



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:51 AM UTC

PDB ID : 6YAH / pdb\_00006yah  
EMDB ID : EMD-10751  
Title : AP2 in clathrin coats assembled on a membrane containing dileucine- and tyrosine-based cargo peptides  
Authors : Kovtun, O.; Kane Dickson, V.; Kelly, B.T.; Owen, D.; Briggs, J.A.G.  
Deposited on : 2020-03-12  
Resolution : 10.20 Å(reported)  
Based on initial model : 1XA7

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.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

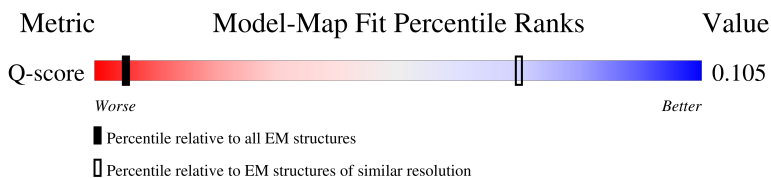
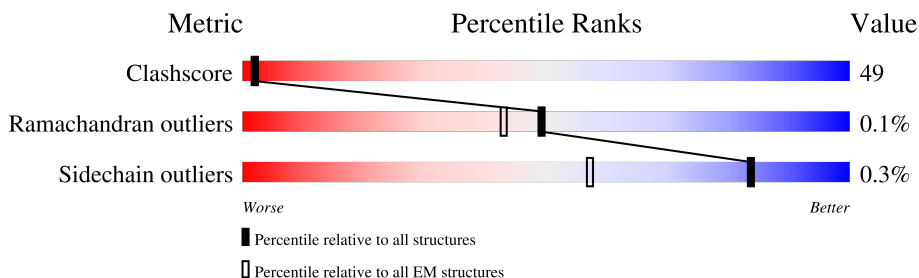
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.20 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<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 119 ( 9.70 - 10.70 )                                     |

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   | A     | 628    | <div> <div>11%</div> <div>27%</div> <div>70%</div> <div>.</div> </div>  |
| 2   | B     | 944    | <div> <div>6%</div> <div>17%</div> <div>44%</div> <div>39%</div> </div> |
| 3   | M     | 446    | <div> <div>28%</div> <div>20%</div> <div>75%</div> <div>..</div> </div> |
| 4   | S     | 142    | <div> <div>53%</div> <div>20%</div> <div>80%</div> <div>.</div> </div>  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14088 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 AP-2 complex subunit alpha-2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 613      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4837  | 3081 | 833 | 902 | 21 |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 8       | ASP      | GLU    | conflict       | UNP P18484 |
| A     | 272     | GLU      | -      | insertion      | UNP P18484 |
| A     | 622     | GLY      | PRO    | conflict       | UNP P18484 |
| A     | 624     | GLY      | -      | expression tag | UNP P18484 |
| A     | 625     | LEU      | -      | expression tag | UNP P18484 |
| A     | 626     | VAL      | -      | expression tag | UNP P18484 |
| A     | 627     | PRO      | -      | expression tag | UNP P18484 |
| A     | 628     | ARG      | -      | expression tag | UNP P18484 |

- Molecule 2 is a protein called AP-2 complex subunit beta.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 579      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4597  | 2928 | 763 | 881 | 25 |         |       |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| B     | -6      | MET      | -      | initiating methionine | UNP P63010 |
| B     | -5      | HIS      | -      | expression tag        | UNP P63010 |
| B     | -4      | HIS      | -      | expression tag        | UNP P63010 |
| B     | -3      | HIS      | -      | expression tag        | UNP P63010 |
| B     | -2      | HIS      | -      | expression tag        | UNP P63010 |
| B     | -1      | HIS      | -      | expression tag        | UNP P63010 |
| B     | 0       | HIS      | -      | expression tag        | UNP P63010 |

- Molecule 3 is a protein called AP-2 complex subunit mu.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | M     | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3454  | 2208 | 601 | 625 | 20 |         |       |

There are 11 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| M     | 237     | MET      | -      | insertion | UNP P84092 |
| M     | 238     | GLU      | -      | insertion | UNP P84092 |
| M     | 239     | GLN      | -      | insertion | UNP P84092 |
| M     | 240     | LYS      | -      | insertion | UNP P84092 |
| M     | 241     | LEU      | -      | insertion | UNP P84092 |
| M     | 242     | ILE      | -      | insertion | UNP P84092 |
| M     | 243     | SER      | -      | insertion | UNP P84092 |
| M     | 244     | GLU      | -      | insertion | UNP P84092 |
| M     | 245     | GLU      | -      | insertion | UNP P84092 |
| M     | 246     | ASP      | -      | insertion | UNP P84092 |
| M     | 247     | LEU      | -      | insertion | UNP P84092 |

