB3   | 1:A:196:LYS:NZ   | 2.32                     | 0.43              |
| 1:A:386:VAL:HG13  | 1:A:489:ILE:HD11 | 2.01                     | 0.43              |
| 1:A:500:ILE:HA    | 1:A:500:ILE:HD12 | 1.84                     | 0.43              |
| 1:A:22:SER:HB3    | 1:A:87:ILE:CD1   | 2.48                     | 0.43              |
| 2:B:326:PHE:O     | 2:B:328:HIS:N    | 2.51                     | 0.43              |
| 2:B:139:VAL:HG11  | 2:B:348:VAL:CG1  | 2.49                     | 0.43              |
| 2:B:406:ARG:O     | 2:B:410:ILE:HG13 | 2.19                     | 0.43              |
| 2:B:168:GLU:N     | 2:B:420:VAL:HG21 | 2.33                     | 0.43              |
| 1:A:109:ASP:O     | 1:A:233:SER:N    | 2.51                     | 0.43              |
| 1:A:263:HIS:HB3   | 1:A:320:SER:OG   | 2.18                     | 0.43              |
| 1:A:200:TYR:O     | 1:A:264:ALA:HA   | 2.18                     | 0.43              |
| 1:A:168:ILE:HD13  | 1:A:334:VAL:HG12 | 2.01                     | 0.43              |
| 2:B:88:PRO:C      | 2:B:90:THR:H     | 2.21                     | 0.43              |
| 1:A:255:GLU:HG2   | 1:A:258:ARG:NH1  | 2.34                     | 0.43              |
| 1:A:87:ILE:HA     | 1:A:87:ILE:HD13  | 1.81                     | 0.43              |
| 2:B:203:SER:HA    | 8:B:620:HOH:O    | 2.19                     | 0.43              |
| 2:B:319:ASP:OD1   | 2:B:320:PRO:HD2  | 2.19                     | 0.43              |
| 2:B:333:THR:HA    | 2:B:353:SER:OG   | 2.19                     | 0.43              |
| 1:A:186:GLN:HB2   | 1:A:228:TYR:HE2  | 1.83                     | 0.43              |
| 1:A:229:THR:HG22  | 1:A:230:ILE:N    | 2.34                     | 0.43              |
| 2:B:161:GLY:O     | 2:B:162:LYS:HB2  | 2.18                     | 0.43              |
| 2:B:268:VAL:HA    | 2:B:271:LEU:HG   | 2.01                     | 0.43              |
| 2:B:330:ASP:O     | 2:B:331:ALA:CB   | 2.67                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:B:428:MET:O      | 2:B:430:LYS:N     | 2.52                     | 0.43              |
| 2:B:35:ALA:HB2     | 2:B:82:ILE:N      | 2.34                     | 0.43              |
| 1:A:228:TYR:CD2    | 1:A:228:TYR:O     | 2.72                     | 0.42              |
| 2:B:200:MET:HB3    | 2:B:206:ILE:CD1   | 2.49                     | 0.42              |
| 2:B:188:GLU:HG3    | 6:B:601:PO4:O3    | 2.18                     | 0.42              |
| 1:A:276:VAL:HG12   | 2:B:286:ALA:HB2   | 2.01                     | 0.42              |
| 1:A:294:TYR:HB3    | 1:A:298:VAL:HG22  | 2.01                     | 0.42              |
| 1:A:173:THR:HG22   | 1:A:352:LEU:HB3   | 2.01                     | 0.42              |
| 2:B:220:GLY:HA3    | 2:B:232:VAL:HB    | 2.01                     | 0.42              |
| 3:G:17[A]:THR:HG22 | 3:G:229[A]:MET:HA | 2.00                     | 0.42              |
| 1:A:127:ARG:NH1    | 1:A:127:ARG:HG2   | 2.35                     | 0.42              |
| 1:A:313:ASN:HD21   | 1:A:315:SER:HB2   | 1.84                     | 0.42              |
| 2:B:253:LEU:CG     | 2:B:255:ILE:HD11  | 2.47                     | 0.42              |
| 2:B:292:MET:CE     | 2:B:293:GLN:HG2   | 2.46                     | 0.42              |
| 2:B:118:ALA:N      | 2:B:295:ARG:HH22  | 2.18                     | 0.42              |
