



## Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 04:06 PM EST

PDB ID : 3J6P  
EMDB ID : EMD-5931  
Title : Pseudo-atomic model of dynein microtubule binding domain-tubulin complex based on a cryoEM map  
Authors : Uchimura, S.; Fujii, T.; Takazaki, H.; Ayukawa, R.; Nishikawa, Y.; Minoura, I.; Hachikubo, Y.; Kurisu, G.; Sutoh, K.; Kon, T.; Namba, K.; Muto, E.  
Deposited on : 2014-03-20  
Resolution : 8.20 Å (reported)  
Based on initial models : 1JFF, 3VKH

This is a Full wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

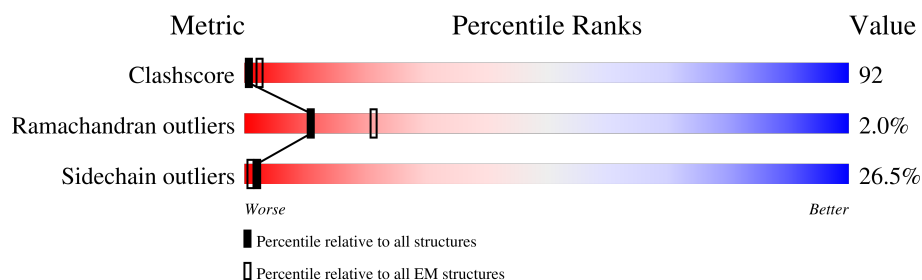
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.20 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 (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore            | 158937                   | 4297                     |
| Ramachandran outliers | 154571                   | 4023                     |
| Sidechain outliers    | 154315                   | 3826                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | D     | 108    | <div> <div>43%</div> <div>21%</div> <div>60%</div> <div>19%</div> </div>               |
| 2   | A     | 451    | <div> <div>14%</div> <div>21%</div> <div>51%</div> <div>19%</div> <div>9%</div> </div> |
| 3   | B     | 445    | <div> <div>12%</div> <div>14%</div> <div>62%</div> <div>18%</div> </div>               |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7563 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Dynein heavy chain, cytoplasmic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | D     | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 862   | 557 | 141 | 157 | 7 |         |       |

- Molecule 2 is a protein called Tubulin alpha-1A chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | A     | 412      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3227  | 2043 | 551 | 613 | 20 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 265     | GLY      | ALA    | CONFLICT | UNP P02550 |

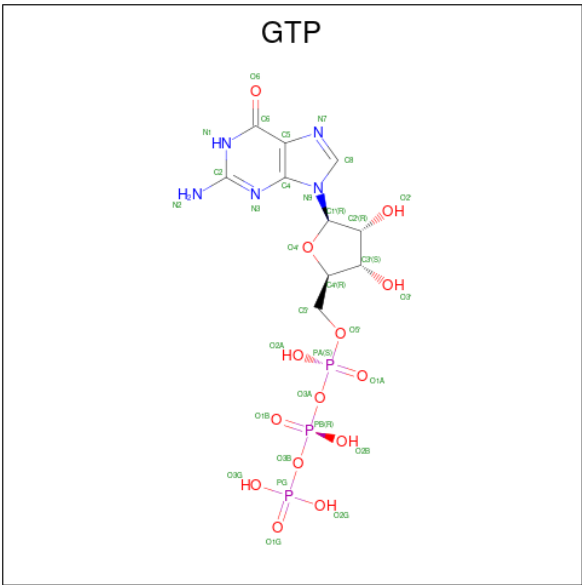
- Molecule 3 is a protein called Tubulin beta chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | B     | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3351  | 2105 | 575 | 646 | 25 |         |       |

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

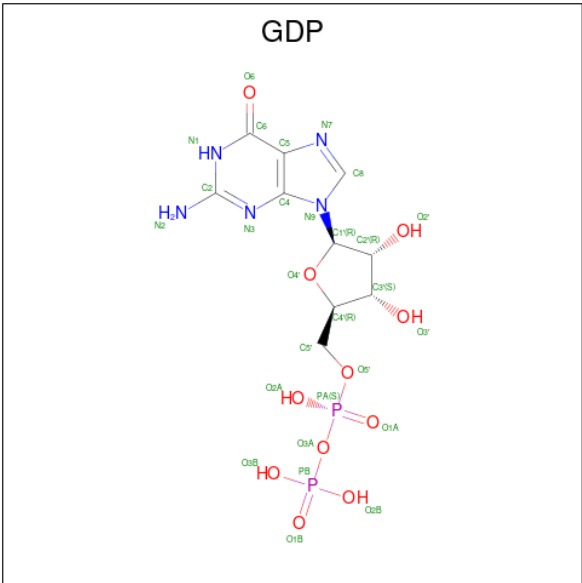
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 4   | A     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



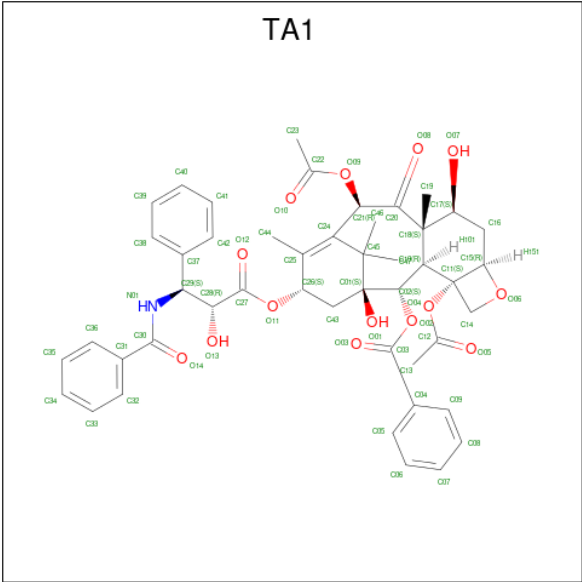
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 5   | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 6   | B     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

- Molecule 7 is TAXOL (three-letter code: TA1) (formula:  $C_{47}H_{51}NO_{14}$ ).

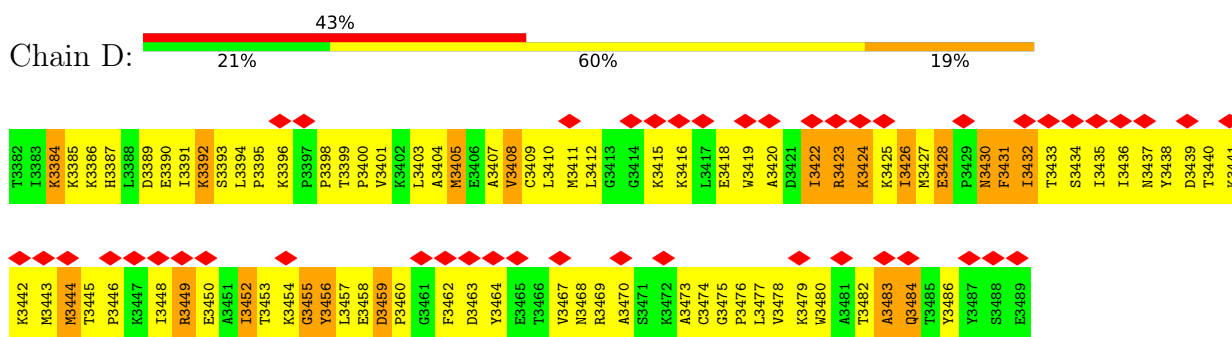


| Mol | Chain | Residues | Atoms |    |   |    | AltConf |
|-----|-------|----------|-------|----|---|----|---------|
| 7   | B     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 62    | 47 | 1 | 14 |         |

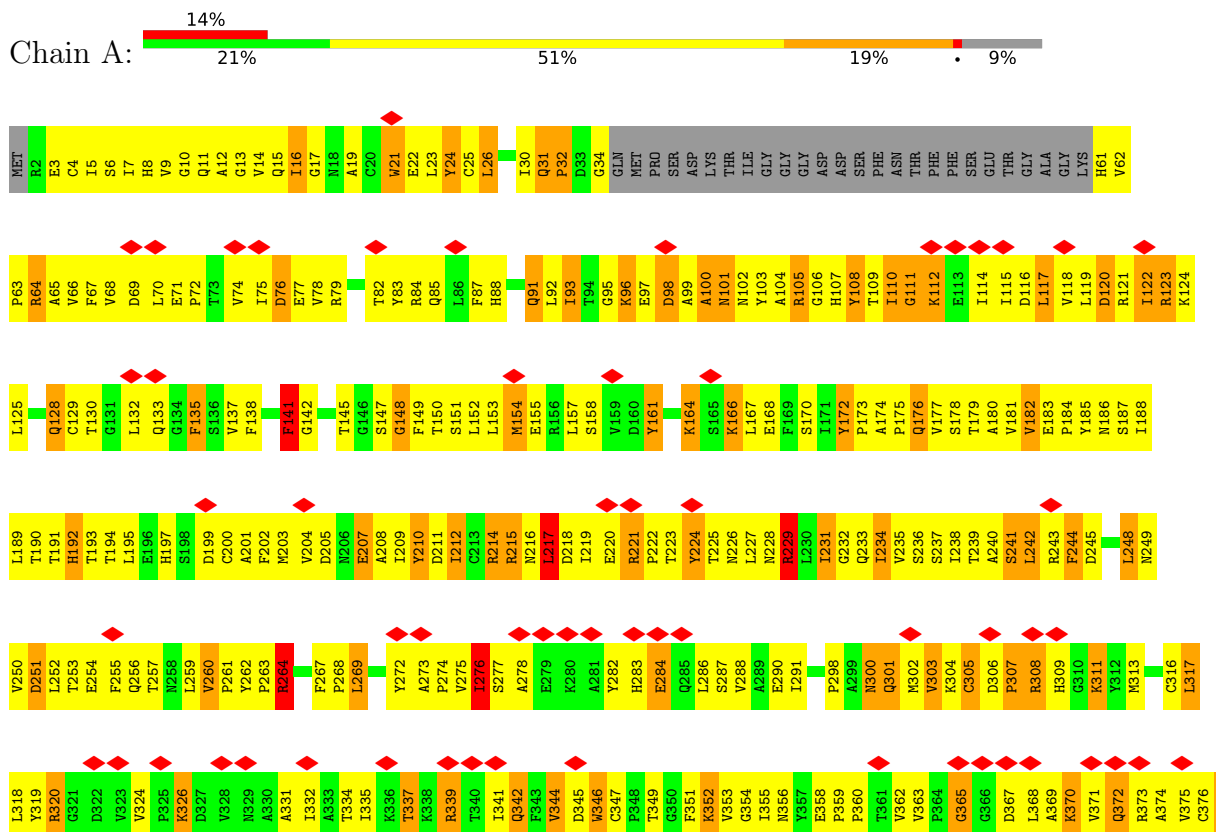
### 3 Residue-property plots

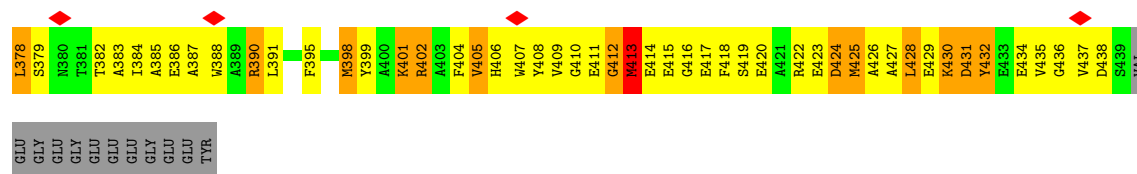
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Dynein heavy chain, cytoplasmic

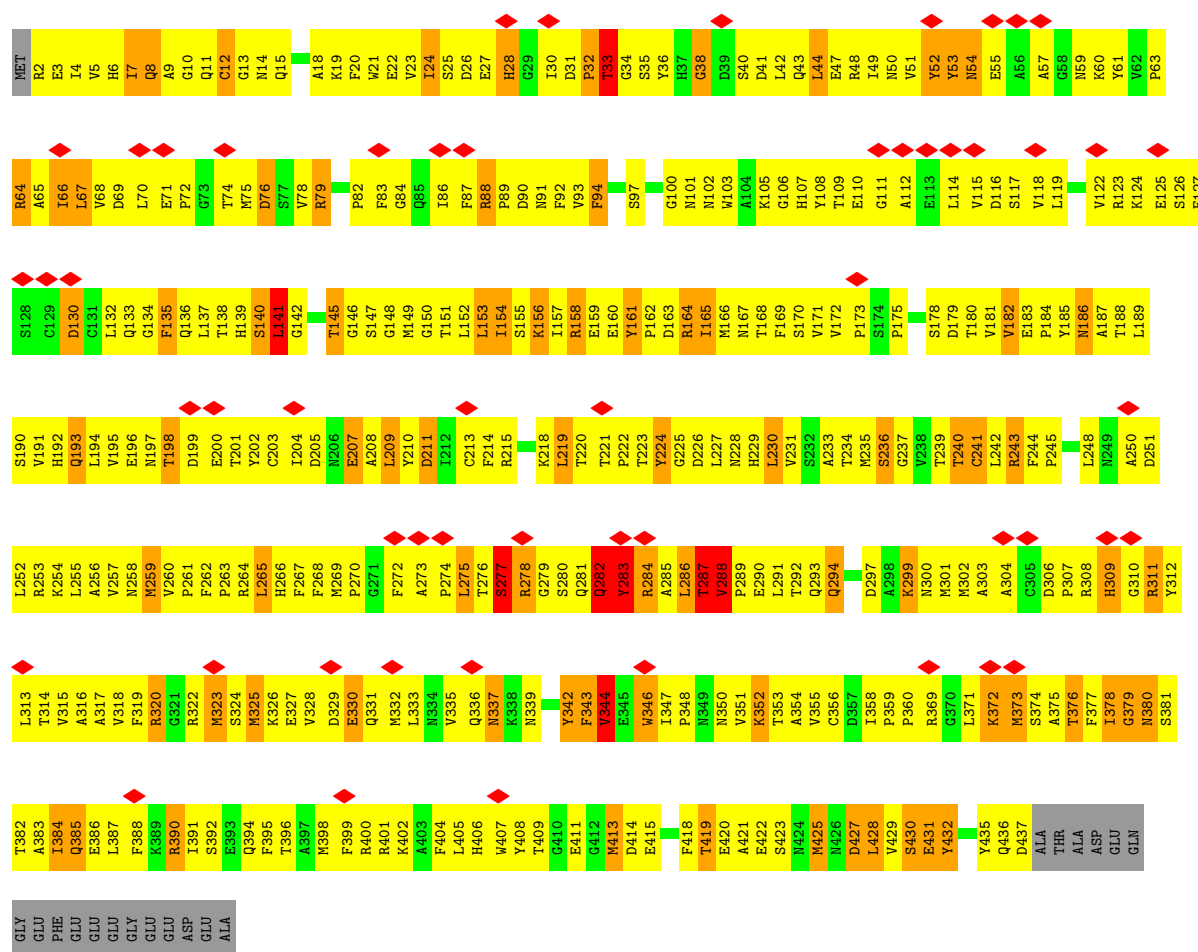
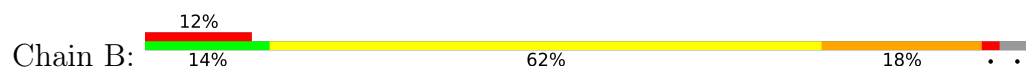


#### • Molecule 2: Tubulin alpha-1A chain





### • Molecule 3: Tubulin beta chain



## 4 Experimental information

| Property                             | Value   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | HELICAL   | Depositor |
| Imposed symmetry                     | HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided | Depositor |
| Number of segments used              | Not provided  |           |
| Resolution determination method      | Not provided  |           |
| CTF correction method                | CTFFIND3 Each particle  | Depositor |
| Microscope                           | JEOL 3200FSC  | Depositor |
| Voltage (kV)                         | 200   | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 20.0  | Depositor |
| Minimum defocus (nm)                 | 1000  | Depositor |
| Maximum defocus (nm)                 | 1500  | Depositor |
| Magnification                        | 109489  | Depositor |
| Image detector                       | TVIPS TEMCAM-F415 (4k x 4k)   | Depositor |
| Maximum map value                    | 0.389   | Depositor |
| Minimum map value                    | -0.163  | Depositor |
| Average map value                    | 0.009   | Depositor |
| Map value standard deviation         | 0.037   | Depositor |
| Recommended contour level            | 0.106   | Depositor |
| Map size (Å)                         | 137.0, 137.0, 137.0   | wwPDB     |
| Map dimensions                       | 100, 100, 100   | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0  | wwPDB     |
| Pixel spacing (Å)                    | 1.37, 1.37, 1.37  | Depositor |



## 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: GDP, MG, TA1, GTP

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   | D     | 0.97         | 0/881         | 1.10        | 0/1186          |
| 2   | A     | 0.99         | 1/3300 (0.0%) | 1.14        | 5/4482 (0.1%)   |
| 3   | B     | 0.99         | 0/3426        | 1.13        | 5/4642 (0.1%)   |
| All | All   | 0.99         | 1/7607 (0.0%) | 1.13        | 10/10310 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | D     | 0                   | 1                   |
| 2   | A     | 0                   | 12                  |
| 3   | B     | 0                   | 10                  |
| All | All   | 0                   | 23                  |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | A     | 30  | ILE  | C-N   | 8.22 | 1.52        | 1.34     |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | A     | 161 | TYR  | CA-CB-CG | -6.75 | 100.57      | 113.40   |
| 2   | A     | 30  | ILE  | O-C-N    | -6.64 | 112.07      | 122.70   |
| 3   | B     | 283 | TYR  | CA-CB-CG | -6.38 | 101.28      | 113.40   |
| 2   | A     | 217 | LEU  | N-CA-CB  | 5.65  | 121.70      | 110.40   |
| 3   | B     | 404 | PHE  | CA-CB-CG | -5.56 | 100.55      | 113.90   |
| 2   | A     | 365 | GLY  | C-N-CA   | -5.55 | 110.64      | 122.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | A     | 229 | ARG  | NE-CZ-NH1 | 5.22  | 122.91      | 120.30   |
| 3   | B     | 373 | MET  | CG-SD-CE  | -5.22 | 91.85       | 100.20   |
| 3   | B     | 52  | TYR  | CA-CB-CG  | -5.20 | 103.53      | 113.40   |
| 3   | B     | 28  | HIS  | CA-CB-CG  | -5.07 | 104.99      | 113.60   |

There are no chirality outliers.

All (23) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 2   | A     | 110  | ILE  | Peptide   |
| 2   | A     | 141  | PHE  | Peptide   |
| 2   | A     | 176  | GLN  | Peptide   |
| 2   | A     | 182  | VAL  | Peptide   |
| 2   | A     | 221  | ARG  | Peptide   |
| 2   | A     | 229  | ARG  | Sidechain |
| 2   | A     | 264  | ARG  | Peptide   |
| 2   | A     | 283  | HIS  | Peptide   |
| 2   | A     | 309  | HIS  | Peptide   |
| 2   | A     | 365  | GLY  | Peptide   |
| 2   | A     | 415  | GLU  | Peptide   |
| 2   | A     | 64   | ARG  | Peptide   |
| 3   | B     | 12   | CYS  | Peptide   |
| 3   | B     | 141  | LEU  | Peptide   |
| 3   | B     | 182  | VAL  | Peptide   |
| 3   | B     | 277  | SER  | Peptide   |
| 3   | B     | 286  | LEU  | Peptide   |
| 3   | B     | 287  | THR  | Peptide   |
| 3   | B     | 288  | VAL  | Peptide   |
| 3   | B     | 33   | THR  | Peptide   |
| 3   | B     | 379  | GLY  | Peptide   |
| 3   | B     | 83   | PHE  | Peptide   |
| 1   | D     | 3455 | GLY  | Peptide   |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | D     | 862   | 0        | 902      | 206     | 0            |
| 2   | A     | 3227  | 0        | 3143     | 596     | 0            |
| 3   | B     | 3351  | 0        | 3229     | 648     | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 32    | 0        | 12       | 3       | 0            |
| 6   | B     | 28    | 0        | 12       | 1       | 0            |
| 7   | B     | 62    | 0        | 51       | 8       | 0            |
| All | All   | 7563  | 0        | 7349     | 1375    | 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 92.