- Molecule 4 is a protein called AP-2 complex subunit sigma.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | S     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1200  | 778 | 200 | 215 | 7 |         |       |

### 3 Residue-property plots

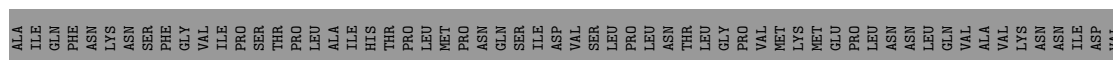
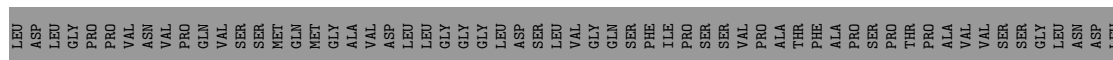
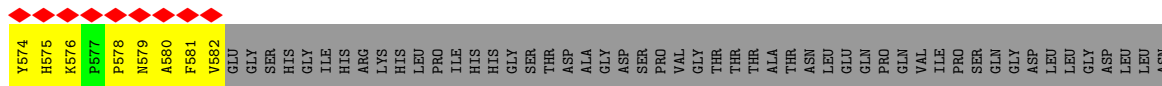
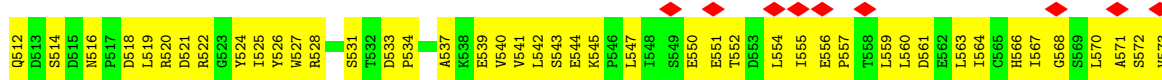
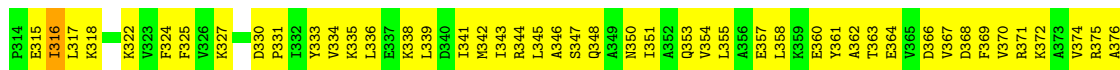
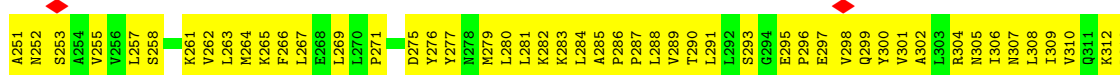
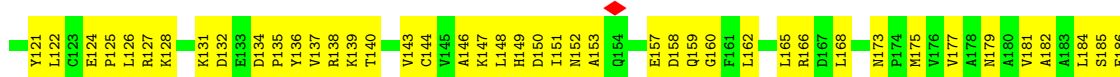
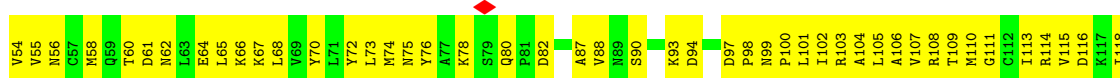
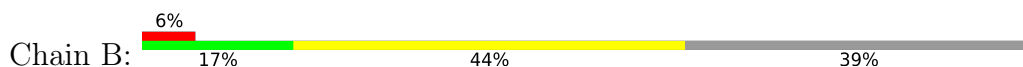
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: AP-2 complex subunit alpha-2