| 2:B:358:MET:HG2    | 2:B:358:MET:O     | 2.19                     | 0.42              |
| 2:B:465:GLU:O      | 2:B:469:LYS:N     | 2.52                     | 0.42              |
| 1:A:199:LEU:HD12   | 1:A:199:LEU:HA    | 1.74                     | 0.42              |
| 1:A:306:LEU:C      | 1:A:308:ARG:H     | 2.23                     | 0.42              |
| 2:B:142:LEU:HG     | 2:B:367:HIS:CD2   | 2.54                     | 0.42              |
| 2:B:452:LEU:HA     | 2:B:453:PRO:HD3   | 1.92                     | 0.42              |
| 3:G:86[A]:MET:O    | 3:G:87[A]:LYS:HG3 | 2.19                     | 0.42              |
| 1:A:468:PHE:O      | 1:A:472:VAL:HG23  | 2.19                     | 0.42              |
| 2:B:259:PHE:CE1    | 2:B:263:GLN:OE1   | 2.72                     | 0.42              |
| 1:A:251:CYS:SG     | 1:A:268:TYR:OH    | 2.69                     | 0.42              |
| 1:A:351:PHE:CZ     | 1:A:353:GLU:HG2   | 2.54                     | 0.42              |
| 1:A:479:LEU:CD1    | 1:A:479:LEU:H     | 2.28                     | 0.42              |
| 2:B:111:LYS:HB2    | 2:B:112:GLN:OE1   | 2.20                     | 0.42              |
| 2:B:182:VAL:HG12   | 2:B:183:PHE:N     | 2.34                     | 0.42              |
| 1:A:202:ILE:HD11   | 1:A:257:PHE:HE2   | 1.85                     | 0.42              |
| 1:A:381:ARG:H      | 1:A:381:ARG:HD2   | 1.85                     | 0.42              |
| 2:B:285:LEU:HG     | 2:B:285:LEU:O     | 2.19                     | 0.42              |
| 2:B:350:PRO:HB2    | 2:B:378:LEU:HD13  | 2.02                     | 0.42              |
| 2:B:428:MET:CB     | 2:B:430:LYS:HE2   | 2.49                     | 0.42              |
| 2:B:164:VAL:HG21   | 7:B:604:ADP:N7    | 2.34                     | 0.42              |
| 1:A:490:SER:HB3    | 1:A:493:SER:HB2   | 2.00                     | 0.42              |
| 2:B:234:LEU:O      | 2:B:238:THR:N     | 2.49                     | 0.42              |
| 2:B:244:ARG:HG3    | 2:B:302:GLY:HA3   | 2.01                     | 0.42              |
| 2:B:158:ALA:H      | 2:B:337:ARG:NH2   | 2.18                     | 0.42              |
| 3:G:81[A]:SER:HA   | 3:G:84[A]:LYS:HE2 | 2.00                     | 0.42              |
| 1:A:202:ILE:O      | 1:A:266:ILE:HG13  | 2.19                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:A:286:ARG:HA     | 2:B:275:ILE:CD1     | 2.50                     | 0.42              |
| 2:B:258:ILE:HD11   | 2:B:292:MET:SD      | 2.60                     | 0.42              |
| 1:A:209:LYS:HE3    | 2:B:356:ARG:CZ      | 2.50                     | 0.42              |
| 2:B:433:PRO:O      | 2:B:435:LYS:N       | 2.53                     | 0.42              |
| 2:B:29:LEU:HD12    | 2:B:58:VAL:HG13     | 2.01                     | 0.42              |
| 1:A:140:ILE:HG12   | 1:A:143:ARG:HH12    | 1.84                     | 0.42              |
| 1:A:164:ARG:HB3    | 1:A:306:LEU:HD12    | 2.01                     | 0.42              |
| 1:A:173:THR:CG2    | 1:A:352:LEU:HB3     | 2.50                     | 0.42              |
| 2:B:138:LYS:HD2    | 2:B:414:LEU:CD2     | 2.48                     | 0.42              |
| 3:G:27[A]:LYS:HE2  | 3:G:222[A]:GLN:OE1  | 2.20                     | 0.42              |
| 3:G:10[A]:ILE:HG21 | 3:G:240[A]:ILE:HG13 | 2.01                     | 0.42              |
| 3:G:36[A]:LYS:HA   | 3:G:36[A]:LYS:HD2   | 1.82                     | 0.42              |