All (1375) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:191:VAL:HA   | 3:B:194:LEU:HD12 | 1.21                     | 1.17              |
| 3:B:250:ALA:HA   | 3:B:254:LYS:HE2  | 1.21                     | 1.16              |
| 2:A:11:GLN:HG3   | 2:A:74:VAL:HG11  | 1.26                     | 1.13              |
| 2:A:259:LEU:HD11 | 2:A:378:LEU:HD13 | 1.27                     | 1.12              |
| 2:A:151:SER:HB3  | 2:A:193:THR:HG21 | 1.32                     | 1.11              |
| 3:B:234:THR:HG21 | 3:B:270:PRO:HB3  | 1.21                     | 1.10              |
| 2:A:71:GLU:HG3   | 3:B:2:ARG:HH21   | 1.15                     | 1.08              |
| 2:A:316:CYS:HB2  | 2:A:378:LEU:HD11 | 1.27                     | 1.08              |
| 1:D:3416:LYS:HG3 | 1:D:3418:GLU:H   | 1.14                     | 1.08              |
| 2:A:303:VAL:HG13 | 2:A:305:CYS:H    | 1.18                     | 1.08              |
| 3:B:57:ALA:HB2   | 3:B:60:LYS:HD2   | 1.30                     | 1.08              |
| 1:D:3424:LYS:HB2 | 3:B:159:GLU:HB2  | 1.34                     | 1.07              |
| 2:A:311:LYS:HG2  | 2:A:344:VAL:HG13 | 1.23                     | 1.07              |
| 3:B:324:SER:HB3  | 3:B:327:GLU:HG2  | 1.08                     | 1.06              |
| 2:A:119:LEU:HA   | 2:A:122:ILE:HD11 | 1.37                     | 1.04              |
| 2:A:7:ILE:HG12   | 2:A:137:VAL:HG22 | 1.35                     | 1.02              |
| 3:B:102:ASN:HB3  | 3:B:105:LYS:H    | 1.22                     | 1.02              |
| 3:B:133:GLN:HE21 | 3:B:252:LEU:HB2  | 1.20                     | 1.02              |
| 1:D:3387:HIS:HD2 | 1:D:3473:ALA:HB2 | 1.24                     | 1.02              |
| 2:A:66:VAL:HG12  | 2:A:91:GLN:HG3   | 1.41                     | 1.02              |
| 2:A:115:ILE:HD11 | 2:A:153:LEU:HD13 | 1.40                     | 1.02              |
| 2:A:269:LEU:HD22 | 2:A:384:ILE:HD11 | 1.42                     | 1.01              |
| 3:B:251:ASP:H    | 3:B:254:LYS:HG3  | 1.27                     | 1.00              |
| 3:B:209:LEU:HB3  | 3:B:227:LEU:HD22 | 1.40                     | 0.99              |
| 3:B:210:TYR:CE1  | 3:B:227:LEU:HD11 | 1.97                     | 0.99              |
| 3:B:21:TRP:HA    | 3:B:24:ILE:HG22  | 1.42                     | 0.98              |
| 2:A:286:LEU:HG   | 2:A:290:GLU:HB2  | 1.45                     | 0.98              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:133:GLN:HG2   | 3:B:252:LEU:HD12  | 1.46                     | 0.98              |
| 3:B:275:LEU:HD23  | 3:B:300:ASN:HD21  | 1.29                     | 0.97              |
| 2:A:362:VAL:HG13  | 2:A:368:LEU:HB2   | 1.45                     | 0.97              |
| 1:D:3390:GLU:HG3  | 2:A:402:ARG:HH22  | 1.29                     | 0.97              |
| 2:A:102:ASN:HB2   | 2:A:408:TYR:CE1   | 2.00                     | 0.96              |
| 2:A:219:ILE:HB    | 2:A:222:PRO:HG3   | 1.46                     | 0.96              |
| 1:D:3424:LYS:HZ2  | 3:B:159:GLU:HB3   | 1.27                     | 0.96              |
| 1:D:3464:TYR:CE1  | 1:D:3478:VAL:HG11 | 2.00                     | 0.96              |
| 1:D:3416:LYS:HE2  | 1:D:3418:GLU:HB2  | 1.45                     | 0.95              |
| 3:B:147:SER:HB3   | 3:B:190:SER:HB3   | 1.48                     | 0.94              |
| 1:D:3455:GLY:HA2  | 1:D:3458:GLU:H    | 1.32                     | 0.94              |
| 3:B:241:CYS:HB2   | 3:B:320:ARG:HE    | 1.31                     | 0.94              |
| 2:A:69:ASP:HB2    | 2:A:75:ILE:HD11   | 1.50                     | 0.94              |
| 3:B:319:PHE:CD2   | 3:B:375:ALA:HB2   | 2.03                     | 0.94              |
| 1:D:3423:ARG:HH12 | 3:B:158:ARG:HD2   | 1.30                     | 0.93              |
| 2:A:26:LEU:HD21   | 2:A:363:VAL:HG13  | 1.49                     | 0.93              |
| 3:B:264:ARG:HB2   | 3:B:266:HIS:CD2   | 2.03                     | 0.93              |
| 3:B:269:MET:SD    | 3:B:303:ALA:HB3   | 2.09                     | 0.93              |
| 3:B:48:ARG:HG2    | 3:B:243:ARG:HB3   | 1.48                     | 0.92              |
| 2:A:210:TYR:HE1   | 2:A:227:LEU:HD21  | 1.32                     | 0.92              |
| 3:B:57:ALA:HB3    | 3:B:60:LYS:H      | 1.32                     | 0.92              |
| 3:B:273:ALA:HB3   | 3:B:274:PRO:HD3   | 1.49                     | 0.92              |
| 2:A:181:VAL:CG2   | 3:B:258:ASN:HB3   | 2.00                     | 0.91              |
| 3:B:133:GLN:CG    | 3:B:252:LEU:HD12  | 1.99                     | 0.91              |
| 2:A:316:CYS:HB2   | 2:A:378:LEU:CD1   | 2.00                     | 0.91              |
| 3:B:140:SER:HB2   | 3:B:142:GLY:CA    | 2.00                     | 0.91              |
| 3:B:27:GLU:OE1    | 7:B:502:TA1:H411  | 1.68                     | 0.91              |
| 3:B:6:HIS:HB3     | 3:B:65:ALA:HB2    | 1.53                     | 0.90              |
| 1:D:3387:HIS:CD2  | 1:D:3473:ALA:HB2  | 2.07                     | 0.90              |
| 2:A:167:LEU:HD23  | 2:A:202:PHE:CE2   | 2.07                     | 0.90              |
| 2:A:273:ALA:HB3   | 2:A:274:PRO:HD3   | 1.51                     | 0.90              |
| 2:A:104:ALA:HB1   | 2:A:411:GLU:HB2   | 1.54                     | 0.90              |
| 2:A:276:ILE:HG23  | 2:A:369:ALA:CB    | 2.01                     | 0.90              |
| 1:D:3424:LYS:HE2  | 3:B:156:LYS:HD2   | 1.52                     | 0.90              |
| 2:A:31:GLN:HB3    | 2:A:32:PRO:HD2    | 1.51                     | 0.90              |
| 3:B:140:SER:HB2   | 3:B:142:GLY:HA3   | 1.53                     | 0.90              |
| 1:D:3431:PHE:CE1  | 1:D:3435:ILE:HD11 | 2.06                     | 0.89              |
| 2:A:179:THR:HG21  | 3:B:248:LEU:CD2   | 2.02                     | 0.89              |
| 2:A:311:LYS:CG    | 2:A:344:VAL:HG13  | 2.03                     | 0.89              |
| 1:D:3384:LYS:HD3  | 1:D:3386:LYS:HB2  | 1.54                     | 0.89              |
| 1:D:3416:LYS:HG3  | 1:D:3418:GLU:N    | 1.88                     | 0.89              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:B:132:LEU:HB3  | 3:B:164:ARG:HD3   | 1.54                     | 0.89              |
| 3:B:241:CYS:HB2  | 3:B:320:ARG:NE    | 1.88                     | 0.88              |
| 2:A:154:MET:HA   | 2:A:157:LEU:HD12  | 1.53                     | 0.88              |
| 3:B:264:ARG:HB2  | 3:B:266:HIS:HD2   | 1.36                     | 0.88              |
| 1:D:3445:THR:HB  | 1:D:3446:PRO:HD3  | 1.54                     | 0.88              |
| 1:D:3457:LEU:HA  | 1:D:3462:PHE:HD2  | 1.39                     | 0.88              |
| 1:D:3464:TYR:HB2 | 1:D:3478:VAL:HG21 | 1.54                     | 0.88              |
| 2:A:110:ILE:HG23 | 2:A:111:GLY:H     | 1.39                     | 0.87              |
| 2:A:422:ARG:HH12 | 2:A:426:ALA:HB2   | 1.39                     | 0.87              |
| 3:B:75:MET:HE1   | 3:B:94:PHE:HB3    | 1.54                     | 0.87              |
| 2:A:132:LEU:CD2  | 2:A:164:LYS:HE3   | 2.04                     | 0.86              |
| 3:B:269:MET:HB2  | 3:B:301:MET:HE3   | 1.57                     | 0.86              |
| 2:A:181:VAL:HG23 | 3:B:258:ASN:HB3   | 1.56                     | 0.86              |
| 2:A:155:GLU:HG2  | 2:A:197:HIS:CE1   | 2.10                     | 0.86              |
| 2:A:174:ALA:HB3  | 2:A:177:VAL:HB    | 1.55                     | 0.86              |
| 2:A:362:VAL:CG1  | 2:A:368:LEU:HB2   | 2.06                     | 0.86              |
| 1:D:3394:LEU:HB3 | 2:A:410:GLY:HA2   | 1.58                     | 0.85              |
| 3:B:315:VAL:HG13 | 3:B:377:PHE:CE1   | 2.11                     | 0.85              |
| 2:A:66:VAL:CG1   | 2:A:91:GLN:HG3    | 2.05                     | 0.85              |
| 3:B:323:MET:HE3  | 3:B:373:MET:SD    | 2.16                     | 0.85              |
| 1:D:3394:LEU:CB  | 2:A:410:GLY:HA2   | 2.07                     | 0.85              |
| 2:A:119:LEU:O    | 2:A:122:ILE:HG12  | 1.76                     | 0.85              |
| 2:A:229:ARG:HG2  | 2:A:229:ARG:HH11  | 1.40                     | 0.85              |
| 2:A:115:ILE:HD13 | 2:A:152:LEU:HD11  | 1.58                     | 0.85              |
| 3:B:301:MET:HE1  | 3:B:377:PHE:HE2   | 1.41                     | 0.85              |
| 3:B:285:ALA:HB1  | 3:B:290:GLU:HG2   | 1.59                     | 0.84              |
| 1:D:3464:TYR:CB  | 1:D:3478:VAL:HG21 | 2.07                     | 0.84              |
| 1:D:3475:GLY:O   | 1:D:3478:VAL:HG12 | 1.76                     | 0.84              |
| 3:B:105:LYS:HG3  | 3:B:110:GLU:HG2   | 1.58                     | 0.84              |
| 2:A:317:LEU:HG   | 2:A:377:MET:HB2   | 1.58                     | 0.84              |
| 3:B:256:ALA:O    | 3:B:260:VAL:HG22  | 1.76                     | 0.84              |
| 3:B:319:PHE:HA   | 3:B:375:ALA:HA    | 1.57                     | 0.84              |
| 3:B:189:LEU:HD23 | 3:B:421:ALA:CB    | 2.08                     | 0.84              |
| 2:A:274:PRO:HG2  | 2:A:374:ALA:CB    | 2.06                     | 0.83              |
| 3:B:6:HIS:HB3    | 3:B:65:ALA:CB     | 2.08                     | 0.83              |
| 3:B:8:GLN:OE1    | 3:B:67:LEU:HD22   | 1.78                     | 0.83              |
| 1:D:3424:LYS:NZ  | 3:B:156:LYS:HA    | 1.93                     | 0.83              |
| 3:B:332:MET:HE3  | 3:B:351:VAL:HG11  | 1.57                     | 0.83              |
| 2:A:112:LYS:O    | 2:A:115:ILE:HG22  | 1.78                     | 0.83              |
| 2:A:174:ALA:HB1  | 2:A:207:GLU:HG2   | 1.60                     | 0.83              |
| 3:B:105:LYS:CG   | 3:B:110:GLU:HG2   | 2.08                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:168:THR:HB    | 3:B:201:THR:HG23  | 1.60                     | 0.83              |
| 2:A:311:LYS:HG2   | 2:A:344:VAL:CG1   | 2.08                     | 0.83              |
| 2:A:71:GLU:HG3    | 3:B:2:ARG:NH2     | 1.93                     | 0.83              |
| 2:A:151:SER:HB3   | 2:A:193:THR:CG2   | 2.08                     | 0.83              |
| 2:A:276:ILE:O     | 2:A:369:ALA:HB2   | 1.79                     | 0.83              |
| 3:B:243:ARG:HH22  | 3:B:252:LEU:HG    | 1.43                     | 0.83              |
| 2:A:68:VAL:HG13   | 2:A:93:ILE:CG2    | 2.09                     | 0.83              |
| 3:B:30:ILE:HD12   | 3:B:53:TYR:CE2    | 2.14                     | 0.83              |
| 2:A:223:THR:HG22  | 2:A:224:TYR:H     | 1.44                     | 0.82              |
| 3:B:75:MET:CE     | 3:B:94:PHE:HB3    | 2.09                     | 0.82              |
| 3:B:133:GLN:NE2   | 3:B:252:LEU:HB2   | 1.94                     | 0.82              |
| 2:A:305:CYS:SG    | 2:A:384:ILE:HD13  | 2.18                     | 0.82              |
| 2:A:115:ILE:CD1   | 2:A:153:LEU:HD13  | 2.08                     | 0.82              |
| 2:A:242:LEU:HG    | 2:A:250:VAL:O     | 1.78                     | 0.82              |
| 3:B:188:THR:HG23  | 3:B:425:MET:HE2   | 1.60                     | 0.82              |
| 3:B:275:LEU:HD23  | 3:B:300:ASN:ND2   | 1.93                     | 0.82              |
| 1:D:3464:TYR:CG   | 1:D:3478:VAL:HG21 | 2.15                     | 0.81              |
| 3:B:172:VAL:HG11  | 3:B:387:LEU:CD2   | 2.09                     | 0.81              |
| 3:B:274:PRO:O     | 3:B:275:LEU:HD13  | 1.80                     | 0.81              |
| 1:D:3482:THR:HG23 | 1:D:3486:TYR:CD2  | 2.16                     | 0.81              |
| 2:A:225:THR:O     | 2:A:229:ARG:HG3   | 1.80                     | 0.81              |
| 2:A:276:ILE:HG23  | 2:A:369:ALA:HB2   | 1.61                     | 0.81              |
| 2:A:301:GLN:HE22  | 2:A:307:PRO:HD3   | 1.43                     | 0.81              |
| 3:B:189:LEU:HD23  | 3:B:421:ALA:HB3   | 1.62                     | 0.81              |
| 2:A:22:GLU:HG2    | 2:A:83:TYR:CE1    | 2.15                     | 0.81              |
| 3:B:103:TRP:HD1   | 3:B:147:SER:HB2   | 1.43                     | 0.81              |
| 3:B:155:SER:HA    | 3:B:197:ASN:HD21  | 1.46                     | 0.81              |
| 2:A:107:HIS:HB2   | 2:A:148:GLY:HA2   | 1.62                     | 0.80              |
| 2:A:362:VAL:HG21  | 2:A:370:LYS:N     | 1.97                     | 0.80              |
| 3:B:70:LEU:H      | 3:B:145:THR:HG21  | 1.46                     | 0.80              |
| 1:D:3464:TYR:CD1  | 1:D:3478:VAL:HG11 | 2.15                     | 0.80              |
| 2:A:119:LEU:HA    | 2:A:122:ILE:CD1   | 2.11                     | 0.80              |
| 1:D:3432:ILE:HD13 | 1:D:3433:THR:H    | 1.46                     | 0.80              |
| 2:A:66:VAL:HA     | 2:A:91:GLN:HG2    | 1.62                     | 0.80              |
| 3:B:234:THR:CG2   | 3:B:270:PRO:HB3   | 2.10                     | 0.80              |
| 3:B:149:MET:O     | 3:B:153:LEU:HD22  | 1.83                     | 0.79              |
| 2:A:223:THR:HB    | 2:A:225:THR:HG22  | 1.63                     | 0.79              |
| 2:A:286:LEU:HG    | 2:A:290:GLU:CB    | 2.12                     | 0.79              |
| 1:D:3433:THR:O    | 1:D:3436:ILE:HG12 | 1.83                     | 0.79              |
| 1:D:3455:GLY:HA2  | 1:D:3457:LEU:HG   | 1.64                     | 0.79              |
| 2:A:132:LEU:HD21  | 2:A:164:LYS:HE3   | 1.63                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:4:ILE:HD11    | 3:B:252:LEU:CD1   | 2.11                     | 0.79              |
| 1:D:3464:TYR:CD1  | 1:D:3478:VAL:HG21 | 2.18                     | 0.79              |
| 2:A:301:GLN:HB2   | 2:A:303:VAL:H     | 1.48                     | 0.79              |
| 1:D:3394:LEU:HD22 | 2:A:410:GLY:CA    | 2.13                     | 0.78              |
| 2:A:431:ASP:O     | 2:A:435:VAL:HG23  | 1.82                     | 0.78              |
| 1:D:3428:GLU:HG2  | 1:D:3431:PHE:H    | 1.47                     | 0.78              |
| 1:D:3424:LYS:HZ1  | 3:B:156:LYS:HA    | 1.48                     | 0.78              |
| 3:B:31:ASP:O      | 3:B:34:GLY:HA3    | 1.83                     | 0.78              |
| 3:B:148:GLY:O     | 3:B:151:THR:HG22  | 1.83                     | 0.78              |
| 1:D:3457:LEU:HA   | 1:D:3462:PHE:CD2  | 2.17                     | 0.78              |
| 2:A:188:ILE:HG23  | 2:A:425:MET:SD    | 2.23                     | 0.78              |
| 2:A:211:ASP:O     | 2:A:215:ARG:HG2   | 1.84                     | 0.78              |
| 3:B:210:TYR:HE1   | 3:B:227:LEU:HD11  | 1.45                     | 0.77              |
| 2:A:103:TYR:HD2   | 2:A:413:MET:HE2   | 1.50                     | 0.77              |
| 2:A:151:SER:CB    | 2:A:193:THR:HG21  | 2.11                     | 0.77              |
| 3:B:150:GLY:HA2   | 3:B:153:LEU:CD2   | 2.15                     | 0.77              |
| 3:B:250:ALA:HB1   | 3:B:254:LYS:HB2   | 1.67                     | 0.77              |
| 3:B:324:SER:HB3   | 3:B:327:GLU:CG    | 2.03                     | 0.77              |
| 3:B:189:LEU:O     | 3:B:192:HIS:HB3   | 1.85                     | 0.77              |
| 3:B:286:LEU:HD22  | 3:B:291:LEU:HD11  | 1.65                     | 0.77              |
| 3:B:115:VAL:HG13  | 3:B:153:LEU:CD1   | 2.15                     | 0.77              |
| 3:B:184:PRO:HG3   | 3:B:394:GLN:CB    | 2.14                     | 0.77              |
| 2:A:303:VAL:HG13  | 2:A:305:CYS:N     | 1.97                     | 0.76              |
| 3:B:250:ALA:CA    | 3:B:254:LYS:HE2   | 2.11                     | 0.76              |
| 2:A:72:PRO:HG3    | 2:A:96:LYS:HA     | 1.67                     | 0.76              |
| 2:A:104:ALA:CB    | 2:A:411:GLU:HB2   | 2.15                     | 0.76              |
| 3:B:30:ILE:HG22   | 3:B:31:ASP:O      | 1.86                     | 0.76              |
| 2:A:205:ASP:HB3   | 2:A:208:ALA:CB    | 2.15                     | 0.76              |
| 2:A:199:ASP:HB3   | 2:A:256:GLN:NE2   | 2.01                     | 0.76              |
| 3:B:242:LEU:HD22  | 3:B:250:ALA:O     | 1.86                     | 0.75              |
| 2:A:74:VAL:O      | 2:A:77:GLU:HB2    | 1.86                     | 0.75              |
| 3:B:323:MET:HG3   | 3:B:328:VAL:CG2   | 2.17                     | 0.75              |
| 2:A:183:GLU:HB3   | 2:A:184:PRO:HD3   | 1.68                     | 0.75              |
| 2:A:362:VAL:HG21  | 2:A:370:LYS:H     | 1.52                     | 0.75              |
| 3:B:204:ILE:HG21  | 3:B:209:LEU:HD21  | 1.69                     | 0.75              |
| 2:A:199:ASP:HB3   | 2:A:256:GLN:HE21  | 1.51                     | 0.75              |
| 3:B:21:TRP:HA     | 3:B:24:ILE:CG2    | 2.17                     | 0.75              |
| 2:A:422:ARG:NH1   | 2:A:426:ALA:HB2   | 2.01                     | 0.75              |
| 3:B:243:ARG:NH2   | 3:B:252:LEU:HG    | 2.00                     | 0.75              |
| 3:B:151:THR:O     | 3:B:154:ILE:HG13  | 1.86                     | 0.75              |
| 3:B:286:LEU:HD13  | 3:B:373:MET:O     | 1.87                     | 0.75              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:B:323:MET:HG3  | 3:B:328:VAL:HG21  | 1.68                     | 0.75              |
| 2:A:69:ASP:HB3   | 2:A:75:ILE:CG1    | 2.17                     | 0.75              |
| 1:D:3455:GLY:CA  | 1:D:3458:GLU:H    | 2.00                     | 0.74              |
| 3:B:19:LYS:O     | 3:B:22:GLU:HB2    | 1.86                     | 0.74              |
| 3:B:57:ALA:HB2   | 3:B:60:LYS:CD     | 2.14                     | 0.74              |
| 3:B:237:GLY:O    | 3:B:241:CYS:HB3   | 1.87                     | 0.74              |
| 3:B:324:SER:O    | 3:B:328:VAL:HG23  | 1.86                     | 0.74              |
| 3:B:371:LEU:HG   | 3:B:372:LYS:N     | 2.00                     | 0.74              |
| 3:B:172:VAL:HG11 | 3:B:387:LEU:HD23  | 1.67                     | 0.74              |
| 3:B:201:THR:OG1  | 3:B:265:LEU:HD11  | 1.87                     | 0.74              |
| 1:D:3459:ASP:HB2 | 1:D:3462:PHE:HB3  | 1.67                     | 0.74              |
| 2:A:7:ILE:CG1    | 2:A:137:VAL:HG22  | 2.15                     | 0.74              |
| 3:B:10:GLY:O     | 3:B:13:GLY:HA3    | 1.87                     | 0.74              |
| 3:B:103:TRP:CD1  | 3:B:147:SER:HB2   | 2.22                     | 0.74              |
| 3:B:119:LEU:HA   | 3:B:122:VAL:CG1   | 2.16                     | 0.74              |
| 2:A:9:VAL:HG11   | 2:A:150:THR:OG1   | 1.87                     | 0.74              |
| 2:A:177:VAL:HG21 | 2:A:207:GLU:HB3   | 1.69                     | 0.74              |
| 2:A:210:TYR:CE1  | 2:A:227:LEU:HD21  | 2.20                     | 0.74              |
| 1:D:3404:ALA:O   | 1:D:3408:VAL:HG22 | 1.88                     | 0.74              |
| 1:D:3405:MET:HA  | 1:D:3408:VAL:CG2  | 2.17                     | 0.74              |
| 2:A:7:ILE:CG1    | 2:A:137:VAL:HG13  | 2.18                     | 0.74              |
| 3:B:318:VAL:HA   | 3:B:354:ALA:HB3   | 1.68                     | 0.74              |
| 3:B:230:LEU:HD21 | 3:B:302:MET:CE    | 2.17                     | 0.74              |
| 3:B:234:THR:HG23 | 3:B:376:THR:CG2   | 2.18                     | 0.74              |
| 3:B:310:GLY:O    | 3:B:342:TYR:HB3   | 1.88                     | 0.74              |
| 1:D:3444:MET:HG2 | 1:D:3446:PRO:HD2  | 1.69                     | 0.74              |
| 2:A:31:GLN:HB3   | 2:A:32:PRO:CD     | 2.18                     | 0.74              |
| 2:A:274:PRO:O    | 2:A:276:ILE:HG22  | 1.87                     | 0.74              |
| 3:B:54:ASN:HD21  | 3:B:64:ARG:HB2    | 1.53                     | 0.73              |
| 3:B:192:HIS:O    | 3:B:195:VAL:HG12  | 1.88                     | 0.73              |
| 2:A:155:GLU:HA   | 2:A:197:HIS:ND1   | 2.02                     | 0.73              |
| 2:A:252:LEU:O    | 2:A:255:PHE:HB2   | 1.88                     | 0.73              |
| 1:D:3424:LYS:HE2 | 3:B:156:LYS:CD    | 2.17                     | 0.73              |
| 3:B:234:THR:HG23 | 3:B:376:THR:HG22  | 1.68                     | 0.73              |
| 3:B:275:LEU:HB2  | 3:B:294:GLN:OE1   | 1.88                     | 0.73              |
| 3:B:259:MET:O    | 3:B:261:PRO:HD3   | 1.89                     | 0.73              |
| 2:A:241:SER:O    | 2:A:244:PHE:HB3   | 1.88                     | 0.73              |
| 2:A:402:ARG:HE   | 2:A:405:VAL:HG12  | 1.52                     | 0.73              |
| 3:B:270:PRO:O    | 3:B:302:MET:HG3   | 1.88                     | 0.73              |
| 2:A:7:ILE:HG13   | 2:A:137:VAL:HG13  | 1.71                     | 0.73              |
| 3:B:184:PRO:HG3  | 3:B:394:GLN:HB3   | 1.69                     | 0.73              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:B:315:VAL:HG13 | 3:B:377:PHE:HE1   | 1.52                     | 0.73              |
| 3:B:154:ILE:HG22 | 3:B:166:MET:SD    | 2.28                     | 0.73              |
| 3:B:219:LEU:HD21 | 3:B:226:ASP:OD2   | 1.89                     | 0.73              |
| 3:B:21:TRP:CZ3   | 3:B:63:PRO:HB3    | 2.23                     | 0.73              |
| 3:B:141:LEU:HB3  | 3:B:187:ALA:HA    | 1.71                     | 0.73              |
| 1:D:3408:VAL:HA  | 1:D:3411:MET:HE2  | 1.71                     | 0.72              |
| 2:A:133:GLN:HB2  | 2:A:243:ARG:HH12  | 1.52                     | 0.72              |
| 3:B:100:GLY:HA3  | 3:B:105:LYS:HE2   | 1.70                     | 0.72              |
| 3:B:169:PHE:CZ   | 3:B:235:MET:HB3   | 2.24                     | 0.72              |
| 2:A:255:PHE:O    | 2:A:259:LEU:HB2   | 1.88                     | 0.72              |
| 3:B:35:SER:HB3   | 3:B:59:ASN:OD1    | 1.88                     | 0.72              |
| 2:A:362:VAL:HG21 | 2:A:370:LYS:CA    | 2.20                     | 0.72              |
| 3:B:67:LEU:HD12  | 3:B:92:PHE:CD1    | 2.24                     | 0.72              |
| 2:A:105:ARG:HG2  | 2:A:411:GLU:HG3   | 1.70                     | 0.72              |
| 3:B:273:ALA:CB   | 3:B:375:ALA:H     | 2.02                     | 0.72              |
| 3:B:199:ASP:O    | 3:B:265:LEU:HB2   | 1.89                     | 0.72              |
| 3:B:286:LEU:HD11 | 3:B:371:LEU:HD21  | 1.72                     | 0.72              |
| 3:B:396:THR:HG23 | 3:B:422:GLU:OE2   | 1.90                     | 0.72              |
| 3:B:413:MET:HG2  | 3:B:418:PHE:HE1   | 1.55                     | 0.72              |
| 3:B:93:VAL:HG11  | 3:B:118:VAL:HG22  | 1.70                     | 0.72              |
| 3:B:304:ALA:HB3  | 3:B:387:LEU:CD1   | 2.20                     | 0.72              |
| 3:B:57:ALA:CB    | 3:B:60:LYS:HD2    | 2.16                     | 0.72              |
| 2:A:69:ASP:HB3   | 2:A:75:ILE:HG12   | 1.72                     | 0.71              |
| 2:A:214:ARG:O    | 2:A:218:ASP:HA    | 1.89                     | 0.71              |
| 2:A:242:LEU:HD21 | 2:A:250:VAL:HB    | 1.71                     | 0.71              |
| 3:B:175:PRO:HD2  | 3:B:207:GLU:OE2   | 1.90                     | 0.71              |
| 3:B:191:VAL:HA   | 3:B:194:LEU:CD1   | 2.12                     | 0.71              |
| 3:B:286:LEU:O    | 3:B:291:LEU:HD13  | 1.90                     | 0.71              |
| 1:D:3444:MET:O   | 1:D:3448:ILE:HB   | 1.90                     | 0.71              |
| 2:A:175:PRO:HD2  | 2:A:207:GLU:HG2   | 1.73                     | 0.71              |
| 2:A:179:THR:HG21 | 3:B:248:LEU:HD22  | 1.71                     | 0.71              |
| 3:B:7:ILE:HB     | 3:B:137:LEU:CD1   | 2.20                     | 0.71              |
| 1:D:3433:THR:HA  | 1:D:3436:ILE:HD13 | 1.73                     | 0.71              |
| 3:B:102:ASN:ND2  | 3:B:408:TYR:HA    | 2.06                     | 0.71              |
| 2:A:174:ALA:CB   | 2:A:177:VAL:HB    | 2.20                     | 0.71              |
| 2:A:385:ALA:HB2  | 2:A:432:TYR:HB3   | 1.72                     | 0.71              |
| 1:D:3449:ARG:O   | 1:D:3453:THR:HG23 | 1.90                     | 0.70              |
| 2:A:166:LYS:HE3  | 2:A:197:HIS:O     | 1.91                     | 0.70              |
| 2:A:274:PRO:HG2  | 2:A:374:ALA:HB1   | 1.73                     | 0.70              |
| 2:A:133:GLN:CB   | 2:A:243:ARG:HH12  | 2.04                     | 0.70              |
| 3:B:332:MET:HE3  | 3:B:351:VAL:CG1   | 2.21                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:48:ARG:CG    | 3:B:243:ARG:HB3  | 2.21                     | 0.70              |
| 3:B:250:ALA:HA   | 3:B:254:LYS:CE   | 2.12                     | 0.70              |
| 3:B:274:PRO:CG   | 3:B:374:SER:HB3  | 2.22                     | 0.70              |
| 2:A:19:ALA:HB2   | 2:A:228:ASN:HB3  | 1.73                     | 0.70              |
| 3:B:119:LEU:HD11 | 3:B:156:LYS:CG   | 2.21                     | 0.70              |
| 2:A:7:ILE:HG12   | 2:A:137:VAL:CG2  | 2.16                     | 0.70              |
| 3:B:149:MET:C    | 3:B:153:LEU:HD22 | 2.12                     | 0.70              |
| 3:B:268:PHE:HB3  | 3:B:379:GLY:H    | 1.57                     | 0.70              |
| 2:A:14:VAL:HG21  | 2:A:75:ILE:CD1   | 2.22                     | 0.70              |
| 2:A:119:LEU:HD23 | 2:A:122:ILE:HD11 | 1.72                     | 0.70              |
| 2:A:303:VAL:CG1  | 2:A:305:CYS:HB2  | 2.20                     | 0.70              |
| 3:B:6:HIS:HD1    | 3:B:21:TRP:HE1   | 1.39                     | 0.70              |
| 3:B:23:VAL:HG13  | 7:B:502:TA1:H321 | 1.73                     | 0.70              |
| 1:D:3439:ASP:HB3 | 1:D:3442:LYS:HG2 | 1.74                     | 0.69              |
| 2:A:405:VAL:O    | 2:A:409:VAL:HG23 | 1.92                     | 0.69              |
| 3:B:119:LEU:HA   | 3:B:122:VAL:HG13 | 1.74                     | 0.69              |
| 1:D:3468:ASN:OD1 | 1:D:3475:GLY:HA2 | 1.92                     | 0.69              |
| 3:B:115:VAL:HG13 | 3:B:153:LEU:HD12 | 1.74                     | 0.69              |
| 1:D:3424:LYS:CE  | 3:B:156:LYS:HD2  | 2.20                     | 0.69              |
| 1:D:3459:ASP:HB2 | 1:D:3462:PHE:CB  | 2.22                     | 0.69              |
| 2:A:207:GLU:O    | 2:A:210:TYR:HB2  | 1.91                     | 0.69              |
| 3:B:89:PRO:HA    | 3:B:92:PHE:CE2   | 2.26                     | 0.69              |
| 3:B:385:GLN:HG2  | 3:B:386:GLU:N    | 2.05                     | 0.69              |
| 3:B:251:ASP:N    | 3:B:254:LYS:HG3  | 2.05                     | 0.69              |
| 3:B:346:TRP:O    | 3:B:348:PRO:HD3  | 1.93                     | 0.69              |
| 2:A:184:PRO:O    | 2:A:188:ILE:HG12 | 1.92                     | 0.69              |
| 3:B:10:GLY:HA2   | 3:B:145:THR:HB   | 1.74                     | 0.69              |
| 3:B:150:GLY:HA2  | 3:B:153:LEU:HD22 | 1.73                     | 0.69              |
| 2:A:84:ARG:HG2   | 2:A:84:ARG:HH11  | 1.57                     | 0.68              |
| 2:A:205:ASP:HB3  | 2:A:208:ALA:HB3  | 1.74                     | 0.68              |
| 3:B:108:TYR:CE1  | 3:B:413:MET:HE1  | 2.27                     | 0.68              |
| 3:B:140:SER:HB2  | 3:B:142:GLY:HA2  | 1.74                     | 0.68              |
| 2:A:5:ILE:O      | 2:A:135:PHE:HA   | 1.93                     | 0.68              |
| 3:B:230:LEU:HD23 | 3:B:231:VAL:N    | 2.08                     | 0.68              |
| 2:A:201:ALA:O    | 2:A:268:PRO:HD2  | 1.94                     | 0.68              |
| 1:D:3392:LYS:HE3 | 1:D:3423:ARG:NH2 | 2.09                     | 0.68              |
| 3:B:8:GLN:CD     | 3:B:67:LEU:HD22  | 2.13                     | 0.68              |
| 3:B:207:GLU:HG2  | 3:B:208:ALA:N    | 2.08                     | 0.68              |
| 2:A:79:ARG:O     | 2:A:84:ARG:HG3   | 1.94                     | 0.68              |
| 3:B:69:ASP:OD1   | 3:B:71:GLU:HB3   | 1.94                     | 0.68              |
| 1:D:3390:GLU:CG  | 2:A:402:ARG:HH22 | 2.04                     | 0.68              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:A:167:LEU:HD23  | 2:A:202:PHE:HE2  | 1.57                     | 0.68              |
| 3:B:6:HIS:HB3     | 3:B:21:TRP:HZ2   | 1.59                     | 0.68              |
| 2:A:188:ILE:HG13  | 2:A:395:PHE:CD2  | 2.29                     | 0.68              |
| 3:B:4:ILE:HD11    | 3:B:252:LEU:HD11 | 1.74                     | 0.68              |
| 3:B:24:ILE:HD11   | 3:B:52:TYR:CE2   | 2.28                     | 0.68              |
| 2:A:371:VAL:HG12  | 2:A:373:ARG:H    | 1.59                     | 0.67              |
| 2:A:242:LEU:HD23  | 2:A:255:PHE:HE1  | 1.58                     | 0.67              |
| 2:A:66:VAL:HG12   | 2:A:91:GLN:CG    | 2.21                     | 0.67              |
| 3:B:173:PRO:HB3   | 3:B:183:GLU:CG   | 2.24                     | 0.67              |
| 1:D:3464:TYR:HB2  | 1:D:3478:VAL:CG2 | 2.23                     | 0.67              |
| 2:A:188:ILE:HD12  | 2:A:425:MET:SD   | 2.34                     | 0.67              |
| 2:A:301:GLN:NE2   | 2:A:307:PRO:HD3  | 2.08                     | 0.67              |
| 2:A:250:VAL:HG21  | 2:A:318:LEU:HD21 | 1.76                     | 0.67              |
| 2:A:105:ARG:HB2   | 2:A:110:ILE:HG22 | 1.77                     | 0.67              |
| 3:B:289:PRO:HG3   | 3:B:331:GLN:OE1  | 1.95                     | 0.67              |
| 1:D:3473:ALA:O    | 1:D:3476:PRO:HD2 | 1.94                     | 0.67              |
| 3:B:371:LEU:HG    | 3:B:372:LYS:H    | 1.59                     | 0.67              |
| 1:D:3424:LYS:HE2  | 3:B:156:LYS:CE   | 2.25                     | 0.67              |
| 2:A:242:LEU:HD23  | 2:A:255:PHE:CE1  | 2.30                     | 0.67              |
| 2:A:251:ASP:H     | 2:A:254:GLU:HG3  | 1.60                     | 0.67              |
| 3:B:155:SER:HA    | 3:B:197:ASN:ND2  | 2.10                     | 0.66              |
| 3:B:413:MET:HG3   | 3:B:414:ASP:N    | 2.08                     | 0.66              |
| 3:B:36:TYR:OH     | 3:B:43:GLN:HB2   | 1.96                     | 0.66              |
| 2:A:69:ASP:CB     | 2:A:75:ILE:HD11  | 2.23                     | 0.66              |
| 2:A:103:TYR:H     | 2:A:408:TYR:HE1  | 1.43                     | 0.66              |
| 1:D:3457:LEU:HD12 | 1:D:3458:GLU:N   | 2.11                     | 0.66              |
| 2:A:172:TYR:HE2   | 2:A:388:TRP:CZ3  | 2.12                     | 0.66              |
| 3:B:11:GLN:HG3    | 3:B:74:THR:CG2   | 2.25                     | 0.66              |
| 3:B:204:ILE:CG2   | 3:B:209:LEU:HD21 | 2.25                     | 0.66              |
| 2:A:11:GLN:O      | 2:A:14:VAL:HB    | 1.96                     | 0.66              |
| 2:A:227:LEU:O     | 2:A:231:ILE:HG12 | 1.95                     | 0.66              |
| 2:A:242:LEU:HD11  | 2:A:250:VAL:HG23 | 1.76                     | 0.66              |
| 3:B:70:LEU:O      | 3:B:72:PRO:HD3   | 1.96                     | 0.66              |
| 3:B:21:TRP:CA     | 3:B:24:ILE:HG22  | 2.20                     | 0.66              |
| 3:B:100:GLY:CA    | 3:B:105:LYS:HE2  | 2.26                     | 0.66              |
| 2:A:256:GLN:O     | 2:A:260:VAL:HG13 | 1.94                     | 0.66              |
| 2:A:360:PRO:HG3   | 2:A:374:ALA:HB3  | 1.78                     | 0.66              |
| 3:B:390:ARG:O     | 3:B:394:GLN:HG3  | 1.95                     | 0.66              |
| 2:A:62:VAL:HG13   | 2:A:63:PRO:HD2   | 1.78                     | 0.65              |
| 3:B:264:ARG:O     | 3:B:265:LEU:HD23 | 1.96                     | 0.65              |
| 2:A:68:VAL:HA     | 2:A:93:ILE:HG22  | 1.78                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:A:98:ASP:O     | 2:A:110:ILE:HD13  | 1.97                     | 0.65              |
| 3:B:71:GLU:HG2   | 3:B:74:THR:H      | 1.62                     | 0.65              |
| 2:A:217:LEU:H    | 2:A:217:LEU:HD23  | 1.60                     | 0.65              |
| 3:B:31:ASP:HB2   | 3:B:34:GLY:HA2    | 1.78                     | 0.65              |
| 3:B:336:GLN:HE22 | 3:B:350:ASN:H     | 1.43                     | 0.65              |
| 2:A:101:ASN:ND2  | 3:B:254:LYS:HD2   | 2.10                     | 0.65              |
| 3:B:132:LEU:O    | 3:B:164:ARG:HG2   | 1.96                     | 0.65              |
| 3:B:140:SER:C    | 3:B:142:GLY:HA3   | 2.17                     | 0.65              |
| 3:B:173:PRO:HD2  | 3:B:391:ILE:HD11  | 1.78                     | 0.65              |
| 3:B:339:ASN:HB3  | 3:B:342:TYR:CE1   | 2.31                     | 0.65              |
| 1:D:3399:THR:OG1 | 1:D:3400:PRO:HD3  | 1.95                     | 0.65              |
| 1:D:3430:ASN:O   | 1:D:3434:SER:HB2  | 1.97                     | 0.65              |
| 3:B:209:LEU:CD1  | 3:B:230:LEU:HD21  | 2.25                     | 0.65              |
| 3:B:259:MET:HA   | 3:B:314:THR:HG21  | 1.79                     | 0.65              |
| 2:A:242:LEU:HD21 | 2:A:318:LEU:HD21  | 1.79                     | 0.65              |
| 3:B:119:LEU:HD11 | 3:B:156:LYS:HG2   | 1.77                     | 0.65              |
| 3:B:272:PHE:CE2  | 3:B:274:PRO:HD2   | 2.32                     | 0.65              |
| 2:A:132:LEU:O    | 2:A:132:LEU:HG    | 1.97                     | 0.65              |
| 2:A:384:ILE:HG22 | 2:A:388:TRP:CD1   | 2.31                     | 0.65              |
| 3:B:202:TYR:HE2  | 3:B:378:ILE:HG21  | 1.61                     | 0.65              |
| 2:A:405:VAL:HG13 | 2:A:409:VAL:CG2   | 2.27                     | 0.65              |
| 3:B:282:GLN:O    | 3:B:282:GLN:HG2   | 1.96                     | 0.65              |
| 1:D:3392:LYS:HE2 | 1:D:3393:SER:HA   | 1.79                     | 0.65              |
| 3:B:172:VAL:HG11 | 3:B:387:LEU:HD21  | 1.77                     | 0.65              |
| 2:A:82:THR:HG22  | 2:A:83:TYR:CD1    | 2.32                     | 0.64              |
| 2:A:242:LEU:CD1  | 2:A:318:LEU:HD22  | 2.27                     | 0.64              |
| 3:B:151:THR:HA   | 3:B:154:ILE:HD11  | 1.79                     | 0.64              |
| 2:A:176:GLN:OE1  | 3:B:333:LEU:HD11  | 1.96                     | 0.64              |
| 3:B:6:HIS:CE1    | 3:B:8:GLN:HG2     | 2.32                     | 0.64              |
| 3:B:241:CYS:O    | 3:B:244:PHE:HB2   | 1.96                     | 0.64              |
| 3:B:325:MET:CE   | 3:B:355:VAL:HG21  | 2.27                     | 0.64              |
| 1:D:3398:PRO:HB2 | 1:D:3401:VAL:HG23 | 1.78                     | 0.64              |
| 1:D:3455:GLY:HA3 | 1:D:3458:GLU:CG   | 2.27                     | 0.64              |
| 2:A:104:ALA:CB   | 2:A:413:MET:HG2   | 2.28                     | 0.64              |
| 2:A:154:MET:HE1  | 2:A:166:LYS:HD2   | 1.79                     | 0.64              |
| 3:B:325:MET:HE3  | 3:B:355:VAL:HG21  | 1.79                     | 0.64              |
| 3:B:110:GLU:HA   | 3:B:110:GLU:OE1   | 1.98                     | 0.64              |
| 3:B:319:PHE:CG   | 3:B:375:ALA:HB2   | 2.31                     | 0.64              |
| 1:D:3419:TRP:CE3 | 1:D:3422:ILE:HG12 | 2.33                     | 0.64              |
| 2:A:185:TYR:OH   | 2:A:399:TYR:HA    | 1.98                     | 0.64              |
| 2:A:203:MET:HG3  | 2:A:267:PHE:HB3   | 1.77                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:416:GLY:O     | 2:A:420:GLU:HG2   | 1.96                     | 0.64              |
| 3:B:264:ARG:HG3   | 3:B:264:ARG:HH11  | 1.62                     | 0.64              |
| 3:B:320:ARG:HA    | 3:B:356:CYS:HB3   | 1.80                     | 0.64              |
| 1:D:3423:ARG:NH2  | 3:B:162:PRO:HB3   | 2.12                     | 0.64              |
| 2:A:248:LEU:HB2   | 2:A:355:ILE:H     | 1.61                     | 0.64              |
| 2:A:386:GLU:OE1   | 2:A:386:GLU:HA    | 1.96                     | 0.64              |
| 3:B:261:PRO:HB2   | 3:B:262:PHE:CD2   | 2.33                     | 0.64              |
| 3:B:102:ASN:HD21  | 3:B:408:TYR:HA    | 1.62                     | 0.64              |
| 3:B:173:PRO:HG2   | 3:B:391:ILE:HD13  | 1.78                     | 0.64              |
| 3:B:188:THR:HG23  | 3:B:425:MET:CE    | 2.26                     | 0.64              |
| 2:A:66:VAL:HG12   | 2:A:91:GLN:HA     | 1.79                     | 0.64              |
| 2:A:103:TYR:CD2   | 2:A:413:MET:HE2   | 2.33                     | 0.64              |
| 2:A:109:THR:HG22  | 2:A:110:ILE:N     | 2.12                     | 0.64              |
| 2:A:311:LYS:H     | 2:A:382:THR:HB    | 1.63                     | 0.64              |
| 3:B:106:GLY:O     | 3:B:111:GLY:HA3   | 1.97                     | 0.64              |
| 2:A:362:VAL:HG21  | 2:A:370:LYS:HA    | 1.78                     | 0.64              |
| 3:B:31:ASP:HB3    | 3:B:32:PRO:HD2    | 1.78                     | 0.64              |
| 3:B:76:ASP:HA     | 3:B:79:ARG:HG3    | 1.80                     | 0.64              |
| 2:A:167:LEU:HA    | 2:A:200:CYS:O     | 1.98                     | 0.63              |
| 2:A:324:VAL:HG12  | 2:A:326:LYS:H     | 1.62                     | 0.63              |
| 2:A:298:PRO:HA    | 2:A:301:GLN:OE1   | 1.99                     | 0.63              |
| 3:B:7:ILE:HB      | 3:B:137:LEU:HD13  | 1.80                     | 0.63              |
| 3:B:288:VAL:HG12  | 3:B:289:PRO:CD    | 2.28                     | 0.63              |
| 1:D:3394:LEU:CG   | 2:A:410:GLY:HA2   | 2.29                     | 0.63              |
| 1:D:3419:TRP:O    | 1:D:3422:ILE:HG13 | 1.98                     | 0.63              |
| 2:A:106:GLY:O     | 2:A:111:GLY:HA2   | 1.99                     | 0.63              |
| 2:A:238:ILE:HD12  | 2:A:255:PHE:CE2   | 2.32                     | 0.63              |
| 2:A:278:ALA:HB2   | 2:A:367:ASP:O     | 1.99                     | 0.63              |
| 1:D:3455:GLY:CA   | 1:D:3458:GLU:HG3  | 2.29                     | 0.63              |
| 1:D:3455:GLY:HA3  | 1:D:3458:GLU:HG3  | 1.79                     | 0.63              |
| 3:B:94:PHE:HD1    | 3:B:94:PHE:H      | 1.46                     | 0.63              |
| 2:A:132:LEU:CG    | 2:A:164:LYS:HE3   | 2.28                     | 0.63              |
| 3:B:328:VAL:O     | 3:B:332:MET:HG2   | 1.99                     | 0.63              |
| 1:D:3416:LYS:CG   | 1:D:3418:GLU:H    | 2.03                     | 0.63              |
| 3:B:286:LEU:HD22  | 3:B:291:LEU:CD1   | 2.28                     | 0.63              |
| 3:B:330:GLU:HG3   | 3:B:331:GLN:N     | 2.13                     | 0.63              |
| 1:D:3469:ARG:HG3  | 1:D:3469:ARG:HH11 | 1.64                     | 0.63              |
| 2:A:84:ARG:HG2    | 2:A:84:ARG:NH1    | 2.12                     | 0.63              |
| 3:B:89:PRO:HA     | 3:B:92:PHE:HE2    | 1.63                     | 0.63              |
| 1:D:3436:ILE:HG13 | 1:D:3437:ASN:HD22 | 1.64                     | 0.63              |
| 2:A:117:LEU:HD11  | 2:A:121:ARG:HH22  | 1.64                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:225:THR:HG23 | 2:A:226:ASN:HD22 | 1.64                     | 0.63              |
| 3:B:198:THR:O    | 3:B:265:LEU:HD13 | 1.98                     | 0.63              |
| 2:A:317:LEU:HB3  | 2:A:319:TYR:HE1  | 1.64                     | 0.62              |
| 2:A:401:LYS:HE3  | 3:B:346:TRP:HB3  | 1.80                     | 0.62              |
| 3:B:182:VAL:HB   | 3:B:186:ASN:HD21 | 1.64                     | 0.62              |
| 3:B:184:PRO:HG3  | 3:B:394:GLN:HB2  | 1.81                     | 0.62              |
| 7:B:502:TA1:H463 | 7:B:502:TA1:H261 | 1.80                     | 0.62              |
| 3:B:220:THR:O    | 3:B:222:PRO:HD3  | 1.99                     | 0.62              |
| 2:A:178:SER:HB2  | 2:A:183:GLU:OE2  | 1.98                     | 0.62              |
| 3:B:67:LEU:N     | 3:B:67:LEU:HD23  | 2.12                     | 0.62              |
| 1:D:3483:ALA:HB1 | 1:D:3484:GLN:NE2 | 2.15                     | 0.62              |
| 2:A:68:VAL:HG13  | 2:A:93:ILE:HG22  | 1.81                     | 0.62              |
| 2:A:179:THR:HG22 | 3:B:352:LYS:HE3  | 1.81                     | 0.62              |
| 2:A:301:GLN:HB2  | 2:A:303:VAL:N    | 2.15                     | 0.62              |
| 2:A:412:GLY:HA2  | 2:A:413:MET:O    | 2.00                     | 0.62              |
| 2:A:179:THR:HG23 | 3:B:353:THR:HB   | 1.81                     | 0.62              |
| 2:A:221:ARG:HG2  | 2:A:221:ARG:O    | 1.99                     | 0.62              |
| 2:A:303:VAL:HG11 | 2:A:305:CYS:HB2  | 1.81                     | 0.62              |
| 2:A:320:ARG:HB2  | 2:A:358:GLU:O    | 1.99                     | 0.62              |
| 2:A:363:VAL:H    | 2:A:368:LEU:HD12 | 1.65                     | 0.62              |
| 2:A:9:VAL:HG21   | 2:A:149:PHE:HD1  | 1.65                     | 0.62              |
| 3:B:20:PHE:CZ    | 3:B:24:ILE:HD13  | 2.34                     | 0.62              |
| 1:D:3424:LYS:HZ2 | 3:B:159:GLU:CB   | 2.09                     | 0.62              |
| 2:A:193:THR:HG23 | 2:A:194:THR:N    | 2.15                     | 0.62              |
| 2:A:275:VAL:HG11 | 2:A:300:ASN:HD21 | 1.64                     | 0.62              |
| 1:D:3416:LYS:HE2 | 1:D:3418:GLU:CB  | 2.23                     | 0.62              |
| 2:A:362:VAL:CG2  | 2:A:370:LYS:HA   | 2.28                     | 0.62              |
| 3:B:55:GLU:HG2   | 3:B:61:TYR:CE1   | 2.35                     | 0.62              |
| 2:A:118:VAL:O    | 2:A:122:ILE:HD13 | 2.00                     | 0.61              |
| 2:A:132:LEU:HG   | 2:A:164:LYS:HE3  | 1.81                     | 0.61              |
| 2:A:175:PRO:HG2  | 2:A:304:LYS:CD   | 2.29                     | 0.61              |
| 3:B:157:ILE:HG21 | 3:B:166:MET:SD   | 2.39                     | 0.61              |
| 3:B:283:TYR:O    | 3:B:284:ARG:HB2  | 2.00                     | 0.61              |
| 3:B:150:GLY:HA2  | 3:B:153:LEU:HD23 | 1.82                     | 0.61              |
| 3:B:288:VAL:HG12 | 3:B:289:PRO:N    | 2.15                     | 0.61              |
| 1:D:3450:GLU:HA  | 1:D:3453:THR:OG1 | 2.01                     | 0.61              |
| 2:A:107:HIS:HD2  | 2:A:108:TYR:CD1  | 2.17                     | 0.61              |
| 2:A:250:VAL:CG2  | 2:A:318:LEU:HD21 | 2.31                     | 0.61              |
| 2:A:408:TYR:CG   | 2:A:418:PHE:HZ   | 2.18                     | 0.61              |
| 3:B:182:VAL:HG12 | 3:B:185:TYR:HB2  | 1.82                     | 0.61              |
| 3:B:326:LYS:HE3  | 3:B:330:GLU:HB3  | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:119:LEU:CA    | 3:B:122:VAL:HG13  | 2.31                     | 0.61              |
| 3:B:278:ARG:HB3   | 3:B:279:GLY:CA    | 2.31                     | 0.61              |
| 3:B:312:TYR:HE2   | 3:B:377:PHE:HZ    | 1.49                     | 0.61              |
| 3:B:408:TYR:CD2   | 3:B:418:PHE:HZ    | 2.18                     | 0.61              |
| 2:A:110:ILE:HG23  | 2:A:111:GLY:N     | 2.14                     | 0.61              |
| 2:A:261:PRO:HB2   | 2:A:262:TYR:CD2   | 2.36                     | 0.61              |
| 3:B:314:THR:H     | 3:B:380:ASN:HB3   | 1.66                     | 0.61              |
| 3:B:388:PHE:HB2   | 3:B:429:VAL:HG22  | 1.83                     | 0.61              |
| 1:D:3384:LYS:HD3  | 1:D:3386:LYS:CB   | 2.28                     | 0.61              |
| 3:B:172:VAL:HG23  | 3:B:203:CYS:HB3   | 1.81                     | 0.61              |
| 3:B:372:LYS:HG3   | 3:B:373:MET:HB2   | 1.83                     | 0.61              |
| 1:D:3422:ILE:HG13 | 1:D:3423:ARG:N    | 2.15                     | 0.61              |
| 2:A:68:VAL:HG13   | 2:A:93:ILE:HG21   | 1.83                     | 0.61              |
| 1:D:3384:LYS:CD   | 1:D:3386:LYS:HB2  | 2.29                     | 0.61              |
| 3:B:209:LEU:HD11  | 3:B:302:MET:CE    | 2.31                     | 0.61              |
| 3:B:188:THR:HG21  | 3:B:422:GLU:HA    | 1.82                     | 0.60              |
| 2:A:115:ILE:CD1   | 2:A:152:LEU:HD11  | 2.28                     | 0.60              |
| 2:A:223:THR:HG22  | 2:A:224:TYR:N     | 2.14                     | 0.60              |
| 2:A:244:PHE:HD1   | 2:A:245:ASP:N     | 1.99                     | 0.60              |
| 2:A:269:LEU:CD2   | 2:A:384:ILE:HD11  | 2.26                     | 0.60              |
| 2:A:419:SER:O     | 2:A:422:ARG:HB3   | 2.01                     | 0.60              |
| 3:B:172:VAL:CG1   | 3:B:173:PRO:HD2   | 2.31                     | 0.60              |
| 3:B:297:ASP:OD2   | 3:B:299:LYS:HE2   | 2.01                     | 0.60              |
| 3:B:327:GLU:HA    | 3:B:330:GLU:HG2   | 1.83                     | 0.60              |
| 2:A:205:ASP:HB3   | 2:A:208:ALA:HB2   | 1.81                     | 0.60              |
| 2:A:275:VAL:HG21  | 2:A:300:ASN:OD1   | 2.01                     | 0.60              |
| 2:A:316:CYS:CB    | 2:A:378:LEU:HD11  | 2.18                     | 0.60              |
| 3:B:315:VAL:CG1   | 3:B:351:VAL:HG13  | 2.31                     | 0.60              |
| 3:B:408:TYR:O     | 3:B:411:GLU:HB2   | 2.02                     | 0.60              |
| 1:D:3418:GLU:O    | 1:D:3422:ILE:HG23 | 2.01                     | 0.60              |
| 2:A:274:PRO:CG    | 2:A:374:ALA:HA    | 2.32                     | 0.60              |
| 3:B:102:ASN:HB3   | 3:B:105:LYS:N     | 2.06                     | 0.60              |
| 3:B:258:ASN:HD22  | 3:B:352:LYS:HG3   | 1.66                     | 0.60              |
| 1:D:3436:ILE:HG13 | 1:D:3437:ASN:ND2  | 2.17                     | 0.60              |
| 1:D:3456:TYR:HA   | 1:D:3459:ASP:OD1  | 2.01                     | 0.60              |
| 2:A:317:LEU:HB3   | 2:A:319:TYR:CE1   | 2.35                     | 0.60              |
| 3:B:168:THR:CB    | 3:B:201:THR:HG23  | 2.30                     | 0.60              |
| 2:A:424:ASP:O     | 2:A:427:ALA:HB3   | 2.01                     | 0.60              |
| 3:B:19:LYS:HG3    | 3:B:228:ASN:HB3   | 1.84                     | 0.60              |
| 3:B:332:MET:CE    | 3:B:351:VAL:HG11  | 2.31                     | 0.60              |
| 1:D:3384:LYS:HZ1  | 1:D:3386:LYS:HE3  | 1.67                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:269:MET:HE3   | 3:B:301:MET:HG2   | 1.82                     | 0.60              |
| 2:A:175:PRO:HG2   | 2:A:304:LYS:CE    | 2.32                     | 0.59              |
| 3:B:119:LEU:HD11  | 3:B:156:LYS:CB    | 2.32                     | 0.59              |
| 2:A:119:LEU:O     | 2:A:123:ARG:HG2   | 2.03                     | 0.59              |
| 2:A:303:VAL:HG13  | 2:A:305:CYS:HB2   | 1.84                     | 0.59              |
| 3:B:107:HIS:CE1   | 3:B:152:LEU:HD13  | 2.37                     | 0.59              |
| 3:B:133:GLN:HG3   | 3:B:252:LEU:HD12  | 1.81                     | 0.59              |
| 1:D:3394:LEU:HD13 | 2:A:409:VAL:C     | 2.21                     | 0.59              |
| 1:D:3456:TYR:O    | 1:D:3459:ASP:HB2  | 2.02                     | 0.59              |
| 2:A:228:ASN:HA    | 2:A:231:ILE:HG13  | 1.83                     | 0.59              |
| 3:B:49:ILE:HG13   | 3:B:50:ASN:N      | 2.16                     | 0.59              |
| 3:B:314:THR:HG22  | 3:B:315:VAL:N     | 2.18                     | 0.59              |
| 1:D:3395:PRO:HD2  | 2:A:410:GLY:HA3   | 1.84                     | 0.59              |
| 1:D:3423:ARG:CZ   | 3:B:162:PRO:HB3   | 2.32                     | 0.59              |
| 3:B:248:LEU:HD23  | 3:B:353:THR:O     | 2.02                     | 0.59              |
| 2:A:239:THR:O     | 2:A:243:ARG:HG2   | 2.01                     | 0.59              |
| 3:B:11:GLN:HG3    | 3:B:74:THR:HG21   | 1.84                     | 0.59              |
| 3:B:150:GLY:CA    | 3:B:153:LEU:HD22  | 2.33                     | 0.59              |
| 3:B:167:ASN:HB3   | 3:B:202:TYR:HE1   | 1.67                     | 0.59              |
| 3:B:255:LEU:O     | 3:B:259:MET:HG3   | 2.01                     | 0.59              |
| 3:B:107:HIS:HB3   | 3:B:108:TYR:CD1   | 2.36                     | 0.59              |
| 3:B:173:PRO:HG2   | 3:B:391:ILE:CD1   | 2.32                     | 0.59              |
| 3:B:273:ALA:CB    | 3:B:274:PRO:HD3   | 2.28                     | 0.59              |
| 1:D:3405:MET:SD   | 1:D:3408:VAL:HG23 | 2.42                     | 0.59              |
| 3:B:172:VAL:HB    | 3:B:205:ASP:OD1   | 2.02                     | 0.59              |
| 3:B:198:THR:O     | 3:B:265:LEU:HD22  | 2.03                     | 0.59              |
| 3:B:209:LEU:HD11  | 3:B:230:LEU:HD21  | 1.85                     | 0.59              |
| 1:D:3424:LYS:CE   | 3:B:156:LYS:HA    | 2.32                     | 0.59              |
| 1:D:3424:LYS:CB   | 3:B:159:GLU:HB2   | 2.22                     | 0.59              |
| 2:A:11:GLN:HG3    | 2:A:74:VAL:CG1    | 2.17                     | 0.59              |
| 2:A:173:PRO:HG2   | 2:A:391:LEU:HD11  | 1.85                     | 0.59              |
| 3:B:139:HIS:HB2   | 3:B:146:GLY:O     | 2.03                     | 0.59              |
| 3:B:48:ARG:O      | 3:B:51:VAL:HG23   | 2.03                     | 0.59              |
| 3:B:86:ILE:HG23   | 3:B:87:PHE:N      | 2.18                     | 0.59              |
| 3:B:156:LYS:HD2   | 3:B:156:LYS:N     | 2.18                     | 0.59              |
| 3:B:209:LEU:HD11  | 3:B:302:MET:HE2   | 1.83                     | 0.59              |
| 1:D:3419:TRP:CZ3  | 1:D:3422:ILE:HG12 | 2.37                     | 0.59              |
| 2:A:23:LEU:HD22   | 2:A:232:GLY:C     | 2.23                     | 0.59              |
| 2:A:407:TRP:HE1   | 3:B:260:VAL:CG2   | 2.15                     | 0.59              |
| 3:B:165:ILE:HG22  | 3:B:199:ASP:OD2   | 2.03                     | 0.59              |
| 2:A:231:ILE:HA    | 2:A:234:ILE:CG2   | 2.32                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:54:ASN:ND2    | 3:B:64:ARG:HB2    | 2.17                     | 0.58              |
| 2:A:120:ASP:O     | 2:A:124:LYS:HB2   | 2.03                     | 0.58              |
| 2:A:273:ALA:CB    | 2:A:274:PRO:HD3   | 2.24                     | 0.58              |
| 3:B:265:LEU:HG    | 3:B:266:HIS:N     | 2.15                     | 0.58              |
| 3:B:273:ALA:HB1   | 3:B:291:LEU:HG    | 1.84                     | 0.58              |
| 1:D:3390:GLU:CD   | 2:A:402:ARG:HH12  | 2.06                     | 0.58              |
| 2:A:179:THR:HG21  | 3:B:248:LEU:HD21  | 1.81                     | 0.58              |
| 2:A:176:GLN:HB3   | 3:B:333:LEU:HD13  | 1.85                     | 0.58              |
| 2:A:256:GLN:HG3   | 2:A:257:THR:N     | 2.18                     | 0.58              |
| 3:B:66:ILE:C      | 3:B:67:LEU:HD23   | 2.23                     | 0.58              |
| 3:B:185:TYR:OH    | 3:B:399:PHE:HA    | 2.04                     | 0.58              |
| 3:B:266:HIS:HB3   | 3:B:432:TYR:OH    | 2.02                     | 0.58              |
| 2:A:105:ARG:C     | 2:A:110:ILE:HG22  | 2.23                     | 0.58              |
| 2:A:423:GLU:O     | 2:A:426:ALA:HB3   | 2.03                     | 0.58              |
| 3:B:125:GLU:HA    | 3:B:125:GLU:OE1   | 2.04                     | 0.58              |
| 2:A:9:VAL:HG22    | 2:A:10:GLY:N      | 2.19                     | 0.58              |
| 2:A:66:VAL:HA     | 2:A:91:GLN:CG     | 2.34                     | 0.58              |
| 2:A:70:LEU:HD12   | 2:A:145:THR:OG1   | 2.03                     | 0.58              |
| 2:A:209:ILE:HG12  | 2:A:302:MET:HG2   | 1.83                     | 0.58              |
| 3:B:5:VAL:CG2     | 3:B:135:PHE:HD2   | 2.17                     | 0.58              |
| 1:D:3412:LEU:HD21 | 1:D:3435:ILE:CD1  | 2.33                     | 0.58              |
| 2:A:166:LYS:HE2   | 2:A:199:ASP:OD1   | 2.03                     | 0.58              |
| 2:A:167:LEU:HD23  | 2:A:202:PHE:CZ    | 2.38                     | 0.58              |
| 3:B:185:TYR:HD1   | 3:B:395:PHE:CE1   | 2.22                     | 0.58              |
| 1:D:3455:GLY:HA3  | 1:D:3458:GLU:HB2  | 1.84                     | 0.58              |
| 2:A:317:LEU:HD23  | 2:A:375:VAL:HG11  | 1.86                     | 0.58              |
| 2:A:413:MET:O     | 2:A:414:GLU:HG3   | 2.04                     | 0.58              |
| 1:D:3469:ARG:HG3  | 1:D:3469:ARG:NH1  | 2.18                     | 0.58              |
| 2:A:24:TYR:CE1    | 2:A:240:ALA:HB2   | 2.39                     | 0.58              |
| 2:A:274:PRO:HG2   | 2:A:374:ALA:CA    | 2.34                     | 0.58              |
| 3:B:171:VAL:HA    | 3:B:204:ILE:O     | 2.04                     | 0.58              |
| 1:D:3405:MET:O    | 1:D:3408:VAL:HG23 | 2.03                     | 0.57              |
| 1:D:3464:TYR:HE1  | 1:D:3468:ASN:OD1  | 1.87                     | 0.57              |
| 2:A:259:LEU:HD11  | 2:A:378:LEU:CD1   | 2.17                     | 0.57              |
| 3:B:119:LEU:O     | 3:B:122:VAL:HG13  | 2.04                     | 0.57              |
| 1:D:3445:THR:O    | 1:D:3449:ARG:HB3  | 2.04                     | 0.57              |
| 2:A:231:ILE:O     | 2:A:234:ILE:HG23  | 2.04                     | 0.57              |
| 3:B:119:LEU:C     | 3:B:122:VAL:HG13  | 2.25                     | 0.57              |
| 1:D:3392:LYS:HE3  | 3:B:158:ARG:HH12  | 1.69                     | 0.57              |
| 1:D:3477:LEU:N    | 1:D:3477:LEU:HD12 | 2.19                     | 0.57              |
| 2:A:105:ARG:CB    | 2:A:110:ILE:HG22  | 2.34                     | 0.57              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:A:401:LYS:HD3   | 3:B:346:TRP:CD2  | 2.39                     | 0.57              |
| 3:B:135:PHE:HZ    | 3:B:161:TYR:CE1  | 2.22                     | 0.57              |
| 1:D:3424:LYS:HE2  | 3:B:156:LYS:HE2  | 1.87                     | 0.57              |
| 3:B:273:ALA:HB2   | 3:B:375:ALA:H    | 1.68                     | 0.57              |
| 2:A:217:LEU:HG    | 2:A:219:ILE:CD1  | 2.34                     | 0.57              |
| 2:A:168:GLU:HG3   | 2:A:201:ALA:CB   | 2.34                     | 0.57              |
| 2:A:405:VAL:HG13  | 2:A:409:VAL:HG23 | 1.86                     | 0.57              |
| 3:B:55:GLU:HG2    | 3:B:61:TYR:HE1   | 1.70                     | 0.57              |
| 3:B:184:PRO:HD2   | 3:B:398:MET:HE1  | 1.85                     | 0.57              |
| 3:B:359:PRO:HB2   | 3:B:371:LEU:O    | 2.05                     | 0.57              |
| 2:A:220:GLU:HA    | 2:A:220:GLU:OE1  | 2.05                     | 0.57              |
| 3:B:107:HIS:HE1   | 3:B:152:LEU:HD13 | 1.68                     | 0.57              |
| 3:B:211:ASP:OD2   | 3:B:215:ARG:HD2  | 2.05                     | 0.57              |
| 2:A:141:PHE:N     | 2:A:142:GLY:HA3  | 2.19                     | 0.57              |
| 2:A:185:TYR:HD1   | 2:A:395:PHE:CE2  | 2.22                     | 0.57              |
| 3:B:67:LEU:HD12   | 3:B:92:PHE:CE1   | 2.39                     | 0.57              |
| 2:A:248:LEU:CB    | 2:A:355:ILE:H    | 2.18                     | 0.57              |
| 3:B:4:ILE:HD11    | 3:B:252:LEU:HD12 | 1.86                     | 0.57              |
| 3:B:307:PRO:O     | 3:B:310:GLY:HA3  | 2.05                     | 0.57              |
| 1:D:3452:ILE:HG22 | 1:D:3453:THR:N   | 2.19                     | 0.57              |
| 3:B:272:PHE:HD2   | 3:B:274:PRO:O    | 1.87                     | 0.57              |
| 2:A:331:ALA:O     | 2:A:335:ILE:HG12 | 2.04                     | 0.56              |
| 2:A:371:VAL:HG12  | 2:A:372:GLN:N    | 2.20                     | 0.56              |
| 3:B:21:TRP:CE3    | 3:B:24:ILE:HG21  | 2.40                     | 0.56              |
| 3:B:230:LEU:CD2   | 3:B:302:MET:HE1  | 2.35                     | 0.56              |
| 1:D:3392:LYS:HE3  | 3:B:158:ARG:NH1  | 2.21                     | 0.56              |
| 2:A:229:ARG:HH11  | 2:A:229:ARG:CG   | 2.16                     | 0.56              |
| 2:A:274:PRO:HG2   | 2:A:374:ALA:HA   | 1.87                     | 0.56              |
| 3:B:180:THR:HG22  | 3:B:182:VAL:H    | 1.69                     | 0.56              |
| 3:B:260:VAL:HG23  | 3:B:260:VAL:O    | 2.04                     | 0.56              |
| 3:B:299:LYS:HD3   | 3:B:299:LYS:N    | 2.20                     | 0.56              |
| 2:A:168:GLU:HG3   | 2:A:201:ALA:HB1  | 1.88                     | 0.56              |
| 2:A:209:ILE:O     | 2:A:212:ILE:HB   | 2.04                     | 0.56              |
| 2:A:241:SER:HB2   | 2:A:356:ASN:ND2  | 2.20                     | 0.56              |
| 3:B:268:PHE:HB3   | 3:B:379:GLY:N    | 2.20                     | 0.56              |
| 3:B:272:PHE:CD2   | 3:B:274:PRO:HD2  | 2.39                     | 0.56              |
| 1:D:3416:LYS:CE   | 1:D:3418:GLU:HB2 | 2.28                     | 0.56              |
| 1:D:3428:GLU:HG2  | 1:D:3431:PHE:HB2 | 1.88                     | 0.56              |
| 2:A:67:PHE:CE2    | 2:A:87:PHE:CE2   | 2.94                     | 0.56              |
| 3:B:230:LEU:HD21  | 3:B:302:MET:HE1  | 1.87                     | 0.56              |
| 2:A:250:VAL:HG13  | 2:A:254:GLU:OE1  | 2.06                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:413:MET:CG    | 3:B:418:PHE:HE1   | 2.18                     | 0.56              |
| 2:A:76:ASP:HA     | 2:A:79:ARG:HG3    | 1.87                     | 0.56              |
| 3:B:64:ARG:HD2    | 3:B:125:GLU:HB3   | 1.88                     | 0.56              |
| 3:B:275:LEU:CD2   | 3:B:300:ASN:HD21  | 2.11                     | 0.56              |
| 1:D:3407:ALA:O    | 1:D:3410:LEU:HB3  | 2.04                     | 0.56              |
| 2:A:362:VAL:HG13  | 2:A:368:LEU:CB    | 2.28                     | 0.56              |
| 3:B:273:ALA:HB3   | 3:B:375:ALA:H     | 1.69                     | 0.56              |
| 3:B:428:LEU:HD12  | 3:B:428:LEU:O     | 2.05                     | 0.56              |
| 1:D:3422:ILE:O    | 1:D:3425:LYS:HB2  | 2.05                     | 0.56              |
| 2:A:16:ILE:HG22   | 2:A:17:GLY:N      | 2.20                     | 0.56              |
| 2:A:92:LEU:HD12   | 2:A:92:LEU:N      | 2.21                     | 0.56              |
| 2:A:152:LEU:HD12  | 2:A:153:LEU:HA    | 1.86                     | 0.56              |
| 2:A:237:SER:HB3   | 2:A:376:CYS:SG    | 2.46                     | 0.56              |
| 3:B:180:THR:HB    | 3:B:183:GLU:OE1   | 2.06                     | 0.56              |
| 3:B:388:PHE:CB    | 3:B:429:VAL:HG22  | 2.36                     | 0.56              |
| 2:A:219:ILE:HG22  | 2:A:222:PRO:HD3   | 1.87                     | 0.56              |
| 3:B:36:TYR:CE2    | 3:B:44:LEU:HB2    | 2.41                     | 0.56              |
| 3:B:132:LEU:HD23  | 3:B:164:ARG:HD2   | 1.88                     | 0.56              |
| 3:B:288:VAL:CB    | 3:B:289:PRO:HD3   | 2.35                     | 0.56              |
| 1:D:3394:LEU:HD13 | 2:A:409:VAL:O     | 2.06                     | 0.55              |
| 2:A:229:ARG:HG2   | 2:A:229:ARG:NH1   | 2.10                     | 0.55              |
| 2:A:225:THR:HG23  | 2:A:226:ASN:N     | 2.21                     | 0.55              |
| 2:A:189:LEU:O     | 2:A:193:THR:HG22  | 2.07                     | 0.55              |
| 3:B:315:VAL:CG1   | 3:B:377:PHE:HE1   | 2.18                     | 0.55              |
| 1:D:3432:ILE:HD13 | 1:D:3433:THR:N    | 2.18                     | 0.55              |
| 2:A:66:VAL:HG12   | 2:A:91:GLN:CA     | 2.36                     | 0.55              |
| 2:A:103:TYR:N     | 2:A:408:TYR:HE1   | 2.04                     | 0.55              |
| 2:A:152:LEU:HD12  | 2:A:153:LEU:N     | 2.21                     | 0.55              |
| 3:B:122:VAL:HG22  | 3:B:123:ARG:N     | 2.21                     | 0.55              |
| 2:A:242:LEU:HD13  | 2:A:318:LEU:HD22  | 1.87                     | 0.55              |
| 1:D:3392:LYS:NZ   | 3:B:158:ARG:HH12  | 2.04                     | 0.55              |
| 1:D:3431:PHE:CZ   | 1:D:3435:ILE:HD11 | 2.42                     | 0.55              |
| 2:A:152:LEU:HD12  | 2:A:152:LEU:C     | 2.26                     | 0.55              |
| 2:A:175:PRO:HG2   | 2:A:304:LYS:HE2   | 1.87                     | 0.55              |
| 3:B:132:LEU:HD23  | 3:B:164:ARG:CD    | 2.36                     | 0.55              |
| 2:A:21:TRP:O      | 2:A:24:TYR:HB2    | 2.06                     | 0.55              |
| 2:A:23:LEU:CD2    | 2:A:233:GLN:HA    | 2.37                     | 0.55              |
| 2:A:359:PRO:HB3   | 2:A:372:GLN:O     | 2.06                     | 0.55              |
| 3:B:7:ILE:HB      | 3:B:137:LEU:HD12  | 1.87                     | 0.55              |
| 3:B:172:VAL:CG2   | 3:B:203:CYS:HB3   | 2.36                     | 0.55              |
| 3:B:223:THR:HG22  | 3:B:224:TYR:N     | 2.21                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:A:185:TYR:CD1   | 2:A:395:PHE:CE2  | 2.95                     | 0.55              |
| 3:B:173:PRO:HB3   | 3:B:183:GLU:HG2  | 1.89                     | 0.55              |