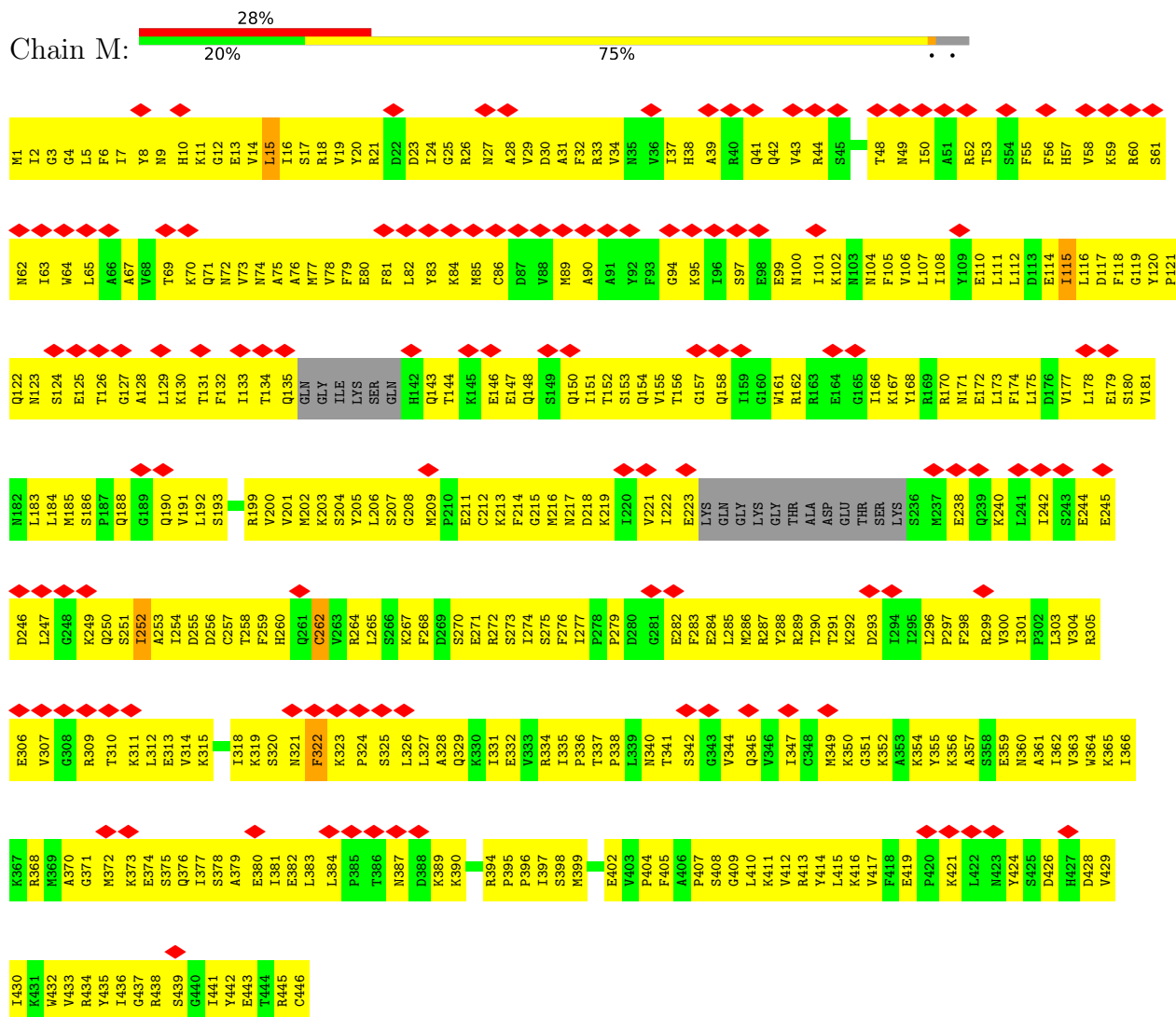


• Molecule 2: AP-2 complex subunit beta



|                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             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|                          | TYR THR ILE ALA SER LYS ARG ASN VAL GLU GLY GLN ASP MET THR LEU GLN SER LEU LYS THR GLY ILE TRP ILE ALA THR LYS LEU ARG ILE GLN PRO GLY ASN PRO ASN TYR THR LEU SER LEU CYS ARG ALA PRO GLU VAL SER GLN TYR ILE TYR VAL TYR ASP                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             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• Molecule 3: AP-2 complex subunit mu







## 4 Experimental information

| Property                             | Value                                                                                      | Source    |
|--------------------------------------|--------------------------------------------------------------------------------------------|-----------|
| EM reconstruction method             | SUBTOMOGRAM AVERAGING                                                                      | Depositor |
| Imposed symmetry                     | POINT, C1                                                                                  | Depositor |
| Number of subtomograms used          | 27630                                                                                      | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                                                                          | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction in no-vaCTF with by multiplication | Depositor |
| Microscope                           | FEI TITAN KRIOS                                                                            | Depositor |
| Voltage (kV)                         | 300                                                                                        | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 3.2                                                                                        | Depositor |
| Minimum defocus (nm)                 | 1500                                                                                       | Depositor |
| Maximum defocus (nm)                 | 6500                                                                                       | Depositor |
| Magnification                        | 81000                                                                                      | Depositor |
| Image detector                       | GATAN K2 QUANTUM (4k x 4k)                                                                 | Depositor |
| Maximum map value                    | 2.548                                                                                      | Depositor |
| Minimum map value                    | -2.356                                                                                     | Depositor |
| Average map value                    | -0.000                                                                                     | Depositor |
| Map value standard deviation         | 0.214                                                                                      | Depositor |
| Recommended contour level            | 0.3                                                                                        | Depositor |
| Map size ( $\text{\AA}$ )            | 214.43999, 214.43999, 214.43999                                                            | wwPDB     |
| Map dimensions                       | 120, 120, 120                                                                              | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                                                                           | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.787, 1.787, 1.787                                                                        | Depositor |