| 1:A:150:ILE:HG21   | 1:A:153:VAL:HG23    | 2.01                     | 0.41              |
| 1:A:16:ARG:O       | 1:A:18:GLY:N        | 2.52                     | 0.41              |
| 1:A:129:VAL:O      | 1:A:308:ARG:NH1     | 2.53                     | 0.41              |
| 1:A:496:LYS:CA     | 1:A:496:LYS:HE2     | 2.49                     | 0.41              |
| 2:B:16:VAL:O       | 2:B:17:ILE:HG13     | 2.20                     | 0.41              |
| 2:B:230:ALA:HB2    | 2:B:264:ALA:CB      | 2.49                     | 0.41              |
| 2:B:97:VAL:C       | 2:B:98:ILE:HG12     | 2.40                     | 0.41              |
| 1:A:306:LEU:O      | 1:A:308:ARG:N       | 2.54                     | 0.41              |
| 2:B:401:LYS:HE3    | 2:B:401:LYS:HB2     | 1.79                     | 0.41              |
| 2:B:25:PHE:HE2     | 2:B:77:ASP:HB2      | 1.84                     | 0.41              |
| 2:B:86:VAL:O       | 2:B:112:GLN:NE2     | 2.53                     | 0.41              |
| 1:A:244:TYR:O      | 1:A:274:GLN:NE2     | 2.54                     | 0.41              |
| 1:A:338:ILE:CB     | 1:A:339:PRO:HD3     | 2.49                     | 0.41              |
| 1:A:44:LEU:HD21    | 1:A:88:VAL:HB       | 2.02                     | 0.41              |
| 2:B:378:LEU:C      | 2:B:381[B]:TYR:HB3  | 2.40                     | 0.41              |
| 2:B:421:ALA:HB2    | 7:B:604:ADP:C6      | 2.54                     | 0.41              |
| 1:A:423:ARG:HG2    | 1:A:454:ASP:O       | 2.21                     | 0.41              |
| 1:A:282:SER:OG     | 1:A:287:ARG:HB2     | 2.20                     | 0.41              |
| 1:A:74:VAL:HG13    | 1:A:74:VAL:O        | 2.20                     | 0.41              |
| 2:B:255:ILE:HD12   | 2:B:255:ILE:N       | 2.36                     | 0.41              |
| 3:G:7[A]:LEU:HD23  | 3:G:10[A]:ILE:HD12  | 2.02                     | 0.41              |
| 1:A:185:ASN:OD1    | 1:A:188:ARG:NH2     | 2.53                     | 0.41              |
| 1:A:270:ASP:H      | 1:A:326:VAL:HB      | 1.84                     | 0.41              |
| 2:B:180:TYR:HB3    | 2:B:181:SER:H       | 1.71                     | 0.41              |
| 2:B:398[B]:GLU:HA  | 2:B:401:LYS:HB3     | 2.01                     | 0.41              |
| 2:B:381[B]:TYR:HB2 | 2:B:403:THR:HG21    | 2.02                     | 0.41              |
| 1:A:42:HIS:CG      | 1:A:43:GLY:N        | 2.89                     | 0.41              |
| 2:B:244:ARG:HG2    | 2:B:245:ASP:N       | 2.32                     | 0.41              |
| 1:A:294:TYR:HA     | 1:A:295:PRO:HD3     | 1.63                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:A:351:PHE:HD2     | 1:A:366:ASN:HB3    | 1.86                     | 0.41              |
| 1:A:381:ARG:CD      | 1:A:381:ARG:H      | 2.33                     | 0.41              |
| 1:A:150:ILE:HG23    | 1:A:430:GLN:HG2    | 2.02                     | 0.41              |
| 1:A:492:GLN:O       | 1:A:496:LYS:HG2    | 2.21                     | 0.41              |
| 2:B:151:LYS:O       | 2:B:330:ASP:N      | 2.53                     | 0.41              |
| 2:B:84:ILE:HD11     | 2:B:238:THR:HB     | 2.02                     | 0.41              |
| 2:B:126:MET:HE1     | 2:B:297:THR:HG21   | 2.03                     | 0.41              |
| 2:B:365:SER:O       | 2:B:368:TYR:HD1    | 2.04                     | 0.41              |