| 3:B:188:THR:CG2   | 3:B:422:GLU:HA   | 2.37                     | 0.55              |
| 3:B:202:TYR:HE2   | 3:B:378:ILE:CG2  | 2.19                     | 0.54              |
| 2:A:9:VAL:HG21    | 2:A:149:PHE:CD1  | 2.41                     | 0.54              |
| 2:A:114:ILE:HG22  | 2:A:118:VAL:CG2  | 2.37                     | 0.54              |
| 3:B:283:TYR:HB3   | 3:B:285:ALA:H    | 1.72                     | 0.54              |
| 1:D:3478:VAL:HG13 | 1:D:3479:LYS:N   | 2.22                     | 0.54              |
| 3:B:264:ARG:HA    | 3:B:264:ARG:NE   | 2.23                     | 0.54              |
| 2:A:104:ALA:HB1   | 2:A:413:MET:HG2  | 1.90                     | 0.54              |
| 2:A:331:ALA:O     | 2:A:334:THR:HG22 | 2.06                     | 0.54              |
| 3:B:299:LYS:HD3   | 3:B:299:LYS:H    | 1.71                     | 0.54              |
| 1:D:3409:CYS:O    | 1:D:3412:LEU:HB2 | 2.08                     | 0.54              |
| 1:D:3484:GLN:NE2  | 1:D:3484:GLN:H   | 2.05                     | 0.54              |
| 2:A:412:GLY:N     | 2:A:413:MET:HB2  | 2.23                     | 0.54              |
| 3:B:132:LEU:CB    | 3:B:164:ARG:HD3  | 2.35                     | 0.54              |
| 3:B:102:ASN:HB2   | 3:B:105:LYS:HB2  | 1.89                     | 0.54              |
| 1:D:3392:LYS:CE   | 3:B:158:ARG:HH12 | 2.21                     | 0.54              |
| 1:D:3438:TYR:CZ   | 1:D:3443:MET:HB2 | 2.43                     | 0.54              |
| 1:D:3455:GLY:HA3  | 1:D:3458:GLU:CB  | 2.38                     | 0.54              |
| 2:A:301:GLN:O     | 2:A:302:MET:HB2  | 2.08                     | 0.54              |
| 3:B:135:PHE:CE1   | 3:B:157:ILE:HG23 | 2.43                     | 0.54              |
| 3:B:189:LEU:HA    | 3:B:421:ALA:HB1  | 1.89                     | 0.54              |
| 3:B:195:VAL:HG13  | 3:B:196:GLU:N    | 2.21                     | 0.54              |
| 3:B:198:THR:HG22  | 3:B:265:LEU:HD13 | 1.89                     | 0.54              |
| 2:A:63:PRO:HG2    | 2:A:87:PHE:HA    | 1.89                     | 0.54              |
| 2:A:177:VAL:HG21  | 2:A:207:GLU:CB   | 2.38                     | 0.54              |
| 2:A:210:TYR:OH    | 3:B:325:MET:HB3  | 2.07                     | 0.54              |
| 2:A:301:GLN:CB    | 2:A:303:VAL:HG12 | 2.38                     | 0.54              |
| 3:B:179:ASP:HB2   | 6:B:501:GDP:H3'  | 1.90                     | 0.54              |
| 3:B:234:THR:HG21  | 3:B:270:PRO:CB   | 2.15                     | 0.54              |
| 3:B:299:LYS:H     | 3:B:299:LYS:CD   | 2.20                     | 0.54              |
| 2:A:26:LEU:CD2    | 2:A:363:VAL:HG13 | 2.30                     | 0.54              |
| 2:A:237:SER:HA    | 2:A:241:SER:OG   | 2.08                     | 0.54              |
| 2:A:66:VAL:HB     | 2:A:91:GLN:O     | 2.08                     | 0.53              |
| 2:A:172:TYR:OH    | 2:A:387:ALA:HB1  | 2.07                     | 0.53              |
| 2:A:172:TYR:CE2   | 2:A:388:TRP:CZ3  | 2.95                     | 0.53              |
| 3:B:264:ARG:HG3   | 3:B:264:ARG:NH1  | 2.23                     | 0.53              |
| 3:B:18:ALA:O      | 3:B:22:GLU:HG3   | 2.09                     | 0.53              |
| 3:B:288:VAL:HG12  | 3:B:289:PRO:HD3  | 1.91                     | 0.53              |
| 3:B:318:VAL:HG23  | 3:B:378:ILE:HD11 | 1.90                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:B:6:HIS:O       | 3:B:65:ALA:HB1   | 2.07                     | 0.53              |
| 3:B:42:LEU:HD21   | 3:B:245:PRO:HD2  | 1.89                     | 0.53              |
| 2:A:118:VAL:HG11  | 2:A:153:LEU:HD22 | 1.90                     | 0.53              |
| 2:A:298:PRO:O     | 2:A:301:GLN:HG2  | 2.09                     | 0.53              |
| 2:A:402:ARG:O     | 2:A:402:ARG:HG3  | 2.08                     | 0.53              |
| 2:A:11:GLN:CG     | 2:A:74:VAL:HG11  | 2.19                     | 0.53              |
| 2:A:274:PRO:HB3   | 2:A:371:VAL:HG21 | 1.91                     | 0.53              |
| 3:B:5:VAL:HG21    | 3:B:135:PHE:HD2  | 1.73                     | 0.53              |
| 3:B:337:ASN:N     | 3:B:337:ASN:HD22 | 2.05                     | 0.53              |
| 3:B:415:GLU:OE2   | 3:B:415:GLU:HA   | 2.08                     | 0.53              |
| 1:D:3394:LEU:HD13 | 2:A:410:GLY:HA2  | 1.90                     | 0.53              |
| 2:A:261:PRO:HG2   | 2:A:313:MET:SD   | 2.49                     | 0.53              |
| 2:A:269:LEU:N     | 2:A:269:LEU:HD23 | 2.24                     | 0.53              |
| 3:B:199:ASP:C     | 3:B:265:LEU:HB2  | 2.29                     | 0.53              |
| 2:A:115:ILE:HG23  | 2:A:116:ASP:N    | 2.24                     | 0.53              |
| 2:A:212:ILE:HD11  | 2:A:302:MET:H    | 1.73                     | 0.53              |
| 2:A:337:THR:O     | 2:A:339:ARG:HB2  | 2.08                     | 0.53              |
| 3:B:119:LEU:HA    | 3:B:122:VAL:HG11 | 1.91                     | 0.53              |
| 3:B:182:VAL:HG12  | 3:B:182:VAL:O    | 2.09                     | 0.53              |
| 1:D:3403:LEU:HD23 | 1:D:3403:LEU:N   | 2.24                     | 0.53              |
| 2:A:68:VAL:HG22   | 2:A:93:ILE:CG2   | 2.39                     | 0.53              |
| 2:A:101:ASN:O     | 2:A:182:VAL:HG21 | 2.08                     | 0.53              |
| 2:A:180:ALA:HA    | 3:B:352:LYS:HZ1  | 1.73                     | 0.53              |
| 2:A:192:HIS:HB2   | 2:A:424:ASP:OD2  | 2.09                     | 0.53              |
| 3:B:168:THR:CG2   | 3:B:201:THR:HG23 | 2.38                     | 0.53              |
| 3:B:204:ILE:HG22  | 3:B:205:ASP:N    | 2.24                     | 0.53              |
| 3:B:285:ALA:CB    | 3:B:290:GLU:HG2  | 2.36                     | 0.53              |
| 3:B:360:PRO:HB2   | 7:B:502:TA1:H281 | 1.91                     | 0.53              |
| 1:D:3428:GLU:HG3  | 1:D:3430:ASN:OD1 | 2.09                     | 0.53              |
| 2:A:78:VAL:HG11   | 2:A:92:LEU:HD21  | 1.91                     | 0.53              |
| 2:A:6:SER:O       | 2:A:65:ALA:HB1   | 2.09                     | 0.52              |
| 2:A:155:GLU:HA    | 2:A:197:HIS:CE1  | 2.43                     | 0.52              |
| 2:A:204:VAL:CG2   | 2:A:302:MET:HB3  | 2.39                     | 0.52              |
| 2:A:217:LEU:HG    | 2:A:219:ILE:HD11 | 1.89                     | 0.52              |
| 3:B:4:ILE:CD1     | 3:B:252:LEU:HD11 | 2.40                     | 0.52              |
| 3:B:135:PHE:CZ    | 3:B:161:TYR:CE1  | 2.97                     | 0.52              |
| 3:B:167:ASN:HA    | 3:B:200:GLU:O    | 2.08                     | 0.52              |
| 3:B:201:THR:HG22  | 3:B:202:TYR:N    | 2.24                     | 0.52              |
| 3:B:172:VAL:CG1   | 3:B:387:LEU:HD21 | 2.39                     | 0.52              |
| 2:A:304:LYS:O     | 2:A:304:LYS:HG3  | 2.10                     | 0.52              |
| 2:A:402:ARG:O     | 2:A:405:VAL:HB   | 2.08                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:3:GLU:OE2     | 3:B:130:ASP:HB3   | 2.08                     | 0.52              |
| 3:B:52:TYR:OH     | 3:B:239:THR:HG21  | 2.09                     | 0.52              |
| 2:A:332:ILE:HD13  | 2:A:351:PHE:CD1   | 2.45                     | 0.52              |
| 3:B:9:ALA:O       | 3:B:13:GLY:HA2    | 2.09                     | 0.52              |
| 3:B:52:TYR:HB2    | 3:B:53:TYR:CE1    | 2.45                     | 0.52              |
| 3:B:57:ALA:HB3    | 3:B:60:LYS:N      | 2.12                     | 0.52              |
| 3:B:309:HIS:N     | 3:B:310:GLY:HA3   | 2.25                     | 0.52              |
| 1:D:3455:GLY:HA2  | 1:D:3458:GLU:N    | 2.13                     | 0.52              |
| 2:A:76:ASP:HA     | 2:A:79:ARG:CG     | 2.40                     | 0.52              |
| 2:A:250:VAL:HG21  | 2:A:318:LEU:CD2   | 2.39                     | 0.52              |
| 3:B:10:GLY:HA3    | 3:B:146:GLY:HA2   | 1.91                     | 0.52              |
| 3:B:229:HIS:ND1   | 3:B:229:HIS:C     | 2.62                     | 0.52              |
| 2:A:88:HIS:O      | 2:A:92:LEU:HD12   | 2.10                     | 0.52              |
| 2:A:251:ASP:O     | 2:A:255:PHE:HD1   | 1.93                     | 0.52              |
| 2:A:288:VAL:HG23  | 2:A:373:ARG:HH11  | 1.74                     | 0.52              |
| 1:D:3394:LEU:HD22 | 2:A:410:GLY:N     | 2.24                     | 0.52              |
| 2:A:388:TRP:CZ3   | 2:A:391:LEU:HD22  | 2.45                     | 0.52              |
| 1:D:3426:ILE:HG22 | 1:D:3427:MET:N    | 2.25                     | 0.52              |
| 2:A:185:TYR:O     | 2:A:189:LEU:HG    | 2.10                     | 0.52              |
| 2:A:251:ASP:N     | 2:A:254:GLU:HG3   | 2.24                     | 0.52              |
| 2:A:377:MET:O     | 2:A:377:MET:HG3   | 2.08                     | 0.52              |
| 2:A:105:ARG:NH2   | 2:A:110:ILE:HD12  | 2.24                     | 0.52              |
| 2:A:185:TYR:HD2   | 2:A:408:TYR:HE2   | 1.59                     | 0.52              |
| 2:A:217:LEU:HA    | 2:A:277:SER:HB3   | 1.92                     | 0.52              |
| 3:B:4:ILE:N       | 3:B:51:VAL:HG12   | 2.25                     | 0.52              |
| 3:B:175:PRO:HD2   | 3:B:207:GLU:CD    | 2.30                     | 0.52              |
| 3:B:253:ARG:O     | 3:B:257:VAL:HG23  | 2.10                     | 0.51              |
| 3:B:352:LYS:HD3   | 3:B:352:LYS:C     | 2.30                     | 0.51              |
| 1:D:3395:PRO:HG2  | 2:A:411:GLU:OE2   | 2.10                     | 0.51              |
| 2:A:208:ALA:HB1   | 2:A:303:VAL:C     | 2.31                     | 0.51              |
| 2:A:352:LYS:HE2   | 2:A:353:VAL:O     | 2.10                     | 0.51              |
| 3:B:44:LEU:O      | 3:B:44:LEU:HD12   | 2.09                     | 0.51              |
| 2:A:372:GLN:HE21  | 2:A:372:GLN:CA    | 2.23                     | 0.51              |
| 3:B:64:ARG:HG3    | 3:B:125:GLU:OE2   | 2.11                     | 0.51              |
| 3:B:313:LEU:HD23  | 3:B:313:LEU:N     | 2.25                     | 0.51              |
| 1:D:3392:LYS:HD2  | 1:D:3423:ARG:NE   | 2.26                     | 0.51              |
| 1:D:3412:LEU:HD21 | 1:D:3435:ILE:HD11 | 1.91                     | 0.51              |
| 3:B:127:GLU:HA    | 3:B:127:GLU:OE1   | 2.10                     | 0.51              |
| 1:D:3444:MET:CE   | 1:D:3448:ILE:HG12 | 2.40                     | 0.51              |
| 2:A:63:PRO:HB2    | 2:A:91:GLN:OE1    | 2.09                     | 0.51              |
| 2:A:248:LEU:O     | 2:A:248:LEU:HD12  | 2.11                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:A:282:TYR:CD1   | 2:A:284:GLU:CG   | 2.94                     | 0.51              |
| 3:B:182:VAL:HG11  | 3:B:408:TYR:OH   | 2.10                     | 0.51              |
| 2:A:147:SER:HB2   | 2:A:190:THR:OG1  | 2.10                     | 0.51              |
| 2:A:221:ARG:N     | 2:A:222:PRO:HD3  | 2.25                     | 0.51              |
| 2:A:363:VAL:HG23  | 2:A:368:LEU:HD11 | 1.93                     | 0.51              |
| 2:A:402:ARG:HE    | 2:A:405:VAL:CG1  | 2.22                     | 0.51              |
| 1:D:3390:GLU:O    | 1:D:3394:LEU:HG  | 2.11                     | 0.51              |
| 2:A:408:TYR:CB    | 2:A:418:PHE:HZ   | 2.24                     | 0.51              |
| 2:A:429:GLU:HG3   | 2:A:430:LYS:N    | 2.26                     | 0.51              |
| 3:B:111:GLY:O     | 3:B:115:VAL:HG23 | 2.11                     | 0.51              |
| 3:B:134:GLY:HA3   | 3:B:165:ILE:O    | 2.11                     | 0.51              |
| 3:B:205:ASP:O     | 3:B:209:LEU:HD22 | 2.11                     | 0.51              |
| 3:B:269:MET:CE    | 3:B:301:MET:HE3  | 2.41                     | 0.51              |
| 1:D:3392:LYS:HE2  | 1:D:3393:SER:CA  | 2.41                     | 0.51              |
| 3:B:4:ILE:H       | 3:B:51:VAL:HG12  | 1.76                     | 0.50              |
| 3:B:287:THR:HG22  | 3:B:288:VAL:H    | 1.76                     | 0.50              |
| 2:A:407:TRP:HE1   | 3:B:260:VAL:HG23 | 1.75                     | 0.50              |
| 2:A:407:TRP:NE1   | 3:B:257:VAL:HA   | 2.27                     | 0.50              |
| 3:B:42:LEU:HD21   | 3:B:245:PRO:CD   | 2.41                     | 0.50              |
| 3:B:287:THR:HG22  | 3:B:288:VAL:N    | 2.26                     | 0.50              |
| 3:B:297:ASP:CG    | 3:B:299:LYS:HE2  | 2.31                     | 0.50              |
| 2:A:102:ASN:ND2   | 2:A:105:ARG:H    | 2.09                     | 0.50              |
| 2:A:114:ILE:HG22  | 2:A:118:VAL:HG23 | 1.93                     | 0.50              |
| 2:A:118:VAL:O     | 2:A:121:ARG:HB2  | 2.12                     | 0.50              |
| 2:A:311:LYS:HD3   | 2:A:342:GLN:O    | 2.12                     | 0.50              |
| 3:B:230:LEU:O     | 3:B:233:ALA:HB3  | 2.11                     | 0.50              |
| 1:D:3392:LYS:HE2  | 1:D:3392:LYS:C   | 2.32                     | 0.50              |
| 1:D:3408:VAL:HG12 | 1:D:3411:MET:CE  | 2.41                     | 0.50              |
| 1:D:3412:LEU:CD2  | 1:D:3431:PHE:CE1 | 2.95                     | 0.50              |
| 2:A:103:TYR:CD2   | 2:A:413:MET:CE   | 2.94                     | 0.50              |
| 2:A:152:LEU:HD12  | 2:A:153:LEU:CA   | 2.42                     | 0.50              |
| 3:B:28:HIS:ND1    | 3:B:49:ILE:HG22  | 2.27                     | 0.50              |
| 3:B:173:PRO:HD2   | 3:B:391:ILE:CD1  | 2.40                     | 0.50              |
| 2:A:103:TYR:CD2   | 2:A:189:LEU:CD1  | 2.94                     | 0.50              |
| 2:A:123:ARG:HA    | 2:A:161:TYR:OH   | 2.11                     | 0.50              |
| 2:A:241:SER:HB2   | 2:A:356:ASN:HD22 | 1.76                     | 0.50              |
| 2:A:287:SER:HA    | 2:A:373:ARG:CZ   | 2.42                     | 0.50              |
| 3:B:8:GLN:HG3     | 3:B:66:ILE:O     | 2.12                     | 0.50              |
| 3:B:123:ARG:O     | 3:B:127:GLU:HG2  | 2.12                     | 0.50              |
| 1:D:3394:LEU:HA   | 2:A:410:GLY:HA3  | 1.93                     | 0.50              |
| 1:D:3408:VAL:HG12 | 1:D:3411:MET:HE1 | 1.94                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:3449:ARG:HH21 | 1:D:3449:ARG:CG  | 2.24                     | 0.50              |
| 2:A:201:ALA:O     | 2:A:267:PHE:HA   | 2.12                     | 0.50              |
| 2:A:224:TYR:CE1   | 3:B:325:MET:HG2  | 2.47                     | 0.50              |
| 1:D:3428:GLU:HG2  | 1:D:3428:GLU:O   | 2.11                     | 0.50              |
| 1:D:3455:GLY:CA   | 1:D:3458:GLU:HB2 | 2.41                     | 0.50              |
| 2:A:22:GLU:HG2    | 2:A:83:TYR:HE1   | 1.72                     | 0.50              |
| 2:A:92:LEU:HD12   | 2:A:92:LEU:H     | 1.76                     | 0.50              |
| 2:A:238:ILE:HD12  | 2:A:255:PHE:CZ   | 2.46                     | 0.50              |
| 2:A:372:GLN:HE21  | 2:A:372:GLN:HA   | 1.75                     | 0.50              |
| 3:B:135:PHE:HZ    | 3:B:161:TYR:CD1  | 2.30                     | 0.50              |
| 3:B:172:VAL:HG12  | 3:B:173:PRO:HD2  | 1.94                     | 0.50              |
| 1:D:3394:LEU:HD22 | 2:A:410:GLY:HA3  | 1.91                     | 0.50              |
| 1:D:3438:TYR:CE2  | 1:D:3443:MET:HB2 | 2.47                     | 0.50              |
| 2:A:23:LEU:HD21   | 2:A:233:GLN:HA   | 1.93                     | 0.50              |
| 2:A:103:TYR:CD2   | 2:A:189:LEU:HD12 | 2.47                     | 0.50              |
| 3:B:5:VAL:CG2     | 3:B:135:PHE:CD2  | 2.95                     | 0.50              |
| 3:B:307:PRO:HB3   | 3:B:312:TYR:CE1  | 2.47                     | 0.50              |
| 2:A:407:TRP:CZ2   | 3:B:256:ALA:HB1  | 2.47                     | 0.49              |
| 3:B:52:TYR:CB     | 3:B:53:TYR:CE1   | 2.95                     | 0.49              |
| 2:A:105:ARG:HB2   | 2:A:110:ILE:CG2  | 2.40                     | 0.49              |
| 2:A:276:ILE:HG12  | 2:A:277:SER:N    | 2.27                     | 0.49              |
| 2:A:107:HIS:CD2   | 2:A:108:TYR:CE1  | 3.00                     | 0.49              |
| 2:A:288:VAL:HA    | 2:A:291:ILE:HD11 | 1.94                     | 0.49              |
| 3:B:250:ALA:HB1   | 3:B:254:LYS:CB   | 2.41                     | 0.49              |
| 2:A:262:TYR:HB3   | 2:A:263:PRO:HD2  | 1.93                     | 0.49              |
| 2:A:401:LYS:CD    | 3:B:346:TRP:CD2  | 2.94                     | 0.49              |
| 2:A:67:PHE:HE2    | 2:A:87:PHE:CE2   | 2.29                     | 0.49              |
| 2:A:107:HIS:HD2   | 2:A:108:TYR:CE1  | 2.31                     | 0.49              |
| 2:A:107:HIS:CD2   | 2:A:108:TYR:CD1  | 2.99                     | 0.49              |
| 2:A:118:VAL:HG11  | 2:A:153:LEU:CD2  | 2.42                     | 0.49              |
| 2:A:412:GLY:H     | 2:A:413:MET:HB2  | 1.77                     | 0.49              |
| 3:B:52:TYR:HB2    | 3:B:53:TYR:CD1   | 2.48                     | 0.49              |
| 3:B:89:PRO:O      | 3:B:92:PHE:HD2   | 1.94                     | 0.49              |
| 1:D:3412:LEU:CD2  | 1:D:3431:PHE:CZ  | 2.95                     | 0.49              |
| 1:D:3449:ARG:HH21 | 1:D:3449:ARG:HG2 | 1.77                     | 0.49              |
| 3:B:135:PHE:CE1   | 3:B:157:ILE:CG2  | 2.95                     | 0.49              |
| 2:A:161:TYR:HB3   | 2:A:164:LYS:HB2  | 1.93                     | 0.49              |
| 3:B:52:TYR:CB     | 3:B:53:TYR:CD1   | 2.95                     | 0.49              |
| 3:B:181:VAL:O     | 3:B:398:MET:HE1  | 2.13                     | 0.49              |
| 3:B:313:LEU:HB2   | 3:B:380:ASN:HB3  | 1.95                     | 0.49              |
| 2:A:97:GLU:HB2    | 2:A:110:ILE:HD11 | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:168:GLU:CG   | 2:A:201:ALA:HB2  | 2.43                     | 0.49              |
| 3:B:7:ILE:HD13   | 3:B:66:ILE:HD11  | 1.94                     | 0.49              |
| 3:B:12:CYS:HB3   | 3:B:140:SER:OG   | 2.13                     | 0.49              |
| 3:B:346:TRP:CE3  | 3:B:347:ILE:HG12 | 2.46                     | 0.49              |
| 2:A:108:TYR:CE1  | 2:A:413:MET:SD   | 3.06                     | 0.49              |
| 3:B:269:MET:HE2  | 3:B:301:MET:HE3  | 1.95                     | 0.49              |
| 2:A:268:PRO:HA   | 2:A:379:SER:O    | 2.13                     | 0.48              |
| 2:A:324:VAL:HG12 | 2:A:326:LYS:N    | 2.26                     | 0.48              |
| 2:A:426:ALA:O    | 2:A:429:GLU:HG2  | 2.13                     | 0.48              |
| 3:B:24:ILE:CD1   | 3:B:52:TYR:CE2   | 2.95                     | 0.48              |
| 3:B:94:PHE:CD1   | 3:B:94:PHE:N     | 2.81                     | 0.48              |
| 2:A:65:ALA:O     | 2:A:91:GLN:HG2   | 2.13                     | 0.48              |
| 2:A:229:ARG:NH2  | 2:A:363:VAL:HG11 | 2.28                     | 0.48              |
| 2:A:248:LEU:HB3  | 2:A:354:GLY:HA2  | 1.94                     | 0.48              |
| 3:B:274:PRO:HG2  | 3:B:374:SER:HB3  | 1.93                     | 0.48              |
| 2:A:118:VAL:HG21 | 2:A:149:PHE:CZ   | 2.49                     | 0.48              |
| 2:A:275:VAL:CG1  | 2:A:300:ASN:HD21 | 2.26                     | 0.48              |
| 2:A:405:VAL:HG12 | 2:A:406:HIS:N    | 2.26                     | 0.48              |
| 3:B:89:PRO:HA    | 3:B:92:PHE:CD2   | 2.48                     | 0.48              |
| 3:B:286:LEU:CD1  | 3:B:371:LEU:HD21 | 2.41                     | 0.48              |
| 2:A:244:PHE:CD1  | 2:A:245:ASP:N    | 2.80                     | 0.48              |
| 2:A:267:PHE:CD1  | 2:A:267:PHE:N    | 2.81                     | 0.48              |
| 2:A:317:LEU:HD23 | 2:A:375:VAL:CG1  | 2.42                     | 0.48              |
| 3:B:67:LEU:HD21  | 3:B:87:PHE:CE2   | 2.48                     | 0.48              |
| 2:A:210:TYR:CE1  | 2:A:227:LEU:CD2  | 2.94                     | 0.48              |
| 2:A:274:PRO:HG3  | 2:A:374:ALA:HA   | 1.96                     | 0.48              |
| 2:A:308:ARG:HH11 | 2:A:390:ARG:HH12 | 1.60                     | 0.48              |
| 3:B:70:LEU:HG    | 3:B:145:THR:HG23 | 1.95                     | 0.48              |
| 3:B:75:MET:HE2   | 3:B:94:PHE:HB3   | 1.95                     | 0.48              |
| 3:B:318:VAL:HG13 | 3:B:354:ALA:HB3  | 1.96                     | 0.48              |
| 3:B:408:TYR:CD2  | 3:B:418:PHE:CZ   | 2.99                     | 0.48              |
| 2:A:132:LEU:HD21 | 2:A:164:LYS:CE   | 2.40                     | 0.48              |
| 3:B:36:TYR:CZ    | 3:B:38:GLY:HA3   | 2.49                     | 0.48              |
| 3:B:103:TRP:CD1  | 3:B:147:SER:CB   | 2.94                     | 0.48              |
| 3:B:107:HIS:CE1  | 3:B:152:LEU:HB2  | 2.48                     | 0.48              |
| 2:A:62:VAL:CG1   | 2:A:63:PRO:HD2   | 2.42                     | 0.48              |
| 2:A:125:LEU:HD23 | 2:A:128:GLN:HE22 | 1.79                     | 0.48              |
| 2:A:228:ASN:HA   | 2:A:231:ILE:CG1  | 2.44                     | 0.48              |
| 3:B:31:ASP:C     | 3:B:34:GLY:HA3   | 2.34                     | 0.48              |
| 3:B:241:CYS:SG   | 3:B:318:VAL:HG11 | 2.54                     | 0.48              |
| 2:A:115:ILE:HD11 | 2:A:153:LEU:CD1  | 2.28                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:B:3:GLU:HA     | 3:B:51:VAL:HG13   | 1.96                     | 0.48              |
| 3:B:42:LEU:HD12  | 3:B:47:GLU:OE1    | 2.14                     | 0.48              |
| 1:D:3392:LYS:HD2 | 1:D:3423:ARG:CZ   | 2.44                     | 0.48              |
| 2:A:9:VAL:HG22   | 2:A:10:GLY:H      | 1.78                     | 0.48              |
| 2:A:107:HIS:CE1  | 2:A:152:LEU:HB3   | 2.48                     | 0.48              |
| 2:A:341:ILE:HG23 | 2:A:342:GLN:N     | 2.29                     | 0.48              |
| 1:D:3398:PRO:HG2 | 1:D:3401:VAL:HG21 | 1.96                     | 0.48              |
| 2:A:11:GLN:HE21  | 2:A:74:VAL:CG1    | 2.26                     | 0.48              |
| 2:A:22:GLU:CG    | 2:A:83:TYR:CE1    | 2.94                     | 0.48              |
| 2:A:172:TYR:CZ   | 2:A:391:LEU:HD13  | 2.48                     | 0.48              |
| 2:A:301:GLN:HB2  | 2:A:303:VAL:HG12  | 1.96                     | 0.48              |
| 3:B:94:PHE:O     | 3:B:114:LEU:HD11  | 2.14                     | 0.48              |
| 1:D:3456:TYR:HA  | 1:D:3456:TYR:HD1  | 1.57                     | 0.47              |
| 2:A:135:PHE:CD1  | 2:A:135:PHE:N     | 2.81                     | 0.47              |
| 3:B:19:LYS:HG3   | 3:B:228:ASN:CB    | 2.44                     | 0.47              |
| 2:A:102:ASN:HD21 | 2:A:105:ARG:H     | 1.62                     | 0.47              |
| 2:A:346:TRP:HZ2  | 2:A:435:VAL:CG1   | 2.27                     | 0.47              |
| 2:A:405:VAL:HA   | 2:A:408:TYR:HD2   | 1.78                     | 0.47              |
| 3:B:255:LEU:O    | 3:B:259:MET:HB2   | 2.14                     | 0.47              |
| 3:B:275:LEU:HD23 | 3:B:300:ASN:CG    | 2.34                     | 0.47              |
| 1:D:3390:GLU:HG3 | 2:A:402:ARG:NH2   | 2.13                     | 0.47              |
| 1:D:3392:LYS:HE2 | 1:D:3393:SER:N    | 2.29                     | 0.47              |
| 1:D:3408:VAL:O   | 1:D:3412:LEU:HD13 | 2.14                     | 0.47              |
| 2:A:17:GLY:HA3   | 2:A:67:PHE:HE1    | 1.80                     | 0.47              |
| 2:A:108:TYR:CD1  | 2:A:108:TYR:N     | 2.82                     | 0.47              |
| 2:A:210:TYR:HE1  | 2:A:227:LEU:CD2   | 2.16                     | 0.47              |
| 3:B:31:ASP:HB3   | 3:B:32:PRO:CD     | 2.43                     | 0.47              |
| 3:B:343:PHE:O    | 3:B:344:VAL:HB    | 2.14                     | 0.47              |
| 3:B:413:MET:HE3  | 3:B:413:MET:HB2   | 1.64                     | 0.47              |
| 3:B:428:LEU:HG   | 3:B:429:VAL:N     | 2.29                     | 0.47              |
| 2:A:101:ASN:HD21 | 3:B:254:LYS:NZ    | 2.13                     | 0.47              |
| 2:A:248:LEU:HB2  | 2:A:355:ILE:N     | 2.28                     | 0.47              |
| 2:A:399:TYR:O    | 2:A:402:ARG:HA    | 2.13                     | 0.47              |
| 3:B:33:THR:HG22  | 3:B:34:GLY:N      | 2.29                     | 0.47              |
| 3:B:53:TYR:CD1   | 3:B:53:TYR:N      | 2.83                     | 0.47              |
| 3:B:427:ASP:O    | 3:B:430:SER:HB3   | 2.14                     | 0.47              |
| 2:A:118:VAL:HG21 | 2:A:149:PHE:HZ    | 1.79                     | 0.47              |
| 2:A:168:GLU:O    | 2:A:201:ALA:HA    | 2.15                     | 0.47              |
| 3:B:231:VAL:HA   | 3:B:302:MET:HE1   | 1.96                     | 0.47              |
| 3:B:259:MET:CE   | 3:B:268:PHE:CZ    | 2.97                     | 0.47              |
| 3:B:269:MET:CG   | 3:B:303:ALA:HB3   | 2.44                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:B:315:VAL:HB   | 3:B:351:VAL:HG13  | 1.96                     | 0.47              |
| 2:A:34:GLY:C     | 2:A:61:HIS:N      | 2.68                     | 0.47              |
| 2:A:164:LYS:HD3  | 2:A:164:LYS:HA    | 1.40                     | 0.47              |
| 2:A:187:SER:O    | 2:A:191:THR:HG22  | 2.15                     | 0.47              |
| 2:A:372:GLN:HA   | 2:A:372:GLN:NE2   | 2.30                     | 0.47              |
| 3:B:272:PHE:CE1  | 7:B:502:TA1:H391  | 2.50                     | 0.47              |
| 3:B:312:TYR:HA   | 3:B:381:SER:HA    | 1.96                     | 0.47              |
| 1:D:3428:GLU:HG2 | 1:D:3431:PHE:N    | 2.22                     | 0.47              |
| 3:B:3:GLU:HA     | 3:B:51:VAL:HA     | 1.96                     | 0.47              |
| 3:B:105:LYS:HG2  | 3:B:110:GLU:HG2   | 1.92                     | 0.47              |
| 3:B:316:ALA:O    | 3:B:378:ILE:HD12  | 2.15                     | 0.47              |
| 1:D:3480:TRP:O   | 1:D:3483:ALA:HB3  | 2.15                     | 0.47              |
| 2:A:9:VAL:O      | 2:A:13:GLY:HA3    | 2.15                     | 0.47              |
| 2:A:175:PRO:HD2  | 2:A:207:GLU:CG    | 2.43                     | 0.47              |
| 2:A:288:VAL:O    | 2:A:291:ILE:HG12  | 2.15                     | 0.47              |
| 1:D:3422:ILE:C   | 1:D:3422:ILE:HD12 | 2.35                     | 0.47              |
| 2:A:67:PHE:N     | 2:A:67:PHE:CD2    | 2.82                     | 0.47              |
| 2:A:82:THR:HG22  | 2:A:83:TYR:N      | 2.29                     | 0.47              |
| 2:A:224:TYR:CD1  | 3:B:325:MET:HG2   | 2.50                     | 0.47              |
| 3:B:132:LEU:HB3  | 3:B:164:ARG:HH11  | 1.79                     | 0.47              |
| 1:D:3449:ARG:HG2 | 1:D:3449:ARG:NH2  | 2.29                     | 0.47              |
| 2:A:87:PHE:N     | 2:A:87:PHE:CD1    | 2.83                     | 0.47              |
| 2:A:388:TRP:HZ3  | 2:A:391:LEU:HD22  | 1.79                     | 0.47              |
| 3:B:70:LEU:H     | 3:B:145:THR:CG2   | 2.22                     | 0.47              |
| 3:B:135:PHE:HD1  | 3:B:166:MET:HG2   | 1.79                     | 0.47              |
| 3:B:262:PHE:HB3  | 3:B:263:PRO:HD2   | 1.97                     | 0.47              |
| 3:B:267:PHE:CD1  | 3:B:267:PHE:N     | 2.82                     | 0.47              |
| 3:B:318:VAL:HG13 | 3:B:354:ALA:CB    | 2.45                     | 0.47              |
| 2:A:175:PRO:CG   | 2:A:304:LYS:HG2   | 2.46                     | 0.46              |
| 2:A:191:THR:HG23 | 2:A:192:HIS:N     | 2.31                     | 0.46              |
| 2:A:204:VAL:HG22 | 2:A:302:MET:HB3   | 1.97                     | 0.46              |
| 2:A:224:TYR:CZ   | 3:B:325:MET:HG2   | 2.50                     | 0.46              |
| 3:B:301:MET:HE1  | 3:B:377:PHE:CE2   | 2.33                     | 0.46              |
| 3:B:326:LYS:HE3  | 3:B:330:GLU:CB    | 2.44                     | 0.46              |
| 3:B:352:LYS:HD3  | 3:B:353:THR:N     | 2.30                     | 0.46              |
| 2:A:14:VAL:HG21  | 2:A:75:ILE:HD11   | 1.96                     | 0.46              |
| 2:A:216:ASN:HD22 | 2:A:216:ASN:HA    | 1.54                     | 0.46              |
| 2:A:242:LEU:HD11 | 2:A:318:LEU:CD2   | 2.45                     | 0.46              |
| 3:B:324:SER:OG   | 3:B:326:LYS:HB3   | 2.16                     | 0.46              |
| 1:D:3384:LYS:HD3 | 1:D:3386:LYS:CG   | 2.45                     | 0.46              |
| 2:A:100:ALA:HB3  | 2:A:105:ARG:HG3   | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:153:LEU:O     | 2:A:157:LEU:HG    | 2.14                     | 0.46              |
| 2:A:177:VAL:HG13  | 3:B:329:ASP:HB3   | 1.96                     | 0.46              |
| 3:B:48:ARG:HG2    | 3:B:243:ARG:CB    | 2.34                     | 0.46              |
| 3:B:107:HIS:CD2   | 3:B:151:THR:CG2   | 2.98                     | 0.46              |
| 3:B:332:MET:O     | 3:B:335:VAL:HB    | 2.16                     | 0.46              |
| 2:A:11:GLN:HE21   | 2:A:74:VAL:CG2    | 2.29                     | 0.46              |
| 2:A:244:PHE:HE2   | 2:A:358:GLU:OE1   | 1.98                     | 0.46              |
| 2:A:259:LEU:O     | 2:A:261:PRO:HD3   | 2.14                     | 0.46              |
| 3:B:135:PHE:CD1   | 3:B:135:PHE:N     | 2.84                     | 0.46              |
| 3:B:315:VAL:HG12  | 3:B:351:VAL:HG13  | 1.97                     | 0.46              |
| 1:D:3442:LYS:HA   | 1:D:3442:LYS:HD3  | 1.79                     | 0.46              |
| 2:A:8:HIS:CD2     | 2:A:17:GLY:HA2    | 2.50                     | 0.46              |
| 2:A:11:GLN:O      | 2:A:15:GLN:HG3    | 2.15                     | 0.46              |
| 2:A:24:TYR:OH     | 2:A:239:THR:HB    | 2.15                     | 0.46              |
| 3:B:319:PHE:HA    | 3:B:375:ALA:CA    | 2.36                     | 0.46              |
| 1:D:3462:PHE:O    | 1:D:3467:VAL:HG23 | 2.15                     | 0.46              |
| 2:A:22:GLU:HG2    | 2:A:83:TYR:CZ     | 2.49                     | 0.46              |
| 3:B:108:TYR:CD1   | 3:B:108:TYR:N     | 2.82                     | 0.46              |
| 3:B:169:PHE:CE2   | 3:B:235:MET:HB3   | 2.49                     | 0.46              |
| 3:B:312:TYR:CD2   | 3:B:315:VAL:HG22  | 2.50                     | 0.46              |
| 1:D:3438:TYR:CD1  | 1:D:3439:ASP:N    | 2.84                     | 0.46              |
| 2:A:10:GLY:O      | 2:A:14:VAL:HG23   | 2.15                     | 0.46              |
| 3:B:210:TYR:O     | 3:B:214:PHE:HB3   | 2.15                     | 0.46              |
| 3:B:425:MET:HA    | 3:B:428:LEU:HD23  | 1.97                     | 0.46              |
| 2:A:105:ARG:O     | 2:A:110:ILE:HG22  | 2.16                     | 0.46              |
| 3:B:4:ILE:HD12    | 3:B:136:GLN:HE21  | 1.81                     | 0.46              |
| 3:B:24:ILE:HD11   | 3:B:52:TYR:HE2    | 1.76                     | 0.46              |
| 1:D:3394:LEU:CD1  | 2:A:410:GLY:HA2   | 2.46                     | 0.46              |
| 1:D:3398:PRO:HB2  | 1:D:3401:VAL:CG2  | 2.44                     | 0.46              |
| 1:D:3482:THR:HG23 | 1:D:3486:TYR:HD2  | 1.77                     | 0.46              |
| 2:A:219:ILE:HG22  | 2:A:221:ARG:N     | 2.31                     | 0.46              |
| 2:A:238:ILE:HD12  | 2:A:255:PHE:HE2   | 1.77                     | 0.46              |
| 3:B:54:ASN:HD21   | 3:B:64:ARG:CB     | 2.22                     | 0.46              |
| 3:B:278:ARG:HB3   | 3:B:279:GLY:HA3   | 1.97                     | 0.46              |
| 2:A:26:LEU:HD23   | 2:A:363:VAL:HA    | 1.98                     | 0.46              |
| 2:A:234:ILE:HD13  | 2:A:235:VAL:N     | 2.31                     | 0.46              |
| 2:A:388:TRP:CE3   | 2:A:388:TRP:HA    | 2.51                     | 0.46              |
| 2:A:412:GLY:CA    | 2:A:413:MET:HB2   | 2.46                     | 0.46              |
| 3:B:70:LEU:HG     | 3:B:145:THR:CG2   | 2.46                     | 0.46              |
| 3:B:161:TYR:CD1   | 3:B:161:TYR:N     | 2.82                     | 0.46              |
| 3:B:172:VAL:HG13  | 3:B:173:PRO:HD2   | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:236:SER:O    | 3:B:240:THR:HG23 | 2.15                     | 0.45              |
| 3:B:425:MET:HE2  | 3:B:425:MET:HB3  | 1.53                     | 0.45              |
| 2:A:72:PRO:HG3   | 2:A:95:GLY:O     | 2.17                     | 0.45              |
| 2:A:251:ASP:CB   | 2:A:254:GLU:HG3  | 2.46                     | 0.45              |
| 3:B:200:GLU:HA   | 3:B:265:LEU:HD12 | 1.98                     | 0.45              |
| 3:B:230:LEU:HD23 | 3:B:231:VAL:HG23 | 1.99                     | 0.45              |
| 1:D:3400:PRO:HA  | 1:D:3403:LEU:HG  | 1.98                     | 0.45              |
| 1:D:3418:GLU:HG3 | 1:D:3420:ALA:H   | 1.82                     | 0.45              |
| 1:D:3455:GLY:CA  | 1:D:3458:GLU:CB  | 2.95                     | 0.45              |
| 2:A:99:ALA:HB1   | 5:A:502:GTP:O2G  | 2.16                     | 0.45              |
| 2:A:181:VAL:HG21 | 3:B:258:ASN:HB3  | 1.93                     | 0.45              |
| 3:B:187:ALA:O    | 3:B:191:VAL:HG12 | 2.16                     | 0.45              |
| 3:B:425:MET:CG   | 3:B:428:LEU:HD23 | 2.47                     | 0.45              |
| 2:A:5:ILE:HD13   | 2:A:125:LEU:HB3  | 1.98                     | 0.45              |
| 3:B:358:ILE:HA   | 3:B:359:PRO:HD3  | 1.50                     | 0.45              |
| 2:A:119:LEU:CD2  | 2:A:153:LEU:CD1  | 2.95                     | 0.45              |
| 2:A:119:LEU:CA   | 2:A:122:ILE:HD11 | 2.27                     | 0.45              |
| 3:B:264:ARG:O    | 3:B:265:LEU:HB3  | 2.16                     | 0.45              |
| 1:D:3399:THR:O   | 1:D:3403:LEU:HG  | 2.17                     | 0.45              |
| 2:A:100:ALA:HB1  | 2:A:102:ASN:OD1  | 2.17                     | 0.45              |
| 2:A:176:GLN:HB3  | 3:B:333:LEU:CD1  | 2.46                     | 0.45              |
| 2:A:217:LEU:H    | 2:A:217:LEU:CD2  | 2.28                     | 0.45              |
| 2:A:276:ILE:HG23 | 2:A:369:ALA:HB1  | 1.95                     | 0.45              |
| 3:B:273:ALA:O    | 3:B:294:GLN:HG2  | 2.16                     | 0.45              |
| 3:B:413:MET:HG2  | 3:B:418:PHE:CE1  | 2.43                     | 0.45              |
| 1:D:3444:MET:O   | 1:D:3444:MET:HE3 | 2.17                     | 0.45              |
| 2:A:217:LEU:CD2  | 2:A:217:LEU:N    | 2.80                     | 0.45              |
| 3:B:140:SER:CB   | 3:B:142:GLY:HA3  | 2.37                     | 0.45              |
| 3:B:242:LEU:HD22 | 3:B:250:ALA:N    | 2.32                     | 0.45              |
| 1:D:3431:PHE:HD1 | 1:D:3431:PHE:HA  | 1.43                     | 0.45              |
| 1:D:3459:ASP:HB2 | 1:D:3462:PHE:HB2 | 1.97                     | 0.45              |
| 7:B:502:TA1:H463 | 7:B:502:TA1:C26  | 2.46                     | 0.45              |
| 1:D:3464:TYR:CD1 | 1:D:3478:VAL:CG1 | 2.94                     | 0.45              |
| 2:A:21:TRP:HE3   | 2:A:21:TRP:N     | 2.14                     | 0.45              |
| 2:A:182:VAL:HG11 | 3:B:257:VAL:CG1  | 2.46                     | 0.45              |
| 3:B:6:HIS:CE1    | 3:B:8:GLN:HE21   | 2.35                     | 0.45              |
| 3:B:11:GLN:O     | 3:B:15:GLN:N     | 2.41                     | 0.45              |
| 3:B:43:GLN:O     | 3:B:49:ILE:HG23  | 2.17                     | 0.45              |
| 3:B:288:VAL:HG12 | 3:B:289:PRO:CA   | 2.47                     | 0.45              |
| 2:A:75:ILE:O     | 2:A:78:VAL:HB    | 2.16                     | 0.45              |
| 2:A:93:ILE:HD12  | 2:A:93:ILE:HA    | 1.76                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:6:SER:OG     | 2:A:65:ALA:HB2   | 2.17                     | 0.44              |
| 2:A:203:MET:SD   | 2:A:388:TRP:CZ2  | 3.10                     | 0.44              |
| 2:A:272:TYR:HE1  | 2:A:376:CYS:HG   | 1.57                     | 0.44              |
| 2:A:360:PRO:HG3  | 2:A:374:ALA:CB   | 2.46                     | 0.44              |
| 3:B:169:PHE:HD2  | 3:B:204:ILE:HD11 | 1.82                     | 0.44              |
| 2:A:12:ALA:HB2   | 5:A:502:GTP:C8   | 2.52                     | 0.44              |
| 2:A:98:ASP:HB3   | 3:B:2:ARG:HH12   | 1.82                     | 0.44              |
| 2:A:166:LYS:H    | 2:A:199:ASP:CG   | 2.20                     | 0.44              |
| 2:A:302:MET:HB2  | 2:A:302:MET:HE3  | 1.88                     | 0.44              |
| 2:A:334:THR:HG23 | 2:A:335:ILE:N    | 2.32                     | 0.44              |
| 2:A:432:TYR:HD1  | 2:A:432:TYR:HA   | 1.36                     | 0.44              |
| 3:B:115:VAL:O    | 3:B:118:VAL:HB   | 2.17                     | 0.44              |
| 3:B:277:SER:N    | 3:B:281:GLN:HB3  | 2.32                     | 0.44              |
| 3:B:346:TRP:CZ2  | 3:B:435:TYR:CD1  | 3.06                     | 0.44              |
| 3:B:431:GLU:OE1  | 3:B:432:TYR:HA   | 2.17                     | 0.44              |
| 1:D:3384:LYS:HG2 | 1:D:3387:HIS:ND1 | 2.32                     | 0.44              |
| 1:D:3395:PRO:HB3 | 3:B:163:ASP:OD1  | 2.17                     | 0.44              |
| 1:D:3418:GLU:HG3 | 1:D:3419:TRP:N   | 2.32                     | 0.44              |
| 2:A:107:HIS:HA   | 2:A:148:GLY:C    | 2.37                     | 0.44              |
| 2:A:195:LEU:HD23 | 2:A:264:ARG:CZ   | 2.47                     | 0.44              |
| 2:A:219:ILE:C    | 2:A:222:PRO:HD3  | 2.38                     | 0.44              |
| 2:A:242:LEU:CD2  | 2:A:318:LEU:CD2  | 2.95                     | 0.44              |
| 3:B:141:LEU:O    | 3:B:186:ASN:HB2  | 2.17                     | 0.44              |
| 3:B:229:HIS:HE2  | 7:B:502:TA1:H361 | 1.83                     | 0.44              |
| 3:B:262:PHE:CE2  | 3:B:435:TYR:CE1  | 3.06                     | 0.44              |
| 1:D:3394:LEU:CD2 | 2:A:410:GLY:CA   | 2.93                     | 0.44              |
| 2:A:23:LEU:CD1   | 2:A:363:VAL:HG22 | 2.46                     | 0.44              |
| 3:B:30:ILE:CD1   | 3:B:53:TYR:CE2   | 2.95                     | 0.44              |
| 3:B:109:THR:HG22 | 3:B:110:GLU:OE2  | 2.17                     | 0.44              |
| 3:B:230:LEU:HD21 | 3:B:302:MET:HE3  | 1.98                     | 0.44              |
| 2:A:3:GLU:C      | 2:A:243:ARG:HH11 | 2.21                     | 0.44              |
| 2:A:5:ILE:HG23   | 2:A:64:ARG:O     | 2.17                     | 0.44              |
| 2:A:22:GLU:CG    | 2:A:83:TYR:HE1   | 2.31                     | 0.44              |
| 2:A:23:LEU:HD12  | 2:A:363:VAL:HG22 | 1.99                     | 0.44              |
| 2:A:119:LEU:HD23 | 2:A:153:LEU:HD11 | 2.00                     | 0.44              |
| 2:A:250:VAL:CG2  | 2:A:318:LEU:CD2  | 2.95                     | 0.44              |
| 3:B:30:ILE:HA    | 3:B:35:SER:O     | 2.18                     | 0.44              |
| 3:B:209:LEU:HG   | 3:B:230:LEU:HD22 | 2.00                     | 0.44              |
| 1:D:3438:TYR:HD1 | 1:D:3439:ASP:N   | 2.15                     | 0.44              |
| 2:A:23:LEU:HD23  | 2:A:236:SER:HB2  | 1.98                     | 0.44              |
| 2:A:103:TYR:CG   | 2:A:189:LEU:HD12 | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:185:TYR:HD1   | 3:B:185:TYR:HA    | 1.69                     | 0.44              |
| 2:A:82:THR:CG2    | 2:A:83:TYR:CD1    | 3.00                     | 0.44              |
| 2:A:177:VAL:CG2   | 2:A:207:GLU:HB3   | 2.44                     | 0.44              |
| 2:A:195:LEU:HD21  | 2:A:428:LEU:CD2   | 2.48                     | 0.44              |
| 2:A:231:ILE:HG12  | 2:A:231:ILE:H     | 1.35                     | 0.44              |
| 3:B:269:MET:CE    | 3:B:301:MET:CE    | 2.95                     | 0.44              |
| 3:B:378:ILE:HG22  | 3:B:379:GLY:N     | 2.33                     | 0.44              |
| 2:A:209:ILE:HG12  | 2:A:302:MET:CG    | 2.47                     | 0.44              |
| 2:A:269:LEU:O     | 2:A:378:LEU:HA    | 2.17                     | 0.44              |
| 3:B:259:MET:HE3   | 3:B:259:MET:HB3   | 1.88                     | 0.44              |
| 3:B:264:ARG:HG2   | 3:B:431:GLU:OE2   | 2.18                     | 0.44              |
| 3:B:332:MET:HE2   | 3:B:353:THR:OG1   | 2.18                     | 0.44              |
| 3:B:392:SER:O     | 3:B:395:PHE:HB3   | 2.17                     | 0.44              |
| 2:A:282:TYR:HD1   | 2:A:282:TYR:HA    | 1.48                     | 0.44              |
| 2:A:133:GLN:HB3   | 2:A:243:ARG:HH12  | 1.80                     | 0.43              |
| 3:B:408:TYR:N     | 3:B:408:TYR:CD1   | 2.86                     | 0.43              |
| 2:A:255:PHE:HE2   | 2:A:378:LEU:HD21  | 1.83                     | 0.43              |
| 2:A:398:MET:HE3   | 2:A:398:MET:HB2   | 1.65                     | 0.43              |
| 3:B:78:VAL:O      | 3:B:84:GLY:HA2    | 2.18                     | 0.43              |
| 3:B:184:PRO:CB    | 3:B:395:PHE:HA    | 2.48                     | 0.43              |
| 3:B:320:ARG:HB2   | 3:B:358:ILE:O     | 2.18                     | 0.43              |
| 1:D:3405:MET:HA   | 1:D:3408:VAL:HG22 | 1.97                     | 0.43              |
| 2:A:242:LEU:CD1   | 2:A:318:LEU:CD2   | 2.94                     | 0.43              |
| 3:B:292:THR:HG21  | 3:B:331:GLN:HG2   | 1.98                     | 0.43              |
| 3:B:314:THR:N     | 3:B:380:ASN:HB3   | 2.33                     | 0.43              |
| 2:A:286:LEU:O     | 2:A:291:ILE:HG23  | 2.18                     | 0.43              |
| 3:B:36:TYR:CD2    | 3:B:44:LEU:HD22   | 2.53                     | 0.43              |
| 3:B:168:THR:HG22  | 3:B:169:PHE:N     | 2.33                     | 0.43              |
| 3:B:191:VAL:CA    | 3:B:194:LEU:HD12  | 2.15                     | 0.43              |
| 3:B:382:THR:HG21  | 3:B:436:GLN:HA    | 2.00                     | 0.43              |
| 3:B:388:PHE:HD1   | 3:B:388:PHE:HA    | 1.59                     | 0.43              |
| 1:D:3391:ILE:HD13 | 1:D:3391:ILE:N    | 2.34                     | 0.43              |
| 1:D:3459:ASP:HA   | 1:D:3460:PRO:HD3  | 1.46                     | 0.43              |
| 2:A:6:SER:HG      | 2:A:21:TRP:HH2    | 1.66                     | 0.43              |
| 2:A:168:GLU:CG    | 2:A:201:ALA:CB    | 2.96                     | 0.43              |
| 2:A:248:LEU:HD13  | 2:A:248:LEU:HA    | 1.56                     | 0.43              |
| 2:A:264:ARG:H     | 2:A:264:ARG:HG2   | 1.62                     | 0.43              |
| 2:A:362:VAL:HB    | 2:A:370:LYS:HD3   | 2.00                     | 0.43              |
| 3:B:10:GLY:C      | 3:B:13:GLY:HA3    | 2.36                     | 0.43              |
| 3:B:204:ILE:CG2   | 3:B:209:LEU:CD2   | 2.95                     | 0.43              |
| 3:B:420:GLU:CG    | 3:B:421:ALA:N     | 2.82                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:3432:ILE:CG1 | 1:D:3433:THR:N   | 2.81                     | 0.43              |
| 1:D:3440:THR:CG2 | 1:D:3441:LYS:N   | 2.82                     | 0.43              |
| 3:B:108:TYR:O    | 3:B:112:ALA:HB2  | 2.19                     | 0.43              |
| 3:B:175:PRO:HD2  | 3:B:207:GLU:OE1  | 2.19                     | 0.43              |
| 3:B:276:THR:HB   | 3:B:281:GLN:HG3  | 2.00                     | 0.43              |
| 2:A:360:PRO:HG2  | 2:A:374:ALA:HB2  | 2.01                     | 0.43              |
| 3:B:282:GLN:HE21 | 3:B:282:GLN:HB3  | 1.47                     | 0.43              |
| 3:B:346:TRP:CE3  | 3:B:347:ILE:CG1  | 3.02                     | 0.43              |
| 3:B:359:PRO:CB   | 3:B:360:PRO:HD2  | 2.47                     | 0.43              |
| 1:D:3405:MET:SD  | 1:D:3408:VAL:CG2 | 3.07                     | 0.43              |
| 1:D:3419:TRP:CE3 | 1:D:3419:TRP:HA  | 2.53                     | 0.43              |
| 2:A:102:ASN:HD21 | 2:A:105:ARG:HG2  | 1.84                     | 0.43              |
| 2:A:220:GLU:C    | 2:A:222:PRO:HD3  | 2.39                     | 0.43              |
| 3:B:44:LEU:O     | 3:B:49:ILE:HG23  | 2.19                     | 0.43              |
| 3:B:325:MET:HE3  | 3:B:355:VAL:CG2  | 2.47                     | 0.43              |
| 3:B:103:TRP:CE3  | 3:B:189:LEU:HD13 | 2.54                     | 0.43              |
| 3:B:137:LEU:HD12 | 3:B:137:LEU:HA   | 1.88                     | 0.43              |
| 3:B:323:MET:HE3  | 3:B:373:MET:CG   | 2.49                     | 0.43              |
| 2:A:142:GLY:HA2  | 2:A:183:GLU:OE1  | 2.18                     | 0.43              |
| 2:A:262:TYR:HA   | 2:A:263:PRO:HD3  | 1.81                     | 0.43              |
| 3:B:195:VAL:CG1  | 3:B:196:GLU:N    | 2.81                     | 0.43              |
| 2:A:7:ILE:HG13   | 2:A:7:ILE:O      | 2.18                     | 0.42              |
| 2:A:185:TYR:HD2  | 2:A:408:TYR:CE2  | 2.37                     | 0.42              |
| 3:B:198:THR:O    | 3:B:198:THR:HG22 | 2.19                     | 0.42              |
| 3:B:425:MET:CA   | 3:B:428:LEU:HD23 | 2.49                     | 0.42              |
| 3:B:428:LEU:HD12 | 3:B:428:LEU:C    | 2.40                     | 0.42              |
| 1:D:3426:ILE:CG2 | 1:D:3427:MET:N   | 2.81                     | 0.42              |
| 1:D:3455:GLY:HA2 | 1:D:3458:GLU:HG3 | 2.01                     | 0.42              |
| 2:A:117:LEU:HD13 | 2:A:117:LEU:HA   | 1.76                     | 0.42              |
| 2:A:225:THR:CG2  | 2:A:226:ASN:N    | 2.82                     | 0.42              |
| 2:A:341:ILE:CG2  | 2:A:342:GLN:N    | 2.82                     | 0.42              |
| 3:B:7:ILE:CG2    | 3:B:137:LEU:CD1  | 2.97                     | 0.42              |
| 3:B:158:ARG:HA   | 3:B:158:ARG:HD3  | 1.75                     | 0.42              |
| 3:B:276:THR:HB   | 3:B:281:GLN:CG   | 2.49                     | 0.42              |
| 1:D:3392:LYS:CE  | 1:D:3393:SER:HA  | 2.48                     | 0.42              |
| 2:A:242:LEU:HD21 | 2:A:318:LEU:CD2  | 2.46                     | 0.42              |
| 2:A:339:ARG:O    | 2:A:339:ARG:HG3  | 2.20                     | 0.42              |
| 3:B:151:THR:CG2  | 3:B:152:LEU:N    | 2.82                     | 0.42              |
| 3:B:275:LEU:HD23 | 3:B:300:ASN:OD1  | 2.19                     | 0.42              |
| 3:B:288:VAL:CG1  | 3:B:289:PRO:HD3  | 2.48                     | 0.42              |
| 1:D:3436:ILE:CG1 | 1:D:3437:ASN:N   | 2.82                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:A:288:VAL:HA   | 2:A:291:ILE:CD1   | 2.49                     | 0.42              |
| 3:B:24:ILE:CG2   | 3:B:25:SER:N      | 2.82                     | 0.42              |
| 3:B:102:ASN:HD21 | 3:B:408:TYR:CA    | 2.29                     | 0.42              |
| 3:B:259:MET:HE3  | 3:B:268:PHE:CE1   | 2.55                     | 0.42              |
| 3:B:269:MET:HG2  | 3:B:303:ALA:CB    | 2.50                     | 0.42              |
| 1:D:3385:LYS:NZ  | 3:B:196:GLU:HG2   | 2.34                     | 0.42              |
| 1:D:3464:TYR:CD1 | 1:D:3478:VAL:CG2  | 2.96                     | 0.42              |
| 2:A:68:VAL:HG11  | 2:A:149:PHE:CZ    | 2.55                     | 0.42              |
| 2:A:147:SER:HB3  | 2:A:186:ASN:HB3   | 2.01                     | 0.42              |
| 2:A:175:PRO:HD3  | 2:A:205:ASP:OD2   | 2.19                     | 0.42              |
| 2:A:237:SER:CB   | 2:A:376:CYS:SG    | 3.07                     | 0.42              |
| 2:A:371:VAL:CG1  | 2:A:372:GLN:N     | 2.82                     | 0.42              |
| 2:A:407:TRP:NE1  | 3:B:260:VAL:CG2   | 2.82                     | 0.42              |
| 2:A:419:SER:O    | 2:A:423:GLU:HG3   | 2.19                     | 0.42              |
| 3:B:4:ILE:N      | 3:B:51:VAL:CG1    | 2.82                     | 0.42              |
| 3:B:4:ILE:CG2    | 3:B:5:VAL:N       | 2.83                     | 0.42              |
| 3:B:86:ILE:CG2   | 3:B:87:PHE:N      | 2.83                     | 0.42              |
| 3:B:168:THR:CG2  | 3:B:169:PHE:N     | 2.83                     | 0.42              |
| 3:B:270:PRO:HB2  | 3:B:302:MET:SD    | 2.59                     | 0.42              |
| 3:B:311:ARG:HH11 | 3:B:311:ARG:CG    | 2.32                     | 0.42              |
| 3:B:319:PHE:N    | 3:B:319:PHE:CD1   | 2.87                     | 0.42              |
| 3:B:399:PHE:HE2  | 3:B:419:THR:HG23  | 1.85                     | 0.42              |
| 3:B:6:HIS:CB     | 3:B:21:TRP:HZ2    | 2.28                     | 0.42              |
| 3:B:40:SER:OG    | 3:B:43:GLN:HG3    | 2.19                     | 0.42              |
| 3:B:133:GLN:HA   | 3:B:133:GLN:OE1   | 2.19                     | 0.42              |
| 3:B:185:TYR:HA   | 3:B:395:PHE:CE1   | 2.54                     | 0.42              |
| 3:B:310:GLY:HA2  | 3:B:383:ALA:HB2   | 2.00                     | 0.42              |
| 3:B:241:CYS:SG   | 3:B:318:VAL:CG1   | 3.08                     | 0.42              |
| 3:B:289:PRO:HA   | 3:B:292:THR:HG23  | 2.01                     | 0.42              |
| 3:B:390:ARG:HD2  | 3:B:390:ARG:HA    | 1.57                     | 0.42              |
| 1:D:3474:CYS:O   | 1:D:3477:LEU:HB2  | 2.20                     | 0.42              |
| 1:D:3478:VAL:CG1 | 1:D:3479:LYS:N    | 2.82                     | 0.42              |
| 2:A:15:GLN:NE2   | 5:A:502:GTP:N7    | 2.67                     | 0.42              |
| 2:A:215:ARG:HG2  | 2:A:215:ARG:H     | 1.65                     | 0.42              |
| 3:B:185:TYR:CD1  | 3:B:395:PHE:CE1   | 3.06                     | 0.42              |
| 1:D:3384:LYS:HB2 | 1:D:3384:LYS:NZ   | 2.35                     | 0.42              |
| 1:D:3436:ILE:CG1 | 1:D:3437:ASN:HD22 | 2.33                     | 0.42              |
| 1:D:3444:MET:HE2 | 1:D:3444:MET:HB3  | 1.86                     | 0.42              |
| 1:D:3467:VAL:O   | 1:D:3470:ALA:HB3  | 2.19                     | 0.42              |
| 2:A:7:ILE:CD1    | 2:A:137:VAL:HG22  | 2.49                     | 0.42              |
| 2:A:152:LEU:O    | 2:A:155:GLU:HB3   | 2.20                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:A:193:THR:CG2  | 2:A:194:THR:N     | 2.83                     | 0.42              |
| 2:A:291:ILE:CD1  | 2:A:373:ARG:HG3   | 2.49                     | 0.42              |
| 2:A:305:CYS:SG   | 2:A:383:ALA:CB    | 3.08                     | 0.42              |
| 2:A:414:GLU:HB2  | 2:A:416:GLY:HA3   | 2.02                     | 0.42              |
| 3:B:68:VAL:CG1   | 3:B:149:MET:SD    | 3.07                     | 0.42              |
| 3:B:140:SER:O    | 3:B:142:GLY:HA3   | 2.19                     | 0.42              |
| 3:B:156:LYS:HZ2  | 3:B:156:LYS:HG3   | 1.68                     | 0.42              |
| 3:B:317:ALA:CB   | 3:B:319:PHE:CE1   | 3.03                     | 0.42              |
| 2:A:158:SER:HB2  | 2:A:197:HIS:ND1   | 2.35                     | 0.42              |
| 2:A:301:GLN:NE2  | 2:A:306:ASP:H     | 2.17                     | 0.42              |
| 3:B:311:ARG:HA   | 3:B:342:TYR:O     | 2.19                     | 0.42              |
| 2:A:9:VAL:HG12   | 2:A:138:PHE:O     | 2.19                     | 0.41              |
| 2:A:117:LEU:HD12 | 2:A:121:ARG:NH1   | 2.35                     | 0.41              |
| 2:A:133:GLN:HG2  | 2:A:252:LEU:HB2   | 2.01                     | 0.41              |
| 2:A:175:PRO:HG2  | 2:A:304:LYS:CG    | 2.50                     | 0.41              |
| 2:A:175:PRO:HG3  | 2:A:304:LYS:HG2   | 2.02                     | 0.41              |
| 3:B:24:ILE:HG23  | 3:B:25:SER:N      | 2.34                     | 0.41              |
| 3:B:28:HIS:O     | 3:B:36:TYR:CE1    | 2.73                     | 0.41              |
| 3:B:88:ARG:HA    | 3:B:89:PRO:HD3    | 1.87                     | 0.41              |
| 3:B:108:TYR:CE1  | 3:B:413:MET:CE    | 3.02                     | 0.41              |
| 3:B:141:LEU:HD13 | 3:B:170:SER:HB2   | 2.01                     | 0.41              |
| 3:B:141:LEU:N    | 3:B:141:LEU:CD1   | 2.83                     | 0.41              |
| 2:A:103:TYR:CD2  | 2:A:189:LEU:HD13  | 2.55                     | 0.41              |
| 3:B:44:LEU:O     | 3:B:49:ILE:HG12   | 2.20                     | 0.41              |
| 3:B:52:TYR:HB3   | 3:B:53:TYR:CE1    | 2.55                     | 0.41              |
| 3:B:115:VAL:HG21 | 3:B:152:LEU:HD23  | 2.02                     | 0.41              |
| 3:B:320:ARG:CB   | 3:B:356:CYS:HB3   | 2.49                     | 0.41              |
| 1:D:3384:LYS:NZ  | 1:D:3386:LYS:HE3  | 2.34                     | 0.41              |
| 1:D:3410:LEU:C   | 1:D:3410:LEU:HD23 | 2.41                     | 0.41              |
| 2:A:269:LEU:HD22 | 2:A:384:ILE:CD1   | 2.32                     | 0.41              |
| 2:A:430:LYS:O    | 2:A:434:GLU:HG3   | 2.20                     | 0.41              |
| 3:B:86:ILE:HG23  | 3:B:87:PHE:CD1    | 2.54                     | 0.41              |
| 3:B:107:HIS:NE2  | 3:B:151:THR:HG23  | 2.35                     | 0.41              |
| 3:B:223:THR:CG2  | 3:B:224:TYR:N     | 2.82                     | 0.41              |
| 3:B:390:ARG:HH11 | 3:B:390:ARG:HD3   | 1.75                     | 0.41              |
| 1:D:3457:LEU:O   | 1:D:3463:ASP:HB3  | 2.20                     | 0.41              |
| 2:A:110:ILE:CG2  | 2:A:111:GLY:N     | 2.82                     | 0.41              |
| 2:A:141:PHE:HB2  | 2:A:173:PRO:HD3   | 2.02                     | 0.41              |
| 2:A:190:THR:O    | 2:A:193:THR:HG22  | 2.20                     | 0.41              |
| 2:A:229:ARG:HH22 | 2:A:363:VAL:HG11  | 1.84                     | 0.41              |
| 2:A:301:GLN:HE21 | 2:A:303:VAL:HG12  | 1.84                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:A:436:GLY:C     | 2:A:438:ASP:H    | 2.23                     | 0.41              |
| 3:B:28:HIS:O      | 3:B:36:TYR:HE1   | 2.03                     | 0.41              |
| 3:B:67:LEU:HD21   | 3:B:87:PHE:CD2   | 2.55                     | 0.41              |
| 3:B:151:THR:OG1   | 3:B:193:GLN:HB2  | 2.20                     | 0.41              |
| 1:D:3384:LYS:HZ2  | 1:D:3386:LYS:HG3 | 1.86                     | 0.41              |
| 1:D:3427:MET:HG3  | 3:B:196:GLU:OE1  | 2.20                     | 0.41              |
| 1:D:3432:ILE:CD1  | 1:D:3433:THR:N   | 2.82                     | 0.41              |
| 2:A:31:GLN:CB     | 2:A:32:PRO:CD    | 2.91                     | 0.41              |
| 2:A:149:PHE:O     | 2:A:152:LEU:HG   | 2.20                     | 0.41              |
| 2:A:104:ALA:CB    | 2:A:413:MET:CG   | 2.97                     | 0.41              |
| 2:A:210:TYR:HD1   | 2:A:210:TYR:HA   | 1.56                     | 0.41              |
| 2:A:217:LEU:HD23  | 2:A:217:LEU:N    | 2.32                     | 0.41              |
| 2:A:238:ILE:HD13  | 2:A:238:ILE:HA   | 1.89                     | 0.41              |
| 2:A:305:CYS:HG    | 2:A:384:ILE:HD13 | 1.80                     | 0.41              |
| 3:B:242:LEU:HB3   | 3:B:250:ALA:O    | 2.20                     | 0.41              |
| 3:B:267:PHE:HB2   | 3:B:384:ILE:CD1  | 2.51                     | 0.41              |
| 1:D:3385:LYS:HZ1  | 3:B:196:GLU:HG2  | 1.86                     | 0.41              |
| 1:D:3456:TYR:O    | 1:D:3462:PHE:HB3 | 2.20                     | 0.41              |
| 1:D:3457:LEU:CD1  | 1:D:3458:GLU:N   | 2.83                     | 0.41              |
| 2:A:19:ALA:CB     | 2:A:228:ASN:HB3  | 2.46                     | 0.41              |
| 3:B:281:GLN:OE1   | 3:B:281:GLN:HA   | 2.20                     | 0.41              |
| 1:D:3433:THR:HA   | 1:D:3436:ILE:CD1 | 2.46                     | 0.41              |
| 2:A:407:TRP:HE1   | 3:B:260:VAL:HG22 | 1.86                     | 0.41              |
| 2:A:422:ARG:HH12  | 2:A:426:ALA:CB   | 2.22                     | 0.41              |
| 3:B:408:TYR:CG    | 3:B:418:PHE:HZ   | 2.39                     | 0.41              |
| 1:D:3384:LYS:HG3  | 1:D:3386:LYS:HB2 | 2.03                     | 0.41              |
| 1:D:3423:ARG:NH1  | 3:B:158:ARG:HD2  | 2.14                     | 0.41              |
| 1:D:3424:LYS:HE3  | 3:B:155:SER:O    | 2.20                     | 0.41              |
| 1:D:3457:LEU:HD12 | 1:D:3458:GLU:CA  | 2.51                     | 0.41              |
| 2:A:63:PRO:CG     | 2:A:87:PHE:HA    | 2.51                     | 0.41              |
| 2:A:69:ASP:CB     | 2:A:75:ILE:CD1   | 2.94                     | 0.41              |
| 2:A:119:LEU:HA    | 2:A:122:ILE:CG1  | 2.51                     | 0.41              |
| 2:A:185:TYR:HD1   | 2:A:185:TYR:HA   | 1.57                     | 0.41              |
| 2:A:244:PHE:HD1   | 2:A:245:ASP:H    | 1.65                     | 0.41              |
| 3:B:76:ASP:HA     | 3:B:79:ARG:CG    | 2.49                     | 0.41              |
| 3:B:88:ARG:O      | 3:B:91:ASN:HB2   | 2.21                     | 0.41              |
| 3:B:133:GLN:HG2   | 3:B:252:LEU:CD1  | 2.34                     | 0.41              |
| 3:B:314:THR:CG2   | 3:B:315:VAL:N    | 2.83                     | 0.41              |
| 2:A:172:TYR:CD1   | 2:A:172:TYR:C    | 2.94                     | 0.41              |
| 2:A:359:PRO:HA    | 2:A:360:PRO:HD3  | 1.92                     | 0.41              |
| 2:A:371:VAL:HG12  | 2:A:373:ARG:N    | 2.30                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:A:407:TRP:NE1   | 3:B:260:VAL:HG23 | 2.36                     | 0.41              |
| 3:B:64:ARG:HG2    | 3:B:125:GLU:HB3  | 2.02                     | 0.41              |
| 3:B:133:GLN:HE22  | 3:B:253:ARG:HG3  | 1.86                     | 0.41              |
| 3:B:223:THR:HG22  | 3:B:225:GLY:H    | 1.86                     | 0.41              |
| 1:D:3412:LEU:HD22 | 1:D:3431:PHE:HZ  | 1.85                     | 0.40              |
| 1:D:3477:LEU:HD12 | 1:D:3477:LEU:H   | 1.85                     | 0.40              |
| 2:A:103:TYR:CE2   | 2:A:413:MET:HE1  | 2.56                     | 0.40              |
| 2:A:404:PHE:CE2   | 3:B:258:ASN:O    | 2.74                     | 0.40              |
| 3:B:4:ILE:CG2     | 3:B:136:GLN:HG2  | 2.51                     | 0.40              |
| 3:B:7:ILE:CB      | 3:B:137:LEU:CD1  | 2.95                     | 0.40              |
| 3:B:7:ILE:CD1     | 3:B:66:ILE:HD11  | 2.51                     | 0.40              |
| 3:B:184:PRO:HB3   | 3:B:394:GLN:HB2  | 2.03                     | 0.40              |
| 3:B:259:MET:CE    | 3:B:268:PHE:CE1  | 3.04                     | 0.40              |
| 3:B:261:PRO:HB2   | 3:B:262:PHE:HD2  | 1.80                     | 0.40              |
| 3:B:325:MET:CE    | 3:B:355:VAL:CG2  | 2.98                     | 0.40              |
| 1:D:3444:MET:HG2  | 1:D:3445:THR:N   | 2.36                     | 0.40              |
| 2:A:72:PRO:HG3    | 2:A:96:LYS:CA    | 2.44                     | 0.40              |
| 2:A:276:ILE:HD13  | 2:A:277:SER:O    | 2.22                     | 0.40              |
| 3:B:167:ASN:HB3   | 3:B:202:TYR:CE1  | 2.50                     | 0.40              |
| 3:B:288:VAL:HB    | 3:B:289:PRO:HD3  | 2.03                     | 0.40              |
| 3:B:396:THR:HA    | 3:B:399:PHE:HB3  | 2.02                     | 0.40              |
| 3:B:406:HIS:CE1   | 3:B:407:TRP:CE2  | 3.09                     | 0.40              |
| 1:D:3418:GLU:CG   | 1:D:3419:TRP:N   | 2.85                     | 0.40              |
| 1:D:3462:PHE:O    | 1:D:3462:PHE:CD1 | 2.74                     | 0.40              |
| 1:D:3464:TYR:CE1  | 1:D:3468:ASN:CG  | 2.95                     | 0.40              |
| 2:A:233:GLN:HG3   | 2:A:272:TYR:CZ   | 2.56                     | 0.40              |
| 2:A:117:LEU:CD1   | 2:A:121:ARG:HH22 | 2.31                     | 0.40              |
| 3:B:64:ARG:HG3    | 3:B:125:GLU:CD   | 2.41                     | 0.40              |
| 3:B:276:THR:O     | 7:B:502:TA1:H192 | 2.21                     | 0.40              |
| 1:D:3477:LEU:N    | 1:D:3477:LEU:CD1 | 2.84                     | 0.40              |
| 2:A:26:LEU:HD12   | 2:A:26:LEU:HA    | 1.90                     | 0.40              |
| 2:A:180:ALA:HB3   | 2:A:183:GLU:HB2  | 2.04                     | 0.40              |
| 2:A:219:ILE:O     | 2:A:222:PRO:HD3  | 2.22                     | 0.40              |
| 2:A:402:ARG:NE    | 2:A:405:VAL:HG12 | 2.28                     | 0.40              |
| 3:B:199:ASP:HA    | 3:B:265:LEU:HB2  | 2.04                     | 0.40              |
| 3:B:425:MET:HA    | 3:B:428:LEU:HB3  | 2.02                     | 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 PDB entries followed by that with respect to all EM entries.