## 5 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |             | Bond angles |                |
|-----|-------|--------------|-------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$    |
| 1   | A     | 0.27         | 0/4922      | 0.59        | 1/6669 (0.0%)  |
| 2   | B     | 0.27         | 0/4669      | 0.63        | 0/6331         |
| 3   | M     | 0.28         | 0/3520      | 0.62        | 2/4735 (0.0%)  |
| 4   | S     | 0.27         | 0/1224      | 0.67        | 2/1650 (0.1%)  |
| All | All   | 0.27         | 0/14335     | 0.62        | 5/19385 (0.0%) |

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 |
|-----|-------|---------------------|---------------------|
| 2   | B     | 0                   | 2                   |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|--------|-------|------------------------|---------------------|
| 1   | A     | 437 | VAL  | N-CA-C | -7.54 | 106.55                 | 113.71              |
| 3   | M     | 262 | CYS  | N-CA-C | -6.59 | 106.45                 | 114.75              |
| 4   | S     | 71  | VAL  | CA-C-N | -6.44 | 113.78                 | 121.90              |
| 4   | S     | 71  | VAL  | C-N-CA | -6.44 | 113.78                 | 121.90              |
| 3   | M     | 15  | LEU  | N-CA-C | -5.64 | 106.76                 | 113.97              |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | B     | 191 | HIS  | Peptide |
| 2   | B     | 251 | ALA  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4837  | 0        | 4952     | 459     | 0            |
| 2   | B     | 4597  | 0        | 4715     | 449     | 0            |
| 3   | M     | 3454  | 0        | 3536     | 411     | 0            |
| 4   | S     | 1200  | 0        | 1195     | 132     | 0            |
| All | All   | 14088 | 0        | 14398    | 1397    | 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 49.