| 2:B:139:VAL:HG22    | 2:B:414:LEU:HD22   | 2.03                     | 0.41              |
| 1:A:84:GLU:CD       | 2:B:54:GLY:HA2     | 2.41                     | 0.41              |
| 1:A:96:ASP:CA       | 1:A:128:ARG:HA     | 2.41                     | 0.41              |
| 1:A:156:LEU:HG      | 1:A:428:LEU:HD11   | 2.02                     | 0.41              |
| 1:A:168:ILE:O       | 1:A:352:LEU:N      | 2.51                     | 0.41              |
| 1:A:294:TYR:HB3     | 1:A:298:VAL:HG21   | 2.02                     | 0.41              |
| 1:A:64:LEU:HD21     | 8:A:633:HOH:O      | 2.19                     | 0.41              |
| 2:B:237:LEU:HD21    | 2:B:295:ARG:HD3    | 2.03                     | 0.41              |
| 2:B:416:GLN:NE2     | 2:B:431:LEU:HD23   | 2.36                     | 0.41              |
| 2:B:177:HIS:NE2     | 2:B:178:GLY:O      | 2.54                     | 0.41              |
| 2:B:186:VAL:O       | 2:B:260:ARG:HG3    | 2.20                     | 0.41              |
| 2:B:332:THR:O       | 2:B:353:SER:HB3    | 2.20                     | 0.41              |
| 1:A:358:TYR:CB      | 2:B:375:GLN:HB2    | 2.49                     | 0.41              |
| 3:G:24[A]:ALA:HB1   | 3:G:226[A]:MET:HG3 | 2.02                     | 0.41              |
| 3:G:259[A]:LEU:HD22 | 3:G:259[A]:LEU:HA  | 1.85                     | 0.41              |
| 2:B:90:THR:HG22     | 2:B:108:ILE:HG21   | 2.03                     | 0.41              |
| 8:A:607:HOH:O       | 2:B:124:ILE:HG13   | 2.20                     | 0.41              |
| 2:B:126:MET:HA      | 2:B:126:MET:CE     | 2.50                     | 0.41              |
| 2:B:63:MET:HG3      | 2:B:82:ILE:HD11    | 2.03                     | 0.41              |
| 1:A:28:THR:C        | 1:A:44:LEU:HD22    | 2.42                     | 0.40              |
| 1:A:251:CYS:SG      | 1:A:308:ARG:NE     | 2.95                     | 0.40              |
| 2:B:235:THR:C       | 2:B:237:LEU:N      | 2.75                     | 0.40              |
| 2:B:332:THR:HB      | 2:B:354:THR:H      | 1.87                     | 0.40              |
| 2:B:164:VAL:HG13    | 2:B:420:VAL:CG1    | 2.50                     | 0.40              |
| 2:B:43:SER:OG       | 2:B:44:ARG:N       | 2.52                     | 0.40              |
| 1:A:189:PHE:CE2     | 1:A:197:LYS:HE2    | 2.56                     | 0.40              |
| 1:A:220:LEU:HA      | 1:A:220:LEU:HD23   | 1.88                     | 0.40              |
| 1:A:165:GLU:O       | 1:A:324:LEU:HB3    | 2.21                     | 0.40              |
| 1:A:354:THR:HG23    | 1:A:355:GLU:N      | 2.36                     | 0.40              |
| 2:B:126:MET:SD      | 2:B:126:MET:N      | 2.94                     | 0.40              |
| 2:B:139:VAL:HA      | 2:B:143:LEU:HB2    | 2.03                     | 0.40              |
| 2:B:247:GLU:O       | 2:B:249:GLN:N      | 2.54                     | 0.40              |
| 2:B:350:PRO:HB3     | 2:B:378:LEU:HD13   | 2.04                     | 0.40              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:B:86:VAL:HG11    | 2:B:114:ALA:HB3     | 2.03                     | 0.40              |
| 1:A:99:VAL:CG1     | 1:A:127:ARG:HB2     | 2.51                     | 0.40              |
| 1:A:81:LEU:H       | 1:A:81:LEU:HD12     | 1.86                     | 0.40              |