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   | D     | 106/108 (98%)  | 100 (94%) | 5 (5%)  | 1 (1%)   | 17          | 57 |
| 2   | A     | 408/451 (90%)  | 374 (92%) | 23 (6%) | 11 (3%)  | 5           | 31 |
| 3   | B     | 424/445 (95%)  | 386 (91%) | 31 (7%) | 7 (2%)   | 9           | 42 |
| All | All   | 938/1004 (93%) | 860 (92%) | 59 (6%) | 19 (2%)  | 11          | 38 |

All (19) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | A     | 276  | ILE  |
| 2   | A     | 437  | VAL  |
| 3   | B     | 38   | GLY  |
| 3   | B     | 130  | ASP  |
| 3   | B     | 282  | GLN  |
| 3   | B     | 287  | THR  |
| 3   | B     | 344  | VAL  |
| 2   | A     | 100  | ALA  |
| 2   | A     | 111  | GLY  |
| 2   | A     | 249  | ASN  |
| 1   | D     | 3483 | ALA  |
| 2   | A     | 342  | GLN  |
| 2   | A     | 413  | MET  |
| 2   | A     | 148  | GLY  |
| 2   | A     | 31   | GLN  |
| 2   | A     | 307  | PRO  |
| 3   | B     | 82   | PRO  |
| 2   | A     | 412  | GLY  |
| 3   | B     | 32   | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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   | D     | 95/95 (100%)  | 73 (77%)  | 22 (23%)  | 1           | 4 |
| 2   | A     | 347/377 (92%) | 260 (75%) | 87 (25%)  | 0           | 3 |
| 3   | B     | 367/381 (96%) | 262 (71%) | 105 (29%) | 0           | 2 |
| All | All   | 809/853 (95%) | 595 (74%) | 214 (26%) | 2           | 3 |