All (1397) 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:M:32:PHE:CE1   | 3:M:55:PHE:CZ    | 2.12                     | 1.35              |
| 3:M:32:PHE:CZ    | 3:M:55:PHE:CE1   | 2.17                     | 1.33              |
| 3:M:32:PHE:CZ    | 3:M:55:PHE:CZ    | 2.30                     | 1.18              |
| 3:M:32:PHE:CE1   | 3:M:55:PHE:CE1   | 2.43                     | 0.99              |
| 3:M:2:ILE:H      | 3:M:119:GLY:HA3  | 1.29                     | 0.95              |
| 1:A:273:ASP:H    | 1:A:277:ARG:HD2  | 1.33                     | 0.94              |
| 3:M:170:ARG:HH21 | 3:M:430:ILE:HG12 | 1.32                     | 0.94              |
| 2:B:54:VAL:O     | 2:B:58:MET:HB2   | 1.70                     | 0.91              |
| 3:M:312:LEU:HB2  | 3:M:383:LEU:HD11 | 1.54                     | 0.89              |
| 3:M:32:PHE:CE1   | 3:M:55:PHE:HZ    | 1.90                     | 0.89              |
| 3:M:32:PHE:CE2   | 3:M:55:PHE:HE1   | 1.93                     | 0.87              |
| 3:M:32:PHE:CZ    | 3:M:55:PHE:HE1   | 1.70                     | 0.87              |
| 2:B:108:ARG:NH2  | 2:B:140:THR:OG1  | 2.09                     | 0.86              |
| 1:A:271:PRO:HA   | 1:A:277:ARG:HD3  | 1.56                     | 0.86              |
| 3:M:322:PHE:H    | 3:M:372:MET:H    | 1.21                     | 0.85              |
| 1:A:518:SER:H    | 1:A:522:GLN:HE22 | 1.24                     | 0.83              |
| 3:M:33:ARG:O     | 3:M:37:ILE:HB    | 1.78                     | 0.83              |
| 3:M:268:PHE:O    | 3:M:272:ARG:N    | 2.11                     | 0.83              |
| 2:B:540:VAL:O    | 2:B:545:LYS:NZ   | 2.12                     | 0.82              |
| 2:B:350:ASN:HB3  | 2:B:353:GLN:HE21 | 1.43                     | 0.81              |
| 3:M:174:PHE:HA   | 3:M:432:TRP:HB2  | 1.63                     | 0.81              |
| 4:S:42:ARG:NH1   | 4:S:59:TYR:OH    | 2.15                     | 0.80              |
| 1:A:43:LYS:HE3   | 1:A:49:ALA:HA    | 1.63                     | 0.80              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:213:LYS:HB2  | 3:M:416:LYS:HB2  | 1.64                     | 0.79              |
| 3:M:32:PHE:CE2   | 3:M:55:PHE:CE1   | 2.70                     | 0.79              |
| 4:S:7:ILE:HD13   | 4:S:16:LEU:HD23  | 1.63                     | 0.79              |
| 4:S:13:LYS:HB2   | 4:S:15:ARG:HH21  | 1.47                     | 0.78              |
| 3:M:319:LYS:NZ   | 3:M:320:SER:O    | 2.15                     | 0.78              |
| 2:B:122:LEU:O    | 2:B:126:LEU:N    | 2.14                     | 0.78              |
| 1:A:83:LEU:O     | 1:A:91:LYS:NZ    | 2.17                     | 0.77              |
| 1:A:240:ALA:HA   | 1:A:253:PRO:HB3  | 1.65                     | 0.77              |
| 3:M:32:PHE:HE1   | 3:M:55:PHE:CZ    | 1.94                     | 0.77              |
| 2:B:496:PRO:O    | 2:B:500:GLN:NE2  | 2.18                     | 0.77              |
| 1:A:383:VAL:HB   | 1:A:387:GLN:HE22 | 1.50                     | 0.76              |
| 1:A:399:ARG:HG3  | 1:A:435:TYR:HB3  | 1.66                     | 0.76              |
| 3:M:260:HIS:NE2  | 3:M:284:GLU:OE1  | 2.18                     | 0.76              |
| 3:M:331:ILE:HB   | 3:M:366:ILE:HB   | 1.67                     | 0.76              |
| 1:A:285:GLU:HA   | 1:A:329:ARG:HH12 | 1.51                     | 0.76              |
| 3:M:323:LYS:HB3  | 3:M:326:LEU:HG   | 1.66                     | 0.76              |
| 1:A:257:LEU:HA   | 1:A:260:LYS:HD2  | 1.66                     | 0.76              |
| 4:S:3:ARG:HA     | 4:S:21:MET:HE1   | 1.67                     | 0.76              |
| 2:B:115:VAL:HG13 | 2:B:116:ASP:H    | 1.51                     | 0.76              |
| 3:M:153:SER:O    | 3:M:157:GLY:N    | 2.17                     | 0.75              |
| 3:M:370:ALA:HB3  | 3:M:373:LYS:HE2  | 1.66                     | 0.75              |
| 3:M:250:GLN:HE21 | 3:M:408:SER:HA   | 1.50                     | 0.75              |
| 2:B:124:GLU:HG3  | 2:B:128:LYS:HE3  | 1.69                     | 0.74              |
| 2:B:229:TYR:O    | 2:B:265:LYS:NZ   | 2.18                     | 0.74              |
| 3:M:323:LYS:NZ   | 3:M:325:SER:OG   | 2.20                     | 0.74              |