| 2:B:343:GLY:O      | 2:B:345:TYR:HD1     | 2.04                     | 0.40              |
| 2:B:362:ILE:HD13   | 2:B:362:ILE:N       | 2.36                     | 0.40              |
| 3:G:250[A]:THR:O   | 3:G:254[A]:VAL:HG23 | 2.21                     | 0.40              |
| 3:G:263[A]:ILE:HA  | 3:G:266[A]:ALA:HB3  | 2.04                     | 0.40              |
| 1:A:149:GLY:HA3    | 1:A:435:PRO:CB      | 2.51                     | 0.40              |
| 1:A:188:ARG:HG3    | 1:A:189:PHE:CE1     | 2.56                     | 0.40              |
| 1:A:335:SER:O      | 1:A:340:THR:HG23    | 2.21                     | 0.40              |
| 2:B:189:ARG:O      | 2:B:192:GLU:HG3     | 2.21                     | 0.40              |
| 2:B:250:ASP:HA     | 2:B:303:SER:O       | 2.21                     | 0.40              |
| 1:A:236:ALA:HB3    | 2:B:294:GLU:HG3     | 2.02                     | 0.40              |
| 2:B:469:LYS:O      | 2:B:469:LYS:HD3     | 2.22                     | 0.40              |
| 1:A:349:GLN:NE2    | 1:A:370:SER:HA      | 2.37                     | 0.40              |
| 1:A:417:LEU:O      | 1:A:420:ARG:HG2     | 2.22                     | 0.40              |
| 3:G:10[A]:ILE:HG13 | 3:G:10[A]:ILE:H     | 1.70                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed        | Favoured  | Allowed   | Outliers  | Percentiles |    |
|-----|-------|-----------------|-----------|-----------|-----------|-------------|----|
| 1   | A     | 499/510 (98%)   | 357 (72%) | 101 (20%) | 41 (8%)   | 1           | 2  |
| 2   | B     | 475/479 (99%)   | 307 (65%) | 109 (23%) | 59 (12%)  | 0           | 1  |
| 3   | G     | 118/270 (44%)   | 96 (81%)  | 18 (15%)  | 4 (3%)    | 3           | 13 |
| All | All   | 1092/1259 (87%) | 760 (70%) | 228 (21%) | 104 (10%) | 0           | 1  |

All (104) Ramachandran outliers are listed below:

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | A     | 15    | GLU  |
| 1   | A     | 17    | ILE  |
| 1   | A     | 44    | LEU  |
| 1   | A     | 50    | GLU  |
| 1   | A     | 78    | ASN  |
| 1   | A     | 80    | LYS  |
| 1   | A     | 84    | GLU  |
| 1   | A     | 92    | GLY  |
| 1   | A     | 95    | VAL  |
| 1   | A     | 109   | ASP  |
| 1   | A     | 111   | LEU  |
| 1   | A     | 117   | GLY  |
| 1   | A     | 134   | PRO  |
| 1   | A     | 208   | GLN  |
| 1   | A     | 236   | ALA  |
| 1   | A     | 295   | PRO  |
| 1   | A     | 338   | ILE  |
| 1   | A     | 357   | PHE  |
| 1   | A     | 451   | GLY  |
| 1   | A     | 458   | PRO  |
| 2   | B     | 53    | LEU  |
| 2   | B     | 97    | VAL  |
| 2   | B     | 138   | LYS  |
| 2   | B     | 143   | LEU  |
| 2   | B     | 188   | GLU  |
| 2   | B     | 210   | ASP  |
| 2   | B     | 211   | ALA  |
| 2   | B     | 245   | ASP  |
| 2   | B     | 248   | GLY  |
| 2   | B     | 269   | SER  |
| 2   | B     | 279   | VAL  |
| 2   | B     | 281   | TYR  |
| 2   | B     | 291   | THR  |
| 2   | B     | 327   | ALA  |
| 2   | B     | 331   | ALA  |
| 2   | B     | 344   | ILE  |
| 2   | B     | 418   | PHE  |
| 2   | B     | 451   | HIS  |
| 2   | B     | 453   | PRO  |
| 3   | G     | 2[A]  | ASP  |
| 3   | G     | 77[A] | ALA  |
| 1   | A     | 19    | ALA  |
| 1   | A     | 72    | GLY  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 116    | ASP  |
| 1   | A     | 191    | ASP  |
| 1   | A     | 194    | ASP  |
| 1   | A     | 454    | ASP  |