All (214) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 3384 | LYS  |
| 1   | D     | 3389 | ASP  |
| 1   | D     | 3392 | LYS  |
| 1   | D     | 3396 | LYS  |
| 1   | D     | 3405 | MET  |
| 1   | D     | 3408 | VAL  |
| 1   | D     | 3415 | LYS  |
| 1   | D     | 3422 | ILE  |
| 1   | D     | 3423 | ARG  |
| 1   | D     | 3424 | LYS  |
| 1   | D     | 3426 | ILE  |
| 1   | D     | 3428 | GLU  |
| 1   | D     | 3430 | ASN  |
| 1   | D     | 3431 | PHE  |
| 1   | D     | 3432 | ILE  |
| 1   | D     | 3444 | MET  |
| 1   | D     | 3449 | ARG  |
| 1   | D     | 3452 | ILE  |
| 1   | D     | 3454 | LYS  |
| 1   | D     | 3456 | TYR  |
| 1   | D     | 3459 | ASP  |
| 1   | D     | 3484 | GLN  |
| 2   | A     | 4    | CYS  |
| 2   | A     | 16   | ILE  |
| 2   | A     | 21   | TRP  |
| 2   | A     | 24   | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 25  | CYS  |
| 2   | A     | 26  | LEU  |
| 2   | A     | 32  | PRO  |
| 2   | A     | 76  | ASP  |
| 2   | A     | 85  | GLN  |
| 2   | A     | 91  | GLN  |
| 2   | A     | 93  | ILE  |
| 2   | A     | 96  | LYS  |
| 2   | A     | 98  | ASP  |
| 2   | A     | 101 | ASN  |
| 2   | A     | 105 | ARG  |
| 2   | A     | 108 | TYR  |
| 2   | A     | 112 | LYS  |
| 2   | A     | 117 | LEU  |
| 2   | A     | 120 | ASP  |
| 2   | A     | 122 | ILE  |
| 2   | A     | 123 | ARG  |
| 2   | A     | 128 | GLN  |
| 2   | A     | 129 | CYS  |
| 2   | A     | 130 | THR  |
| 2   | A     | 135 | PHE  |
| 2   | A     | 141 | PHE  |
| 2   | A     | 154 | MET  |
| 2   | A     | 164 | LYS  |
| 2   | A     | 166 | LYS  |
| 2   | A     | 170 | SER  |
| 2   | A     | 172 | TYR  |
| 2   | A     | 192 | HIS  |
| 2   | A     | 207 | GLU  |
| 2   | A     | 210 | TYR  |
| 2   | A     | 212 | ILE  |
| 2   | A     | 214 | ARG  |
| 2   | A     | 215 | ARG  |
| 2   | A     | 217 | LEU  |
| 2   | A     | 224 | TYR  |
| 2   | A     | 229 | ARG  |
| 2   | A     | 231 | ILE  |
| 2   | A     | 234 | ILE  |
| 2   | A     | 241 | SER  |
| 2   | A     | 242 | LEU  |
| 2   | A     | 244 | PHE  |
| 2   | A     | 248 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 251 | ASP  |
| 2   | A     | 253 | THR  |
| 2   | A     | 260 | VAL  |
| 2   | A     | 264 | ARG  |
| 2   | A     | 269 | LEU  |
| 2   | A     | 276 | ILE  |
| 2   | A     | 284 | GLU  |
| 2   | A     | 300 | ASN  |
| 2   | A     | 301 | GLN  |
| 2   | A     | 303 | VAL  |
| 2   | A     | 305 | CYS  |
| 2   | A     | 308 | ARG  |
| 2   | A     | 311 | LYS  |
| 2   | A     | 317 | LEU  |
| 2   | A     | 320 | ARG  |
| 2   | A     | 326 | LYS  |
| 2   | A     | 337 | THR  |
| 2   | A     | 339 | ARG  |
| 2   | A     | 344 | VAL  |
| 2   | A     | 345 | ASP  |
| 2   | A     | 346 | TRP  |
| 2   | A     | 347 | CYS  |
| 2   | A     | 349 | THR  |
| 2   | A     | 352 | LYS  |
| 2   | A     | 370 | LYS  |
| 2   | A     | 372 | GLN  |
| 2   | A     | 377 | MET  |
| 2   | A     | 378 | LEU  |
| 2   | A     | 390 | ARG  |
| 2   | A     | 398 | MET  |
| 2   | A     | 401 | LYS  |
| 2   | A     | 402 | ARG  |
| 2   | A     | 405 | VAL  |
| 2   | A     | 413 | MET  |
| 2   | A     | 417 | GLU  |
| 2   | A     | 424 | ASP  |
| 2   | A     | 425 | MET  |
| 2   | A     | 428 | LEU  |
| 2   | A     | 430 | LYS  |
| 2   | A     | 431 | ASP  |
| 2   | A     | 432 | TYR  |
| 3   | B     | 7   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B     | 8   | GLN  |
| 3   | B     | 14  | ASN  |
| 3   | B     | 24  | ILE  |
| 3   | B     | 26  | ASP  |
| 3   | B     | 33  | THR  |
| 3   | B     | 41  | ASP  |
| 3   | B     | 44  | LEU  |
| 3   | B     | 53  | TYR  |
| 3   | B     | 54  | ASN  |
| 3   | B     | 64  | ARG  |
| 3   | B     | 66  | ILE  |
| 3   | B     | 67  | LEU  |
| 3   | B     | 76  | ASP  |
| 3   | B     | 79  | ARG  |
| 3   | B     | 88  | ARG  |
| 3   | B     | 90  | ASP  |
| 3   | B     | 94  | PHE  |
| 3   | B     | 97  | SER  |
| 3   | B     | 101 | ASN  |
| 3   | B     | 116 | ASP  |
| 3   | B     | 117 | SER  |
| 3   | B     | 124 | LYS  |
| 3   | B     | 126 | SER  |
| 3   | B     | 135 | PHE  |
| 3   | B     | 138 | THR  |
| 3   | B     | 140 | SER  |
| 3   | B     | 141 | LEU  |
| 3   | B     | 145 | THR  |
| 3   | B     | 153 | LEU  |
| 3   | B     | 154 | ILE  |
| 3   | B     | 156 | LYS  |
| 3   | B     | 158 | ARG  |
| 3   | B     | 160 | GLU  |
| 3   | B     | 161 | TYR  |
| 3   | B     | 164 | ARG  |
| 3   | B     | 165 | ILE  |
| 3   | B     | 178 | SER  |
| 3   | B     | 186 | ASN  |
| 3   | B     | 193 | GLN  |
| 3   | B     | 198 | THR  |
| 3   | B     | 207 | GLU  |
| 3   | B     | 209 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B     | 211 | ASP  |
| 3   | B     | 213 | CYS  |
| 3   | B     | 218 | LYS  |
| 3   | B     | 219 | LEU  |
| 3   | B     | 221 | THR  |
| 3   | B     | 224 | TYR  |
| 3   | B     | 230 | LEU  |
| 3   | B     | 236 | SER  |
| 3   | B     | 240 | THR  |
| 3   | B     | 241 | CYS  |
| 3   | B     | 243 | ARG  |
| 3   | B     | 259 | MET  |
| 3   | B     | 265 | LEU  |
| 3   | B     | 275 | LEU  |
| 3   | B     | 277 | SER  |
| 3   | B     | 278 | ARG  |
| 3   | B     | 280 | SER  |
| 3   | B     | 282 | GLN  |
| 3   | B     | 283 | TYR  |
| 3   | B     | 284 | ARG  |
| 3   | B     | 288 | VAL  |
| 3   | B     | 293 | GLN  |
| 3   | B     | 294 | GLN  |
| 3   | B     | 299 | LYS  |
| 3   | B     | 306 | ASP  |
| 3   | B     | 308 | ARG  |
| 3   | B     | 309 | HIS  |
| 3   | B     | 311 | ARG  |
| 3   | B     | 320 | ARG  |
| 3   | B     | 322 | ARG  |
| 3   | B     | 323 | MET  |
| 3   | B     | 325 | MET  |
| 3   | B     | 330 | GLU  |
| 3   | B     | 337 | ASN  |
| 3   | B     | 342 | TYR  |
| 3   | B     | 343 | PHE  |
| 3   | B     | 344 | VAL  |
| 3   | B     | 346 | TRP  |
| 3   | B     | 352 | LYS  |
| 3   | B     | 369 | ARG  |
| 3   | B     | 372 | LYS  |
| 3   | B     | 376 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B     | 378 | ILE  |
| 3   | B     | 380 | ASN  |
| 3   | B     | 384 | ILE  |
| 3   | B     | 385 | GLN  |
| 3   | B     | 390 | ARG  |
| 3   | B     | 400 | ARG  |
| 3   | B     | 401 | ARG  |
| 3   | B     | 402 | LYS  |
| 3   | B     | 405 | LEU  |
| 3   | B     | 409 | THR  |
| 3   | B     | 413 | MET  |
| 3   | B     | 419 | THR  |
| 3   | B     | 423 | SER  |
| 3   | B     | 425 | MET  |
| 3   | B     | 427 | ASP  |
| 3   | B     | 428 | LEU  |
| 3   | B     | 430 | SER  |
| 3   | B     | 431 | GLU  |
| 3   | B     | 432 | TYR  |
| 3   | B     | 437 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 3437 | ASN  |
| 1   | D     | 3484 | GLN  |
| 2   | A     | 11   | GLN  |
| 2   | A     | 15   | GLN  |
| 2   | A     | 61   | HIS  |
| 2   | A     | 101  | ASN  |
| 2   | A     | 102  | ASN  |
| 2   | A     | 107  | HIS  |
| 2   | A     | 128  | GLN  |
| 2   | A     | 133  | GLN  |
| 2   | A     | 139  | HIS  |
| 2   | A     | 216  | ASN  |
| 2   | A     | 226  | ASN  |
| 2   | A     | 256  | GLN  |
| 2   | A     | 301  | GLN  |
| 2   | A     | 372  | GLN  |
| 2   | A     | 380  | ASN  |
| 3   | B     | 8    | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B     | 14  | ASN  |
| 3   | B     | 43  | GLN  |
| 3   | B     | 54  | ASN  |
| 3   | B     | 91  | ASN  |
| 3   | B     | 101 | ASN  |
| 3   | B     | 102 | ASN  |
| 3   | B     | 107 | HIS  |
| 3   | B     | 133 | GLN  |
| 3   | B     | 136 | GLN  |
| 3   | B     | 139 | HIS  |
| 3   | B     | 167 | ASN  |
| 3   | B     | 186 | ASN  |
| 3   | B     | 258 | ASN  |
| 3   | B     | 282 | GLN  |
| 3   | B     | 300 | ASN  |
| 3   | B     | 334 | ASN  |
| 3   | B     | 336 | GLN  |
| 3   | B     | 337 | ASN  |
| 3   | B     | 349 | ASN  |
| 3   | B     | 380 | ASN  |
| 3   | B     | 406 | HIS  |
| 3   | B     | 424 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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 | $\# Z  > 2$ |
| 6   | GDP  | B     | 501 | -    | 24,30,30     | 2.59 | 9 (37%)     | 30,47,47    | 2.92 | 8 (26%)     |
| 7   | TA1  | B     | 502 | -    | 68,68,68     | 2.01 | 19 (27%)    | 105,105,105 | 1.39 | 11 (10%)    |
| 5   | GTP  | A     | 502 | 4    | 26,34,34     | 1.28 | 4 (15%)     | 32,54,54    | 1.11 | 3 (9%)      |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 6   | GDP  | B     | 501 | -    | -       | 4/12/32/32   | 0/3/3/3 |
| 7   | TA1  | B     | 502 | -    | -       | 9/41/127/127 | 0/7/7/7 |
| 5   | GTP  | A     | 502 | 4    | -       | 3/18/38/38   | 0/3/3/3 |