| 1:A:41:ARG:O     | 1:A:45:LYS:N     | 2.15                     | 0.73              |
| 1:A:520:LEU:HD13 | 1:A:555:VAL:HG23 | 1.70                     | 0.73              |
| 2:B:111:GLY:O    | 2:B:114:ARG:NH1  | 2.19                     | 0.73              |
| 4:S:102:ASP:O    | 4:S:106:ASN:ND2  | 2.21                     | 0.73              |
| 3:M:60:ARG:NH1   | 3:M:86:CYS:SG    | 2.61                     | 0.73              |
| 3:M:264:ARG:H    | 3:M:274:ILE:HB   | 1.53                     | 0.73              |
| 1:A:469:VAL:O    | 1:A:476:GLN:NE2  | 2.21                     | 0.73              |
| 1:A:527:HIS:HA   | 1:A:530:PHE:HB2  | 1.70                     | 0.73              |
| 3:M:180:SER:HA   | 3:M:438:ARG:HB3  | 1.70                     | 0.73              |
| 3:M:347:ILE:HB   | 3:M:378:SER:H    | 1.54                     | 0.73              |
| 2:B:361:TYR:HA   | 2:B:364:GLU:HG2  | 1.68                     | 0.73              |
| 3:M:32:PHE:CZ    | 3:M:55:PHE:HZ    | 1.97                     | 0.73              |
| 3:M:1:MET:N      | 3:M:118:PHE:O    | 2.21                     | 0.73              |
| 3:M:255:ASP:OD2  | 3:M:291:THR:N    | 2.22                     | 0.72              |
| 3:M:351:GLY:HA3  | 3:M:366:ILE:HG12 | 1.69                     | 0.72              |
| 1:A:62:LEU:HB3   | 1:A:72:ILE:HG13  | 1.71                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:214:CYS:O    | 2:B:219:GLN:NE2  | 2.22                     | 0.72              |
| 2:B:309:ILE:O    | 2:B:313:ARG:N    | 2.19                     | 0.72              |
| 1:A:198:ASP:O    | 1:A:232:ARG:NH2  | 2.21                     | 0.72              |
| 2:B:364:GLU:HB2  | 2:B:369:PHE:HZ   | 1.54                     | 0.72              |
| 1:A:66:PHE:HD1   | 1:A:71:ASP:HA    | 1.54                     | 0.72              |
| 1:A:398:ASP:H    | 1:A:401:ASN:HD21 | 1.37                     | 0.72              |
| 1:A:380:GLU:HG3  | 1:A:382:ASP:H    | 1.54                     | 0.72              |
| 2:B:516:ASN:OD1  | 2:B:519:LEU:N    | 2.23                     | 0.72              |
| 1:A:147:PHE:HB3  | 1:A:151:ILE:HG12 | 1.71                     | 0.72              |
| 2:B:543:SER:O    | 2:B:545:LYS:NZ   | 2.22                     | 0.72              |
| 1:A:43:LYS:HA    | 1:A:47:ASP:HB2   | 1.71                     | 0.72              |
| 2:B:457:GLU:HA   | 2:B:495:LYS:HE2  | 1.71                     | 0.72              |
| 3:M:342:SER:HB2  | 3:M:382:GLU:HB2  | 1.72                     | 0.72              |
| 3:M:349:MET:HG3  | 3:M:376:GLN:H    | 1.53                     | 0.72              |
| 2:B:98:PRO:O     | 2:B:103:ARG:NH2  | 2.23                     | 0.71              |
| 2:B:485:LEU:HB2  | 2:B:522:ARG:HH21 | 1.55                     | 0.71              |
| 4:S:42:ARG:O     | 4:S:61:ARG:NH1   | 2.21                     | 0.71              |
| 2:B:135:PRO:O    | 2:B:139:LYS:HB2  | 1.90                     | 0.71              |
| 2:B:404:ASN:O    | 2:B:408:GLN:N    | 2.23                     | 0.71              |
| 3:M:95:LYS:NZ    | 3:M:97:SER:OG    | 2.24                     | 0.71              |
| 1:A:77:MET:SD    | 1:A:77:MET:N     | 2.64                     | 0.71              |
| 1:A:384:SER:O    | 1:A:388:ARG:NH1  | 2.24                     | 0.71              |
| 2:B:210:ALA:O    | 2:B:214:CYS:N    | 2.24                     | 0.71              |
| 1:A:194:HIS:HA   | 1:A:197:ASN:HD22 | 1.56                     | 0.71              |
| 3:M:4:GLY:HA2    | 3:M:19:VAL:HA    | 1.72                     | 0.70              |
| 3:M:60:ARG:HH12  | 3:M:83:TYR:HA    | 1.55                     | 0.70              |
| 1:A:193:VAL:O    | 1:A:197:ASN:ND2  | 2.25                     | 0.70              |
| 2:B:149:HIS:HA   | 2:B:153:ALA:HB2  | 1.72                     | 0.70              |
| 3:M:304:VAL:HG22 | 3:M:314:VAL:HG13 | 1.72                     | 0.70              |
| 3:M:337:THR:HG22 | 3:M:362:ILE:HG13 | 1.73                     | 0.70              |
| 3:M:100:ASN:O    | 3:M:104:ASN:ND2  | 2.19                     | 0.70              |
| 1:A:365:ALA:O    | 1:A:368:THR:OG1  | 2.08                     | 0.70              |
| 2:B:28:GLU:HG2   | 2:B:29:LYS:H     | 1.57                     | 0.70              |