| 2   | B     | 40     | GLY  |
| 2   | B     | 43     | SER  |
| 2   | B     | 71     | ARG  |
| 2   | B     | 162    | LYS  |
| 2   | B     | 174    | ALA  |
| 2   | B     | 205    | VAL  |
| 2   | B     | 285    | LEU  |
| 2   | B     | 393[B] | MET  |
| 2   | B     | 431    | LEU  |
| 2   | B     | 434    | LEU  |
| 1   | A     | 16     | ARG  |
| 1   | A     | 21     | THR  |
| 1   | A     | 34     | ILE  |
| 1   | A     | 395    | ALA  |
| 1   | A     | 455    | LYS  |
| 2   | B     | 67     | GLU  |
| 2   | B     | 89     | GLU  |
| 2   | B     | 223    | ASN  |
| 2   | B     | 246    | GLN  |
| 2   | B     | 276    | PRO  |
| 2   | B     | 278    | ALA  |
| 2   | B     | 323    | ALA  |
| 2   | B     | 324    | THR  |
| 2   | B     | 391[B] | LEU  |
| 2   | B     | 428    | MET  |
| 2   | B     | 476    | GLU  |
| 3   | G     | 31[A]  | ALA  |
| 3   | G     | 40[A]  | VAL  |
| 1   | A     | 145    | PRO  |
| 1   | A     | 307    | GLU  |
| 2   | B     | 98     | ILE  |
| 2   | B     | 160    | VAL  |
| 2   | B     | 270    | ALA  |
| 2   | B     | 351    | LEU  |
| 2   | B     | 432    | VAL  |
| 2   | B     | 435    | LYS  |
| 2   | B     | 444    | ILE  |
| 2   | B     | 454    | GLU  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 38     | ILE  |
| 1   | A     | 199    | LEU  |
| 1   | A     | 210    | ARG  |
| 1   | A     | 262    | LYS  |
| 1   | A     | 270    | ASP  |
| 2   | B     | 31     | PRO  |
| 2   | B     | 440    | GLY  |
| 1   | A     | 187    | LYS  |
| 1   | A     | 288    | PRO  |
| 2   | B     | 390[B] | ILE  |
| 1   | A     | 23     | VAL  |
| 2   | B     | 28     | GLY  |
| 2   | B     | 68     | GLY  |
| 2   | B     | 429    | GLY  |
| 2   | B     | 58     | VAL  |
| 2   | B     | 107    | PRO  |
| 2   | B     | 357    | ILE  |
| 2   | B     | 159    | GLY  |
| 2   | B     | 173    | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |    |
|-----|-------|----------------|-----------|-----------|-------------|----|
| 1   | A     | 404/416 (97%)  | 348 (86%) | 56 (14%)  | 3           | 11 |
| 2   | B     | 381/384 (99%)  | 323 (85%) | 58 (15%)  | 3           | 8  |
| 3   | G     | 103/228 (45%)  | 93 (90%)  | 10 (10%)  | 8           | 24 |
| All | All   | 888/1028 (86%) | 764 (86%) | 124 (14%) | 3           | 11 |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 21  | THR  |
| 1   | A     | 30  | ARG  |
| 1   | A     | 45  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 47  | VAL  |
| 1   | A     | 50  | GLU  |
| 1   | A     | 56  | SER  |
| 1   | A     | 62  | MET  |
| 1   | A     | 78  | ASN  |
| 1   | A     | 81  | LEU  |
| 1   | A     | 83  | LYS  |
| 1   | A     | 104 | LEU  |
| 1   | A     | 111 | LEU  |
| 1   | A     | 113 | ASN  |
| 1   | A     | 127 | ARG  |
| 1   | A     | 137 | ILE  |
| 1   | A     | 144 | GLU  |
| 1   | A     | 164 | ARG  |
| 1   | A     | 178 | ILE  |
| 1   | A     | 180 | ILE  |
| 1   | A     | 188 | ARG  |
| 1   | A     | 189 | PHE  |
| 1   | A     | 191 | ASP  |
| 1   | A     | 200 | TYR  |
| 1   | A     | 206 | ILE  |
| 1   | A     | 209 | LYS  |
| 1   | A     | 212 | THR  |
| 1   | A     | 219 | ARG  |
| 1   | A     | 231 | VAL  |
| 1   | A     | 233 | SER  |
| 1   | A     | 237 | SER  |
| 1   | A     | 244 | TYR  |
| 1   | A     | 251 | CYS  |
| 1   | A     | 257 | PHE  |
| 1   | A     | 269 | ASP  |
| 1   | A     | 281 | MET  |
| 1   | A     | 292 | GLU  |
| 1   | A     | 313 | ASN  |