All (32) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | B     | 501 | GDP  | O4'-C1' | 6.27  | 1.49        | 1.41     |
| 6   | B     | 501 | GDP  | O6-C6   | 5.65  | 1.34        | 1.23     |
| 7   | B     | 502 | TA1  | C06-C05 | 5.25  | 1.50        | 1.38     |
| 7   | B     | 502 | TA1  | C18-C10 | 5.08  | 1.68        | 1.57     |
| 6   | B     | 501 | GDP  | C2-N1   | 4.64  | 1.49        | 1.37     |
| 7   | B     | 502 | TA1  | C08-C07 | -4.57 | 1.25        | 1.38     |
| 7   | B     | 502 | TA1  | C05-C04 | 4.36  | 1.46        | 1.39     |
| 7   | B     | 502 | TA1  | C45-C24 | 3.96  | 1.61        | 1.54     |
| 6   | B     | 501 | GDP  | PB-O2B  | -3.78 | 1.40        | 1.54     |
| 5   | A     | 502 | GTP  | C5-C6   | -3.74 | 1.39        | 1.47     |
| 7   | B     | 502 | TA1  | O02-C03 | 3.60  | 1.42        | 1.34     |
| 6   | B     | 501 | GDP  | C8-N7   | 3.55  | 1.41        | 1.35     |
| 7   | B     | 502 | TA1  | C36-C31 | 3.37  | 1.45        | 1.39     |
| 7   | B     | 502 | TA1  | C25-C24 | 3.33  | 1.39        | 1.34     |
| 7   | B     | 502 | TA1  | C46-C45 | 3.09  | 1.59        | 1.53     |
| 7   | B     | 502 | TA1  | C11-C10 | 3.05  | 1.61        | 1.54     |
| 7   | B     | 502 | TA1  | C43-C01 | 3.02  | 1.60        | 1.54     |
| 6   | B     | 501 | GDP  | C5-C6   | -2.85 | 1.41        | 1.47     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | B     | 502 | TA1  | C43-C26 | 2.83  | 1.58        | 1.52     |
| 5   | A     | 502 | GTP  | C6-N1   | 2.52  | 1.41        | 1.37     |
| 7   | B     | 502 | TA1  | C26-C25 | 2.51  | 1.56        | 1.51     |
| 7   | B     | 502 | TA1  | C18-C20 | 2.49  | 1.62        | 1.55     |
| 7   | B     | 502 | TA1  | C04-C03 | -2.40 | 1.44        | 1.50     |
| 6   | B     | 501 | GDP  | C2-N3   | -2.39 | 1.27        | 1.33     |
| 7   | B     | 502 | TA1  | C01-C45 | 2.38  | 1.66        | 1.56     |
| 5   | A     | 502 | GTP  | C8-N7   | -2.35 | 1.31        | 1.35     |
| 6   | B     | 501 | GDP  | PB-O3B  | 2.31  | 1.63        | 1.54     |
| 7   | B     | 502 | TA1  | C16-C15 | 2.25  | 1.56        | 1.52     |
| 7   | B     | 502 | TA1  | C37-C29 | 2.12  | 1.54        | 1.52     |
| 7   | B     | 502 | TA1  | C10-C02 | 2.10  | 1.62        | 1.57     |
| 5   | A     | 502 | GTP  | O4'-C1' | 2.07  | 1.44        | 1.41     |
| 6   | B     | 501 | GDP  | O3'-C3' | 2.05  | 1.47        | 1.43     |