| 2:B:492:PHE:HD1  | 2:B:499:THR:HB   | 1.56                     | 0.70              |
| 2:B:6:TYR:HB3    | 3:M:102:LYS:HG2  | 1.74                     | 0.70              |
| 2:B:234:ASP:OD1  | 2:B:235:ARG:NH1  | 2.25                     | 0.70              |
| 2:B:476:GLU:O    | 2:B:481:GLN:NE2  | 2.25                     | 0.69              |
| 3:M:320:SER:N    | 3:M:373:LYS:O    | 2.23                     | 0.69              |
| 1:A:519:PRO:O    | 1:A:523:PHE:HB2  | 1.91                     | 0.69              |
| 1:A:550:ASN:HB3  | 1:A:599:LEU:HD22 | 1.73                     | 0.69              |
| 1:A:78:GLU:N     | 1:A:78:GLU:OE1   | 2.24                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:166:ARG:HH12 | 2:B:197:LEU:H    | 1.39                     | 0.69              |
| 3:M:2:ILE:N      | 3:M:119:GLY:HA3  | 2.07                     | 0.69              |
| 4:S:7:ILE:HB     | 4:S:16:LEU:HB3   | 1.72                     | 0.69              |
| 1:A:79:ALA:HA    | 1:A:82:LEU:HD12  | 1.72                     | 0.69              |
| 3:M:144:THR:H    | 3:M:147:GLU:HB3  | 1.57                     | 0.69              |
| 3:M:309:ARG:NH1  | 3:M:387:ASN:O    | 2.26                     | 0.69              |
| 4:S:51:GLU:HA    | 4:S:56:LYS:HA    | 1.73                     | 0.69              |
| 2:B:185:SER:O    | 2:B:188:SER:OG   | 2.10                     | 0.69              |
| 3:M:115:ILE:O    | 3:M:122:GLN:N    | 2.25                     | 0.69              |
| 1:A:59:VAL:HG21  | 1:A:82:LEU:HD11  | 1.74                     | 0.68              |
| 1:A:481:LYS:O    | 1:A:516:ARG:NH2  | 2.27                     | 0.68              |
| 2:B:304:ARG:HH21 | 2:B:574:TYR:HA   | 1.57                     | 0.68              |
| 1:A:335:GLY:O    | 1:A:339:GLN:NE2  | 2.27                     | 0.68              |
| 2:B:19:LYS:O     | 2:B:23:ASN:N     | 2.25                     | 0.68              |
| 2:B:50:LEU:O     | 2:B:54:VAL:N     | 2.21                     | 0.68              |
| 1:A:519:PRO:O    | 1:A:523:PHE:CB   | 2.41                     | 0.68              |
| 3:M:304:VAL:HG13 | 3:M:314:VAL:HG22 | 1.75                     | 0.68              |
| 1:A:21:ARG:O     | 1:A:24:LYS:NZ    | 2.23                     | 0.68              |
| 2:B:184:LEU:HB2  | 2:B:196:LEU:HD11 | 1.74                     | 0.68              |
| 2:B:34:VAL:HG11  | 2:B:68:LEU:HD22  | 1.74                     | 0.68              |
| 3:M:214:PHE:HA   | 3:M:415:LEU:HA   | 1.73                     | 0.68              |
| 1:A:448:ASN:HB3  | 1:A:451:ARG:HH21 | 1.58                     | 0.68              |
| 2:B:135:PRO:HB3  | 2:B:173:ASN:HD21 | 1.59                     | 0.68              |
| 2:B:249:SER:HA   | 2:B:252:ASN:HD21 | 1.58                     | 0.68              |
| 2:B:264:MET:HA   | 2:B:267:LEU:HB2  | 1.75                     | 0.68              |
| 3:M:170:ARG:HG3  | 3:M:172:GLU:HG3  | 1.76                     | 0.68              |
| 1:A:334:LEU:HD13 | 1:A:353:MET:HG3  | 1.75                     | 0.67              |
| 1:A:455:ASP:OD2  | 1:A:493:HIS:ND1  | 2.26                     | 0.67              |
| 3:M:90:ALA:O     | 3:M:94:GLY:N     | 2.26                     | 0.67              |
| 2:B:305:ASN:HD21 | 2:B:573:VAL:HG22 | 1.59                     | 0.67              |
| 4:S:119:LEU:HD22 | 4:S:124:ARG:HD2  | 1.75                     | 0.67              |
| 1:A:533:CYS:SG   | 1:A:538:ARG:NH1  | 2.68                     | 0.67              |
| 2:B:166:ARG:NH2  | 2:B:197:LEU:O    | 2.27                     | 0.67              |
| 2:B:401:THR:HG22 | 3:M:389:LYS:HD3  | 1.75                     | 0.67              |
| 1:A:19:ASP:OD1   | 1:A:20:ILE:N     | 2.28                     | 0.67              |
| 1:A:514:ASP:O    | 1:A:517:SER:OG   | 2.11                     | 0.67              |
| 2:B:32:GLU:HA    | 2:B:35:LYS:HD2   | 1.74                     | 0.67              |
| 2:B:43:VAL:HG23  | 2:B:45:LYS:HG2   | 1.76                     | 0.67              |
| 3:M:319:LYS:HD2  | 3:M:374:GLU:HB2  | 1.76                     | 0.67              |
| 3:M:267:LYS:NZ   | 3:M:271:GLU:OE2  | 2.28                     | 0.67              |
| 4:S:60:ARG:N     | 4:S:67:PHE:O     | 2.28                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:89:THR:N     | 4:S:142:GLU:OXT  | 2.19                     | 0.66              |