| 1   | A     | 316 | PHE  |
| 1   | A     | 324 | LEU  |
| 1   | A     | 339 | PRO  |
| 1   | A     | 341 | ASN  |
| 1   | A     | 347 | ASP  |
| 1   | A     | 357 | PHE  |
| 1   | A     | 358 | TYR  |
| 1   | A     | 374 | VAL  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 390    | MET  |
| 1   | A     | 392    | LEU  |
| 1   | A     | 410[B] | LEU  |
| 1   | A     | 418    | LEU  |
| 1   | A     | 432    | GLN  |
| 1   | A     | 439    | GLU  |
| 1   | A     | 446    | TYR  |
| 1   | A     | 450    | ARG  |
| 1   | A     | 468    | PHE  |
| 1   | A     | 477    | GLN  |
| 1   | A     | 492    | GLN  |
| 2   | B     | 12     | GLN  |
| 2   | B     | 14     | VAL  |
| 2   | B     | 31     | PRO  |
| 2   | B     | 58     | VAL  |
| 2   | B     | 66     | THR  |
| 2   | B     | 83     | LYS  |
| 2   | B     | 89     | GLU  |
| 2   | B     | 91     | LEU  |
| 2   | B     | 95     | MET  |
| 2   | B     | 96     | ASN  |
| 2   | B     | 105    | ARG  |
| 2   | B     | 113    | PHE  |
| 2   | B     | 125    | GLU  |
| 2   | B     | 126    | MET  |
| 2   | B     | 143    | LEU  |
| 2   | B     | 148    | LYS  |
| 2   | B     | 154    | LEU  |
| 2   | B     | 166    | ILE  |
| 2   | B     | 170    | ILE  |
| 2   | B     | 188    | GLU  |
| 2   | B     | 192    | GLU  |
| 2   | B     | 194    | ASN  |
| 2   | B     | 195    | ASP  |
| 2   | B     | 207    | ASN  |
| 2   | B     | 212    | THR  |
| 2   | B     | 214    | LYS  |
| 2   | B     | 231    | ARG  |
| 2   | B     | 246    | GLN  |
| 2   | B     | 249    | GLN  |
| 2   | B     | 252    | LEU  |
| 2   | B     | 259    | PHE  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | B     | 269    | SER  |
| 2   | B     | 271    | LEU  |
| 2   | B     | 284    | THR  |
| 2   | B     | 285    | LEU  |
| 2   | B     | 292    | MET  |
| 2   | B     | 299    | THR  |
| 2   | B     | 318    | THR  |
| 2   | B     | 329    | LEU  |
| 2   | B     | 335    | LEU  |
| 2   | B     | 341    | GLU  |
| 2   | B     | 349    | ASP  |
| 2   | B     | 359    | ASP  |
| 2   | B     | 362    | ILE  |
| 2   | B     | 368    | TYR  |
| 2   | B     | 380[B] | ASP  |
| 2   | B     | 402    | LEU  |
| 2   | B     | 412    | ARG  |
| 2   | B     | 425    | THR  |
| 2   | B     | 427    | HIS  |
| 2   | B     | 437    | THR  |
| 2   | B     | 441    | PHE  |
| 2   | B     | 449    | TYR  |
| 2   | B     | 453    | PRO  |
| 2   | B     | 457    | PHE  |
| 2   | B     | 460    | VAL  |
| 2   | B     | 471    | ASP  |
| 2   | B     | 475    | GLU  |
| 3   | G     | 28[A]  | TYR  |
| 3   | G     | 30[A]  | ARG  |
| 3   | G     | 208[A] | ASN  |
| 3   | G     | 211[A] | TYR  |
| 3   | G     | 226[A] | MET  |
| 3   | G     | 229[A] | MET  |
| 3   | G     | 234[A] | LYS  |
| 3   | G     | 247[A] | PHE  |
| 3   | G     | 259[A] | LEU  |
| 3   | G     | 269[A] | LEU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 70  | ASN  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 78     | ASN  |
| 1   | A     | 208    | GLN  |
| 1   | A     | 366    | ASN  |
| 1   | A     | 477    | GLN  |
| 1   | A     | 492    | GLN  |
| 2   | B     | 24     | GLN  |
| 2   | B     | 73     | GLN  |
| 2   | B     | 96     | ASN  |
| 2   | B     | 207    | ASN  |
| 2   | B     | 246    | GLN  |
| 2   | B     | 249    | GLN  |
| 2   | B     | 263    | GLN  |
| 2   | B     | 416    | GLN  |
| 2   | B     | 427    | HIS  |