All (22) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | B     | 501 | GDP  | C8-N7-C5    | 9.27  | 120.65      | 102.99   |
| 6   | B     | 501 | GDP  | N2-C2-N3    | 6.26  | 131.93      | 119.74   |
| 6   | B     | 501 | GDP  | C5-C6-N1    | 6.07  | 124.67      | 113.95   |
| 7   | B     | 502 | TA1  | C06-C05-C04 | -4.84 | 114.61      | 120.34   |
| 7   | B     | 502 | TA1  | C07-C08-C09 | 4.67  | 127.31      | 120.19   |
| 6   | B     | 501 | GDP  | O6-C6-C5    | -4.23 | 116.11      | 124.37   |
| 6   | B     | 501 | GDP  | N2-C2-N1    | -4.17 | 107.83      | 116.71   |
| 7   | B     | 502 | TA1  | C05-C04-C03 | -3.93 | 111.54      | 120.40   |
| 6   | B     | 501 | GDP  | C2-N1-C6    | -3.73 | 118.24      | 125.10   |
| 7   | B     | 502 | TA1  | C09-C04-C03 | 3.55  | 128.41      | 120.40   |
| 6   | B     | 501 | GDP  | C2'-C3'-C4' | 3.36  | 109.17      | 102.64   |
| 7   | B     | 502 | TA1  | C17-C18-C20 | 3.10  | 109.75      | 102.59   |
| 7   | B     | 502 | TA1  | C45-C01-C02 | 2.98  | 115.17      | 111.91   |
| 7   | B     | 502 | TA1  | O04-C11-C14 | -2.90 | 101.75      | 108.09   |
| 5   | A     | 502 | GTP  | O2G-PG-O3B  | 2.65  | 113.52      | 104.64   |
| 7   | B     | 502 | TA1  | O01-C01-C43 | 2.55  | 113.40      | 107.03   |
| 7   | B     | 502 | TA1  | C14-C11-C15 | -2.28 | 82.98       | 85.40    |
| 6   | B     | 501 | GDP  | O2'-C2'-C3' | 2.26  | 119.14      | 111.82   |
| 7   | B     | 502 | TA1  | C10-C18-C17 | -2.17 | 102.31      | 106.54   |
| 7   | B     | 502 | TA1  | O06-C15-C11 | 2.12  | 92.96       | 90.58    |
| 5   | A     | 502 | GTP  | O5'-C5'-C4' | 2.08  | 116.14      | 108.99   |
| 5   | A     | 502 | GTP  | O3G-PG-O3B  | 2.03  | 111.44      | 104.64   |

There are no chirality outliers.

All (16) torsion outliers are listed below:

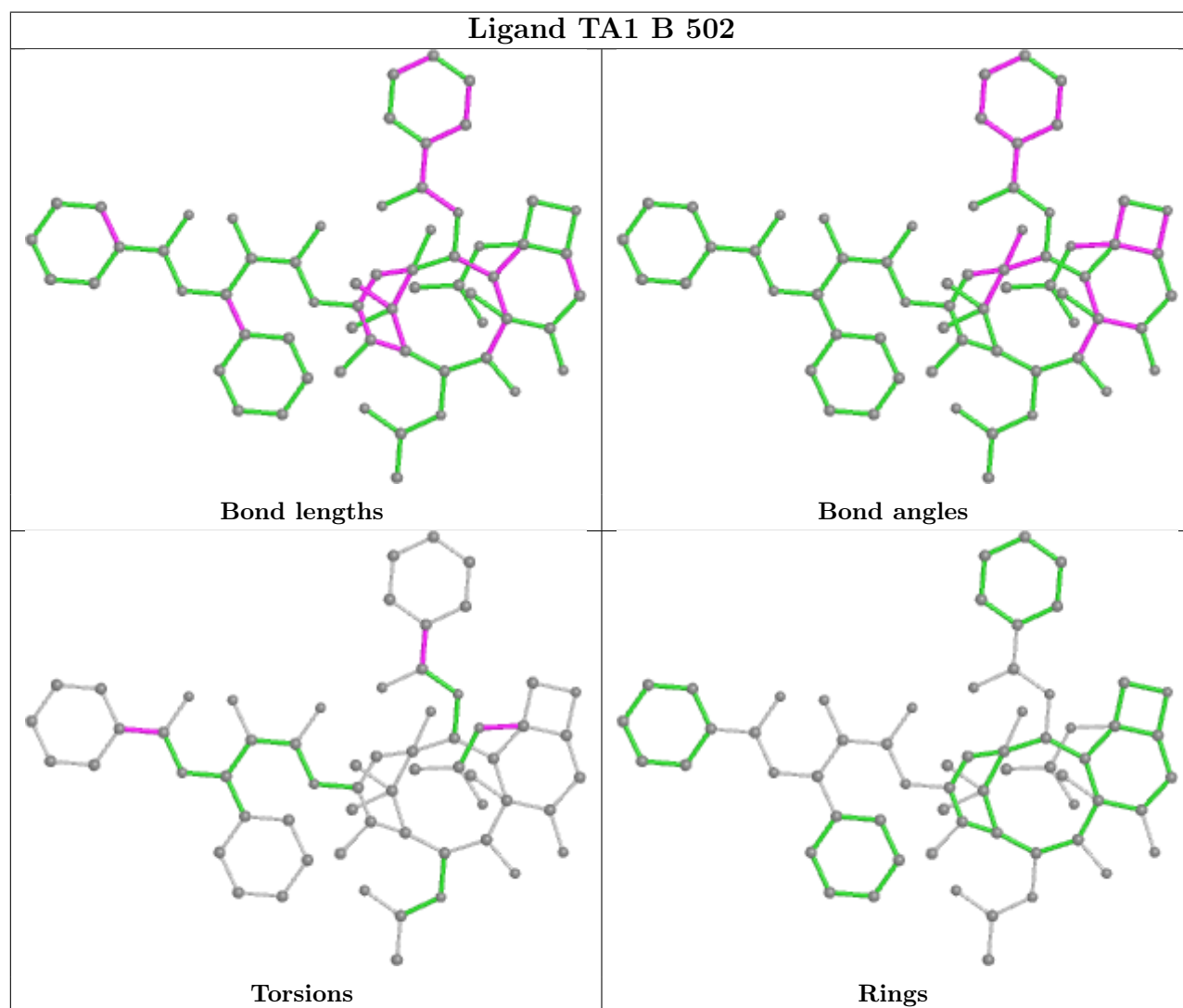
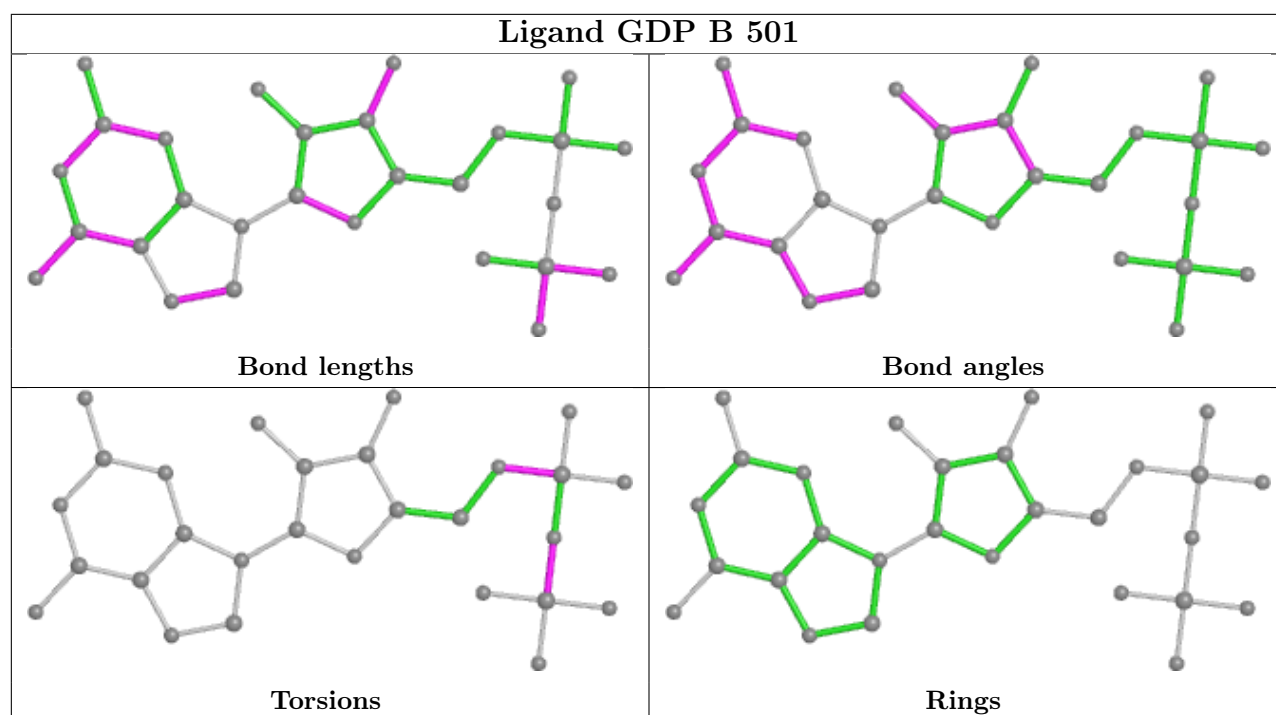
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | B     | 501 | GDP  | PA-O3A-PB-O2B   |
| 6   | B     | 501 | GDP  | C5'-O5'-PA-O3A  |
| 6   | B     | 501 | GDP  | C5'-O5'-PA-O1A  |
| 7   | B     | 502 | TA1  | O02-C03-C04-C05 |
| 7   | B     | 502 | TA1  | O02-C03-C04-C09 |
| 7   | B     | 502 | TA1  | O03-C03-C04-C09 |
| 7   | B     | 502 | TA1  | O03-C03-C04-C05 |
| 7   | B     | 502 | TA1  | N01-C30-C31-C36 |
| 7   | B     | 502 | TA1  | O14-C30-C31-C36 |
| 7   | B     | 502 | TA1  | N01-C30-C31-C32 |
| 7   | B     | 502 | TA1  | O14-C30-C31-C32 |
| 5   | A     | 502 | GTP  | C3'-C4'-C5'-O5' |
| 5   | A     | 502 | GTP  | O4'-C4'-C5'-O5' |
| 6   | B     | 501 | GDP  | PA-O3A-PB-O3B   |
| 7   | B     | 502 | TA1  | C15-C11-O04-C12 |
| 5   | A     | 502 | GTP  | C5'-O5'-PA-O1A  |

There are no ring outliers.

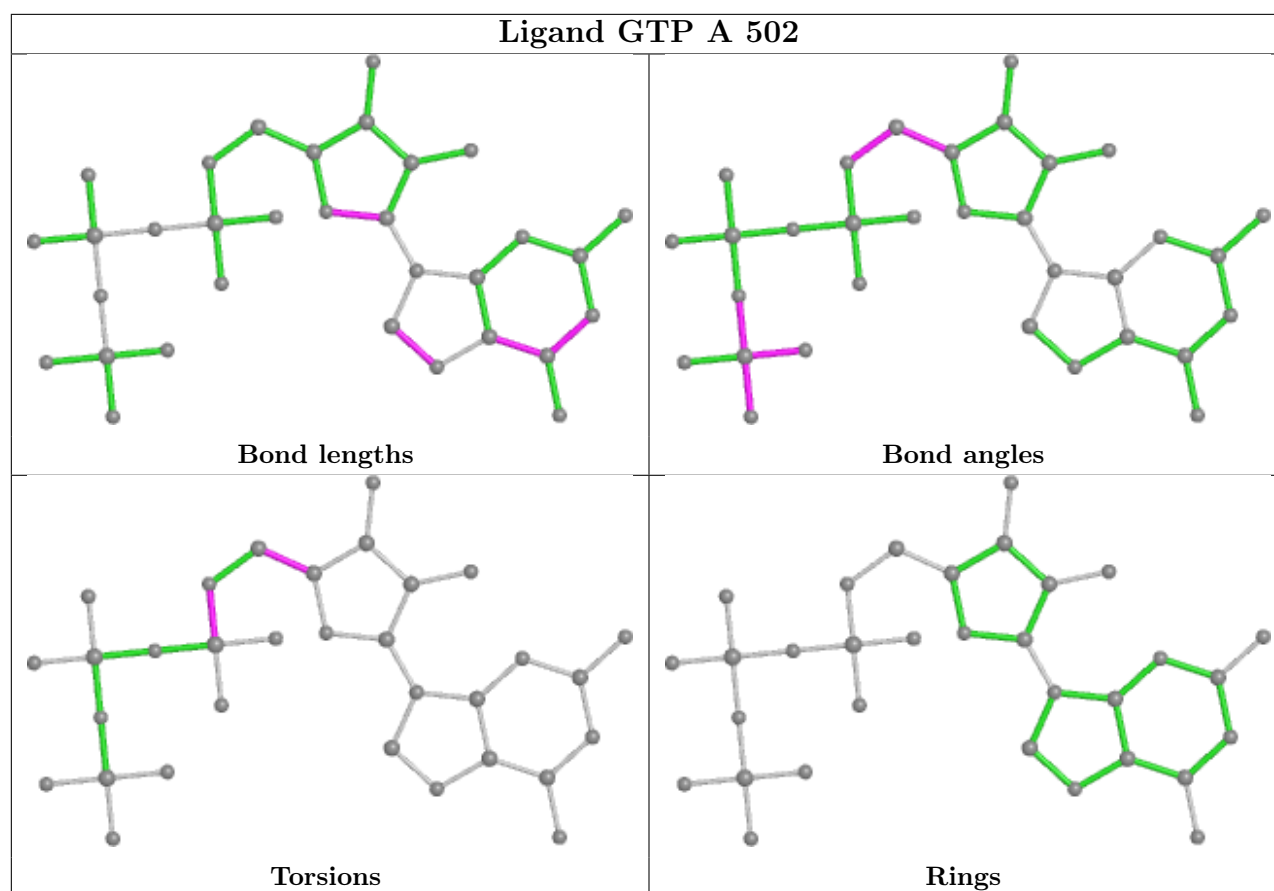
3 monomers are involved in 12 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6   | B     | 501 | GDP  | 1       | 0            |
| 7   | B     | 502 | TA1  | 8       | 0            |
| 5   | A     | 502 | GTP  | 3       | 0            |

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

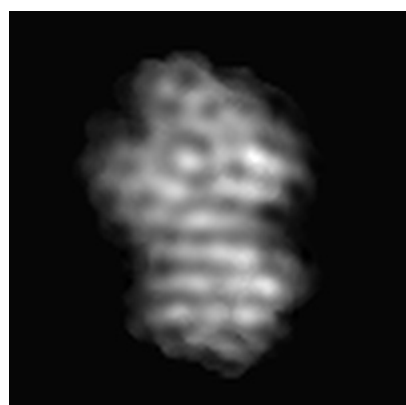
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5931. These allow visual inspection of the internal detail of the map and identification of artifacts.

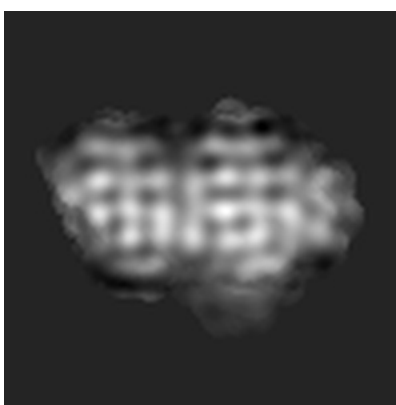
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



X



Y

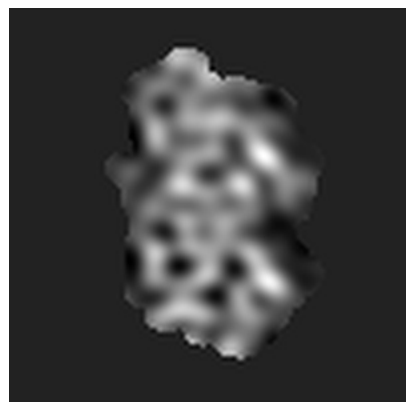


Z

The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

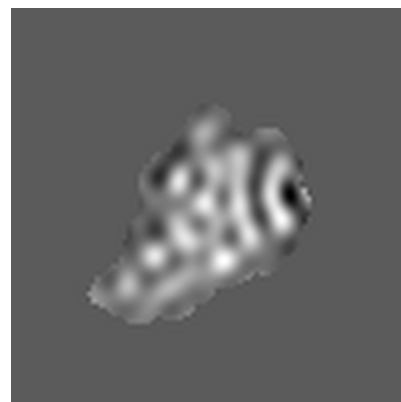
#### 6.2.1 Primary map



X Index: 50



Y Index: 50

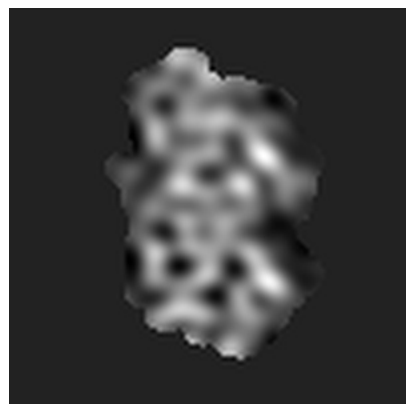


Z Index: 50

The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

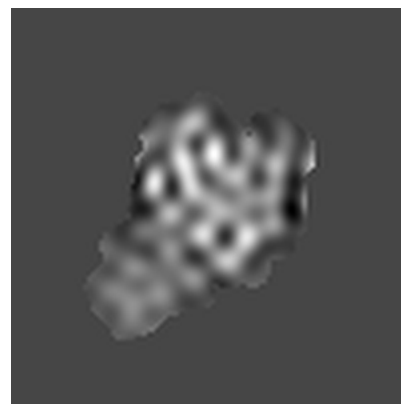
### 6.3.1 Primary map



X Index: 50



Y Index: 54



Z Index: 63

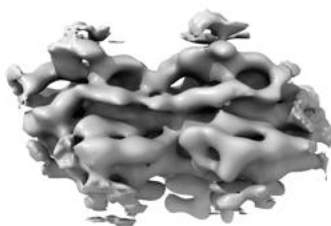
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

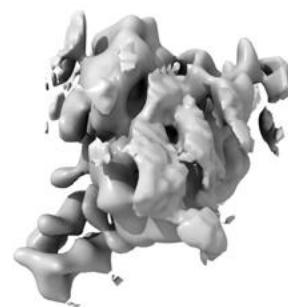
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.106. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

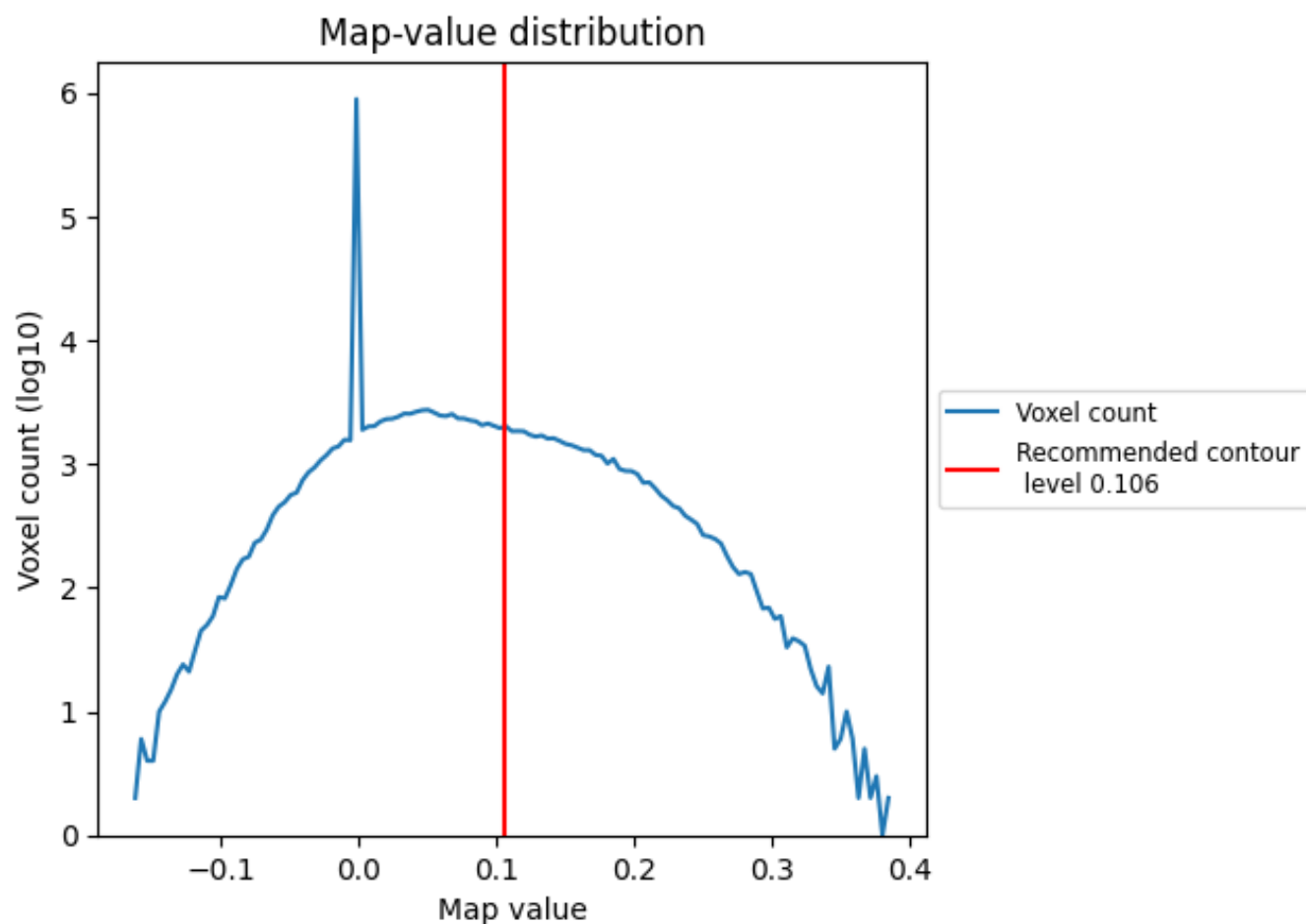
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

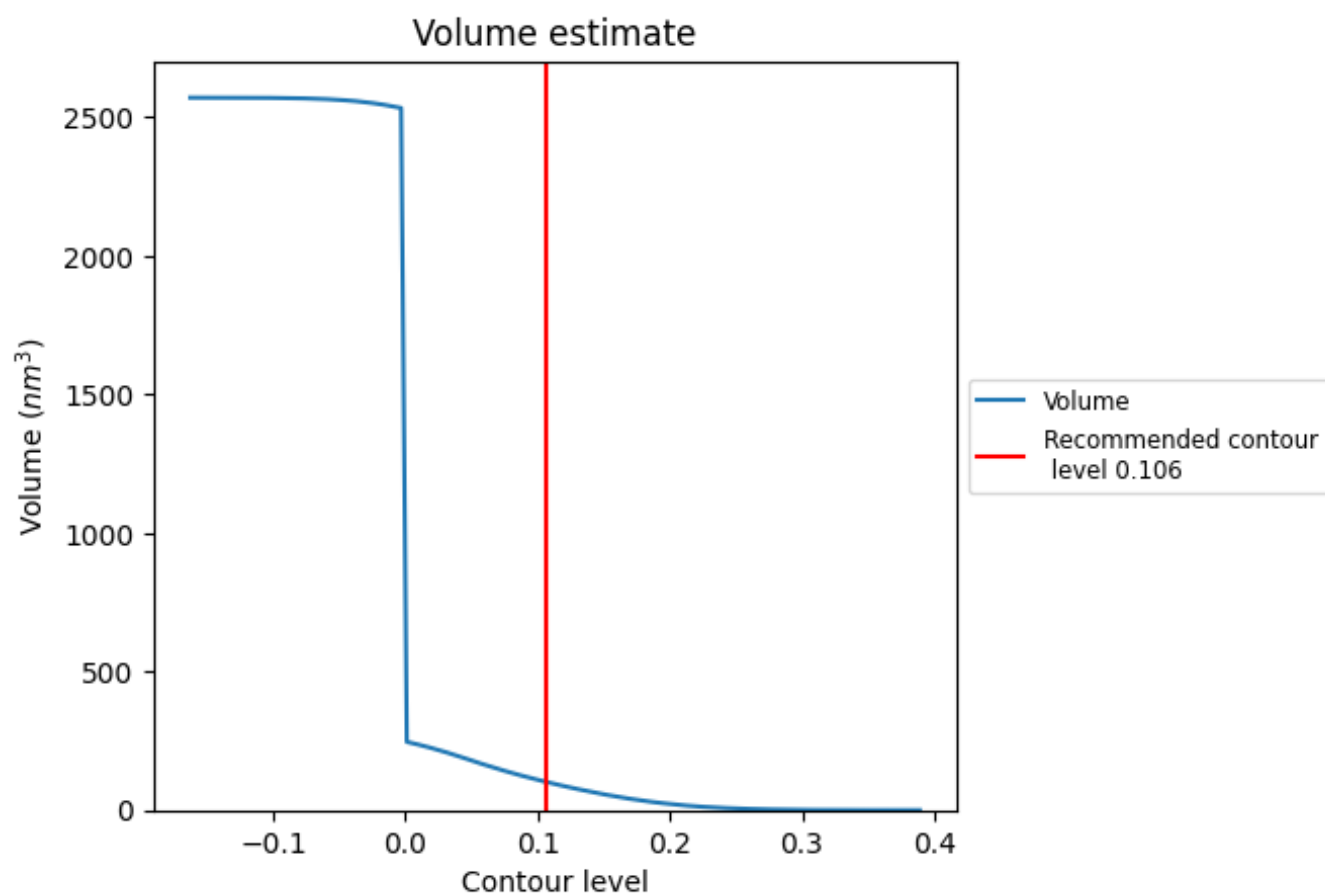
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

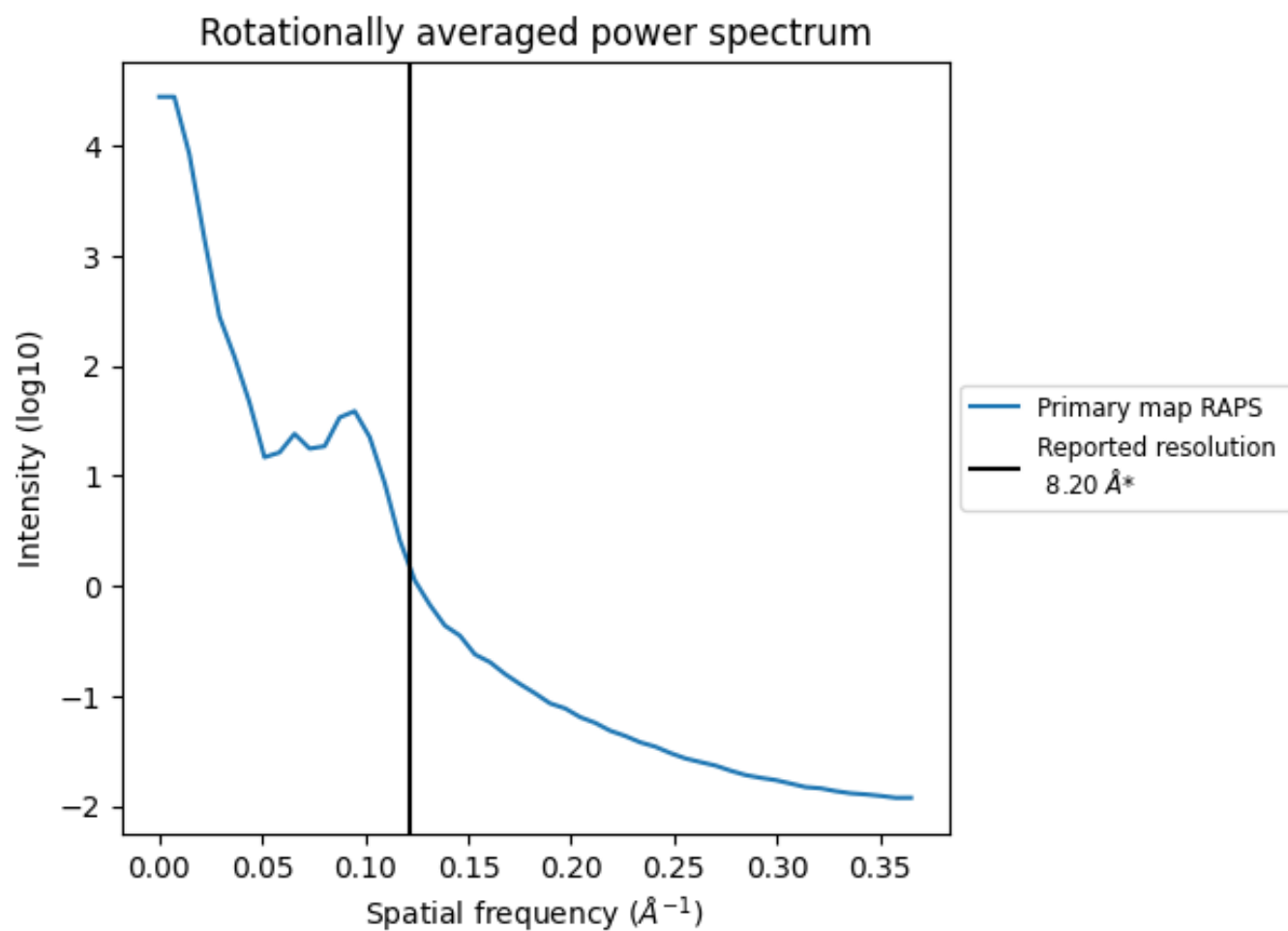
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 102  $\text{nm}^3$ ; this corresponds to an approximate mass of 93 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.122 Å<sup>-1</sup>



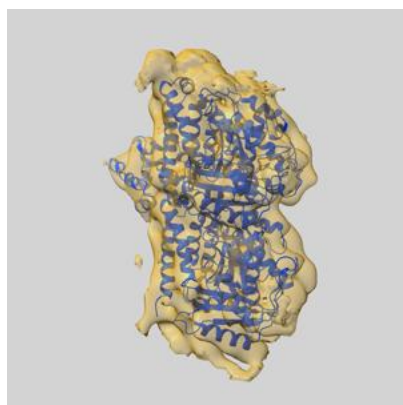
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

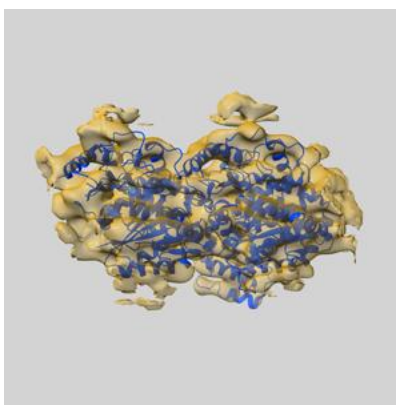
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5931 and PDB model 3J6P. Per-residue inclusion information can be found in section [3](#) on page [6](#).

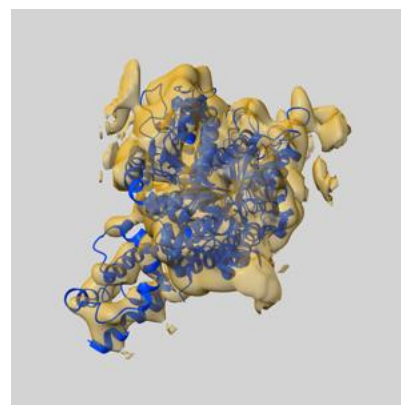
### 9.1 Map-model overlay [i](#)



X



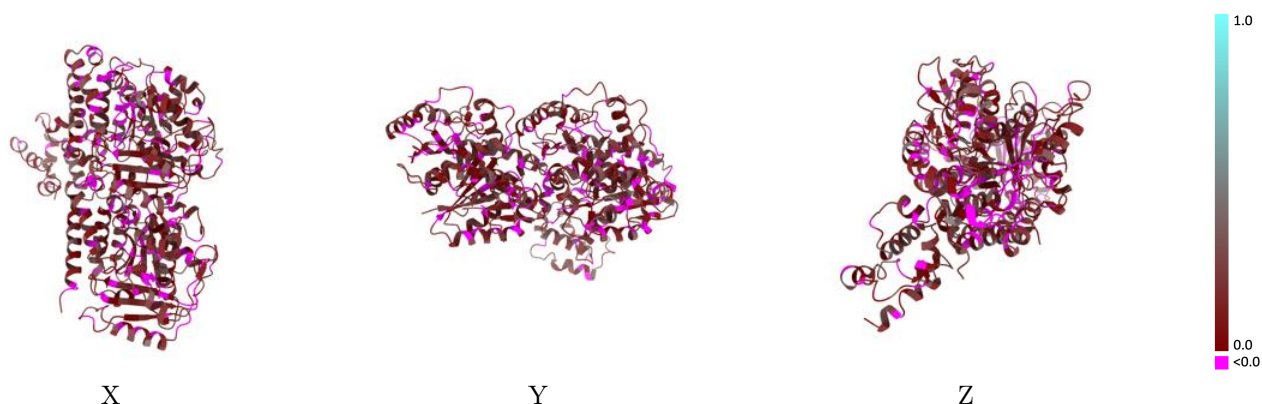
Y



Z

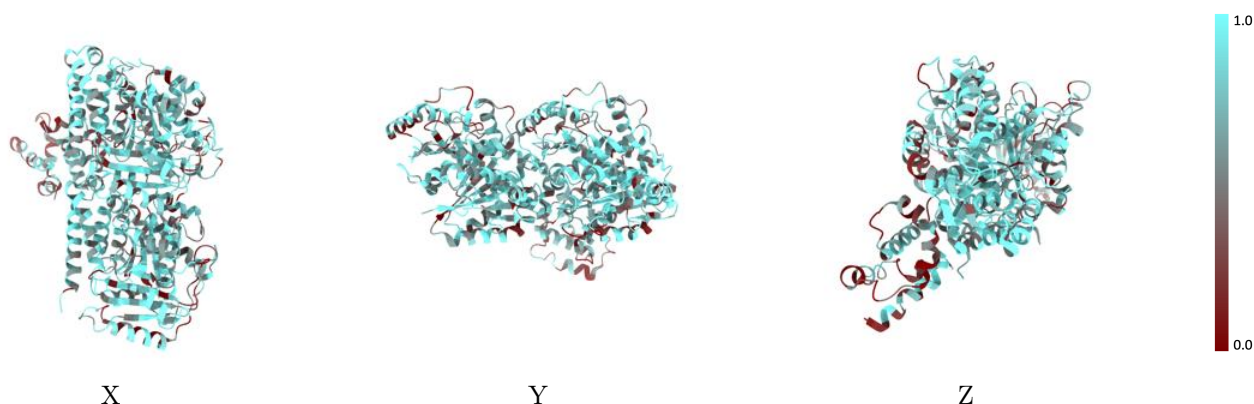
The images above show the 3D surface view of the map at the recommended contour level 0.106 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



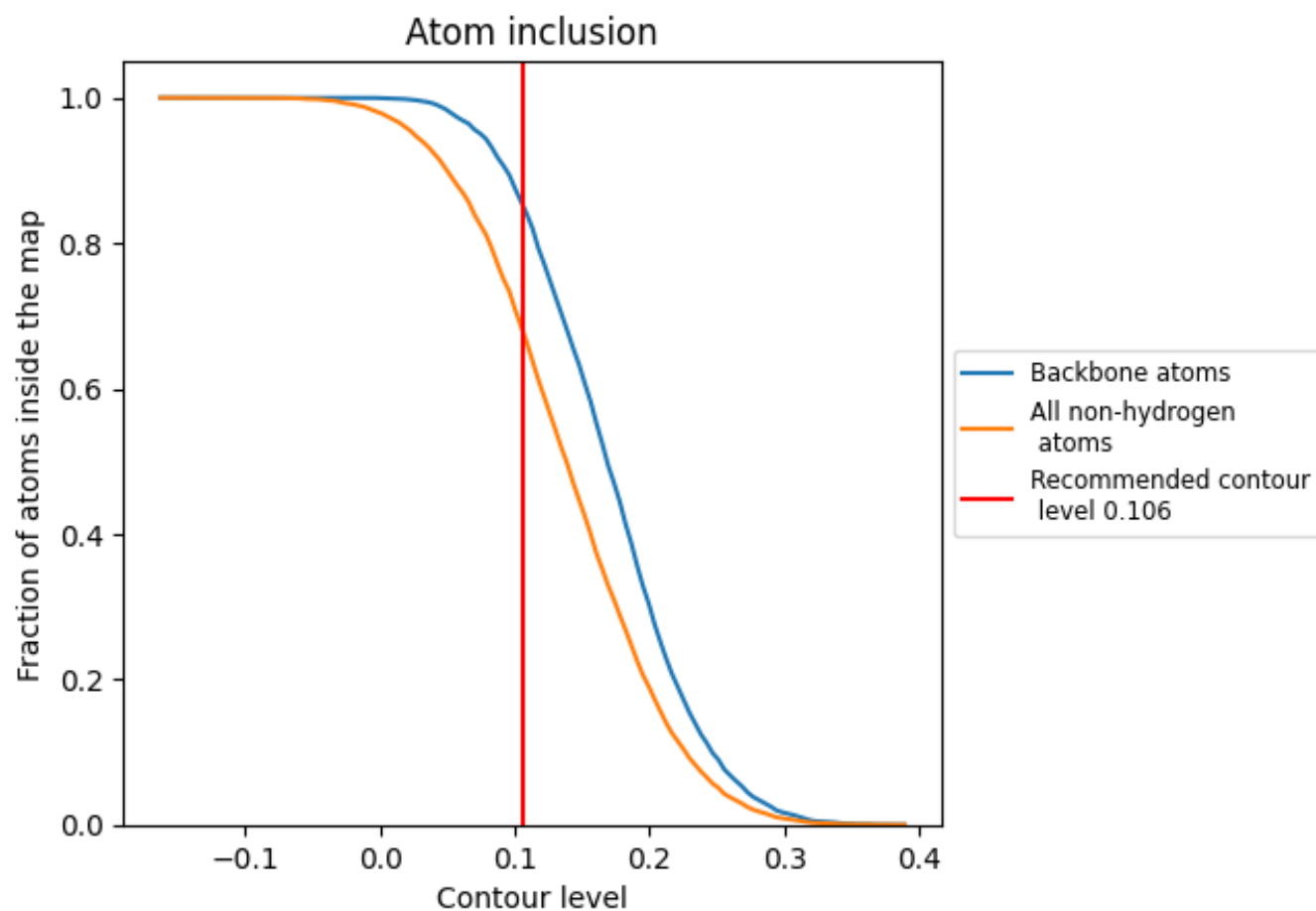
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.106).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.106) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.6789 | <div></div> 0.1140 |
| A     | <div></div> 0.6962 | <div></div> 0.1060 |
| B     | <div></div> 0.7163 | <div></div> 0.1140 |
| D     | <div></div> 0.4653 | <div></div> 0.1430 |