| 2   | B     | 442    | GLN  |
| 3   | G     | 85[A]  | GLN  |
| 3   | G     | 252[A] | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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 |
| 5   | ATP  | A     | 603 | 4    | 26,33,33     | 1.14 | 3 (11%)  | 31,52,52    | 1.70 | 6 (19%)  |
| 6   | PO4  | B     | 601 | -    | 4,4,4        | 1.95 | 3 (75%)  | 6,6,6       | 0.41 | 0        |
| 7   | ADP  | B     | 604 | -    | 24,29,29     | 1.10 | 2 (8%)   | 29,45,45    | 1.62 | 6 (20%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | ATP  | A     | 603 | 4    | -       | 5/18/38/38 | 0/3/3/3 |
| 7   | ADP  | B     | 604 | -    | -       | 7/12/32/32 | 0/3/3/3 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | A     | 603 | ATP  | PG-O3G  | -2.64 | 1.44        | 1.54     |
| 5   | A     | 603 | ATP  | C2-N3   | 2.63  | 1.36        | 1.32     |
| 7   | B     | 604 | ADP  | C2'-C1' | -2.42 | 1.50        | 1.53     |
| 6   | B     | 601 | PO4  | P-O3    | -2.32 | 1.47        | 1.54     |
| 7   | B     | 604 | ADP  | C2-N3   | 2.15  | 1.35        | 1.32     |
| 6   | B     | 601 | PO4  | P-O4    | -2.05 | 1.48        | 1.54     |
| 6   | B     | 601 | PO4  | P-O2    | -2.05 | 1.48        | 1.54     |
| 5   | A     | 603 | ATP  | C2'-C1' | -2.01 | 1.50        | 1.53     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | A     | 603 | ATP  | C1'-N9-C4   | 5.64  | 136.54      | 126.64   |
| 7   | B     | 604 | ADP  | O3'-C3'-C2' | 4.27  | 125.64      | 111.82   |
| 5   | A     | 603 | ATP  | O5'-C5'-C4' | 3.84  | 122.21      | 108.99   |
| 7   | B     | 604 | ADP  | O2'-C2'-C3' | 3.42  | 122.87      | 111.82   |
| 7   | B     | 604 | ADP  | C5-C6-N6    | 3.28  | 125.33      | 120.35   |
| 7   | B     | 604 | ADP  | O2B-PB-O1B  | 3.06  | 122.65      | 110.68   |
| 5   | A     | 603 | ATP  | PB-O3B-PG   | 2.33  | 140.83      | 132.83   |
| 5   | A     | 603 | ATP  | O3'-C3'-C4' | 2.31  | 117.73      | 111.05   |
| 5   | A     | 603 | ATP  | C4-C5-N7    | 2.24  | 111.74      | 109.40   |
| 7   | B     | 604 | ADP  | O4'-C4'-C3' | -2.23 | 100.69      | 105.11   |
| 7   | B     | 604 | ADP  | N3-C2-N1    | -2.05 | 125.48      | 128.68   |
| 5   | A     | 603 | ATP  | O2'-C2'-C3' | 2.01  | 118.32      | 111.82   |

There are no chirality outliers.

All (12) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | A     | 603 | ATP  | PB-O3B-PG-O2G   |
| 7   | B     | 604 | ADP  | PA-O3A-PB-O2B   |
| 7   | B     | 604 | ADP  | C5'-O5'-PA-O2A  |
| 7   | B     | 604 | ADP  | O4'-C4'-C5'-O5' |
| 7   | B     | 604 | ADP  | C3'-C4'-C5'-O5' |
| 5   | A     | 603 | ATP  | C3'-C4'-C5'-O5' |
| 5   | A     | 603 | ATP  | O4'-C4'-C5'-O5' |
| 5   | A     | 603 | ATP  | C4'-C5'-O5'-PA  |
| 7   | B     | 604 | ADP  | PA-O3A-PB-O1B   |
| 7   | B     | 604 | ADP  | C5'-O5'-PA-O3A  |
| 7   | B     | 604 | ADP  | C5'-O5'-PA-O1A  |
| 5   | A     | 603 | ATP  | PB-O3B-PG-O1G   |

There are no ring outliers.

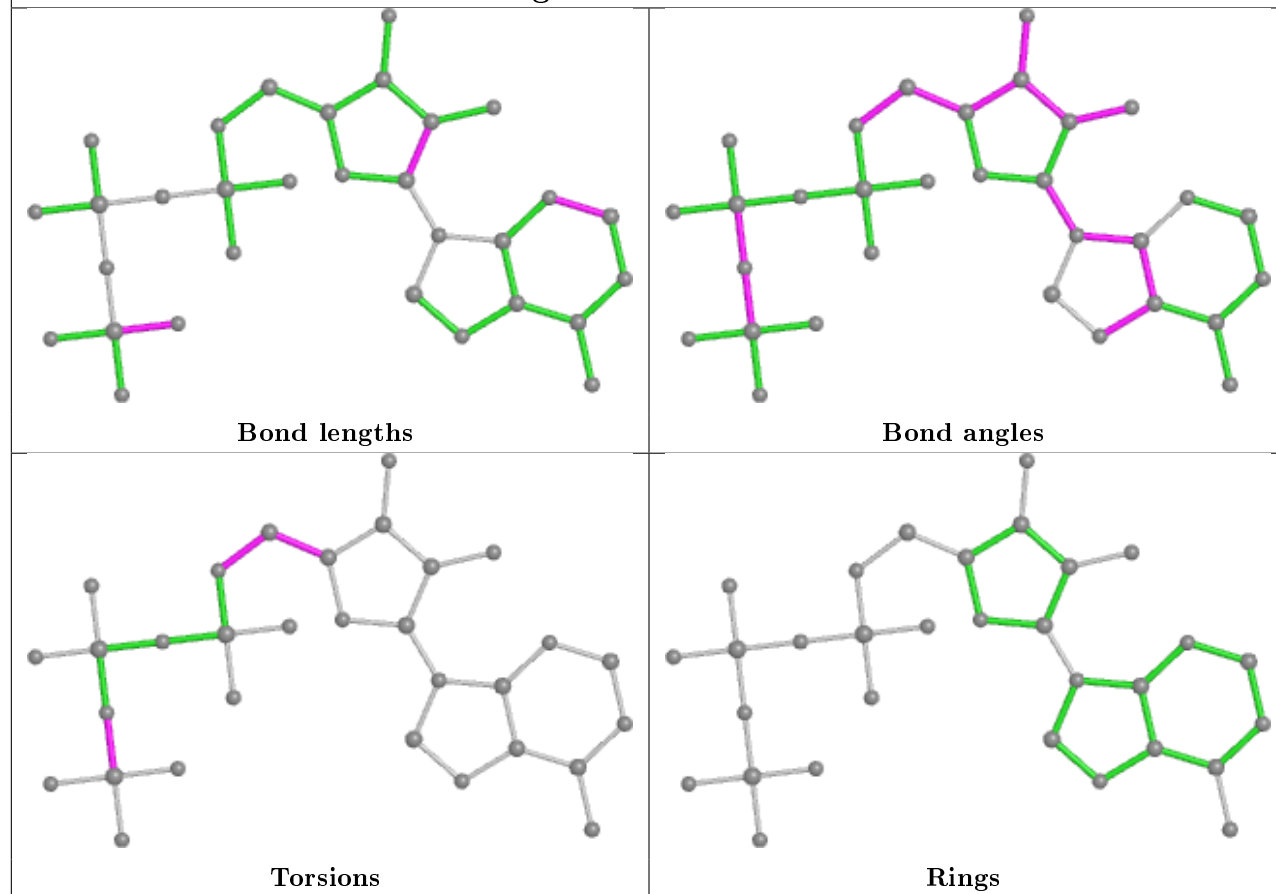
3 monomers are involved in 14 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | A     | 603 | ATP  | 6       | 0            |
| 6   | B     | 601 | PO4  | 1       | 0            |
| 7   | B     | 604 | ADP  | 7       | 0            |

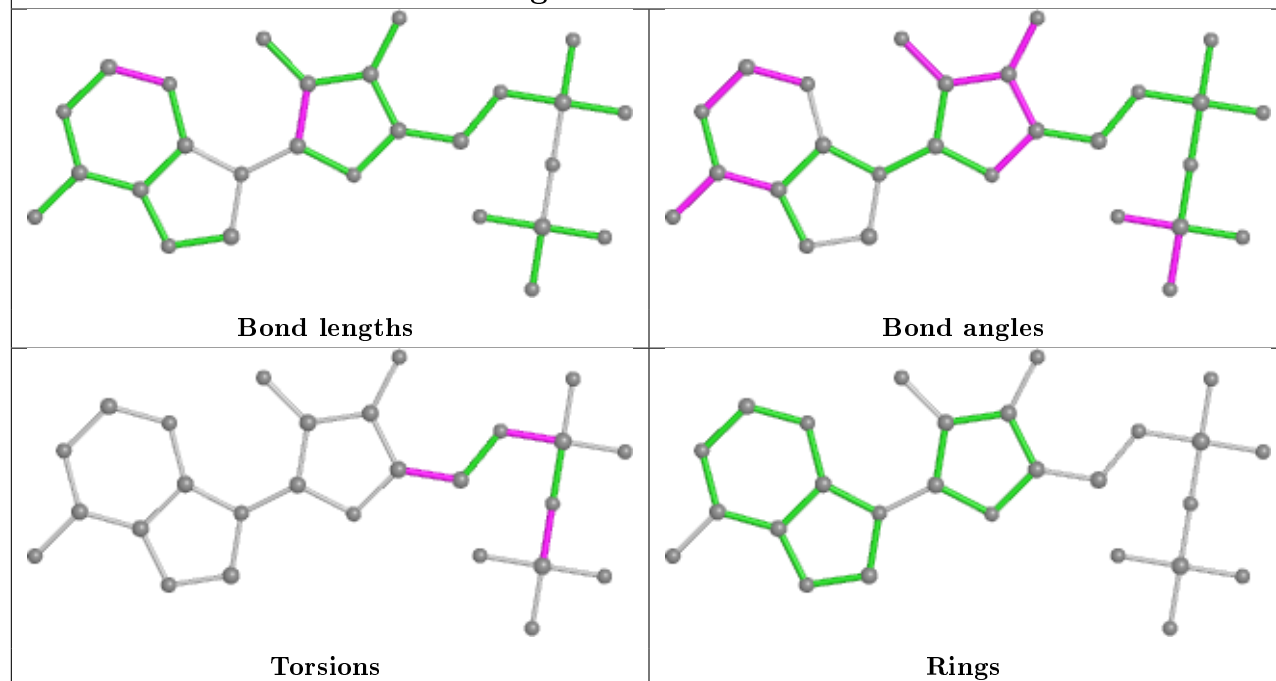
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



## Ligand ATP A 603



## Ligand ADP B 604



## 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.