| 3:M:356:LYS:HG3  | 3:M:359:GLU:HB3  | 1.78                     | 0.66              |
| 3:M:114:GLU:O    | 3:M:122:GLN:NE2  | 2.20                     | 0.66              |
| 3:M:268:PHE:HA   | 3:M:273:SER:H    | 1.59                     | 0.66              |
| 4:S:18:LYS:NZ    | 4:S:19:TRP:O     | 2.29                     | 0.66              |
| 3:M:329:GLN:NE2  | 3:M:402:GLU:OE2  | 2.28                     | 0.66              |
| 4:S:106:ASN:OD1  | 4:S:109:LYS:NZ   | 2.27                     | 0.66              |
| 4:S:8:GLN:HG3    | 4:S:66:TYR:HB2   | 1.76                     | 0.66              |
| 3:M:48:THR:HB    | 3:M:55:PHE:HB2   | 1.76                     | 0.66              |
| 4:S:118:PHE:HA   | 4:S:124:ARG:H    | 1.61                     | 0.66              |
| 1:A:106:SER:OG   | 1:A:110:ARG:NH1  | 2.30                     | 0.66              |
| 2:B:245:THR:OG1  | 2:B:276:TYR:OH   | 2.13                     | 0.66              |
| 2:B:47:VAL:HG23  | 2:B:72:TYR:HE1   | 1.61                     | 0.65              |
| 3:M:335:ILE:O    | 3:M:362:ILE:N    | 2.25                     | 0.65              |
| 1:A:503:ILE:O    | 1:A:507:PHE:N    | 2.29                     | 0.65              |
| 3:M:212:CYS:HB3  | 3:M:417:VAL:HG12 | 1.78                     | 0.65              |
| 3:M:443:GLU:OE1  | 3:M:443:GLU:N    | 2.29                     | 0.65              |
| 1:A:533:CYS:O    | 1:A:538:ARG:NH2  | 2.30                     | 0.65              |
| 2:B:234:ASP:O    | 2:B:238:GLN:N    | 2.28                     | 0.65              |
| 1:A:119:ASP:HB3  | 1:A:127:PHE:HB3  | 1.78                     | 0.65              |
| 2:B:492:PHE:CD1  | 2:B:499:THR:HB   | 2.31                     | 0.65              |
| 3:M:350:LYS:NZ   | 3:M:368:ARG:O    | 2.29                     | 0.65              |
| 4:S:116:GLU:O    | 4:S:124:ARG:NH1  | 2.27                     | 0.65              |
| 3:M:9:ASN:ND2    | 3:M:13:GLU:O     | 2.30                     | 0.65              |
| 4:S:5:ILE:N      | 4:S:18:LYS:O     | 2.25                     | 0.65              |
| 4:S:103:LEU:O    | 4:S:107:PHE:N    | 2.29                     | 0.65              |
| 2:B:37:VAL:HG13  | 2:B:47:VAL:HG21  | 1.78                     | 0.65              |
| 3:M:97:SER:H     | 3:M:100:ASN:HB2  | 1.61                     | 0.65              |
| 2:B:134:ASP:OD2  | 2:B:137:VAL:N    | 2.28                     | 0.64              |
| 3:M:161:TRP:HB2  | 3:M:279:PRO:HB3  | 1.77                     | 0.64              |
| 1:A:432:ALA:O    | 1:A:436:ALA:N    | 2.29                     | 0.64              |
| 2:B:450:TRP:O    | 2:B:454:GLU:HG2  | 1.97                     | 0.64              |
| 3:M:311:LYS:HE3  | 3:M:382:GLU:HG2  | 1.78                     | 0.64              |
| 1:A:316:LEU:O    | 1:A:320:HIS:NE2  | 2.29                     | 0.64              |
| 1:A:431:LEU:HA   | 1:A:434:LYS:HD2  | 1.78                     | 0.64              |
| 2:B:557:PRO:O    | 2:B:561:ASP:N    | 2.24                     | 0.64              |
| 4:S:3:ARG:HB2    | 4:S:70:CYS:HB3   | 1.79                     | 0.64              |
| 1:A:364:GLU:N    | 1:A:364:GLU:OE1  | 2.28                     | 0.64              |
| 2:B:364:GLU:HB2  | 2:B:369:PHE:CZ   | 2.33                     | 0.64              |
| 1:A:162:ASP:HA   | 1:A:203:VAL:HG13 | 1.79                     | 0.64              |
| 2:B:343:ILE:HG13 | 2:B:376:ALA:HB1  | 1.80                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:124:GLU:OE2  | 2:B:131:LYS:NZ   | 2.31                     | 0.64              |
| 3:M:7:ILE:H      | 3:M:16:ILE:HG22  | 1.63                     | 0.64              |
| 1:A:205:THR:HA   | 1:A:257:LEU:HD13 | 1.79                     | 0.64              |
| 3:M:356:LYS:HB3  | 3:M:361:ALA:HB3  | 1.79                     | 0.64              |
| 1:A:173:LEU:HG   | 1:A:177:ARG:HH21 | 1.62                     | 0.64              |
| 2:B:41:MET:SD    | 2:B:75:ASN:ND2   | 2.71                     | 0.64              |
| 2:B:116:ASP:N    | 2:B:116:ASP:OD1  | 2.31                     | 0.63              |
| 2:B:250:HIS:CE1  | 3:M:265:LEU:HD12 | 2.33                     | 0.63              |
| 3:M:337:THR:N    | 3:M:360:ASN:O    | 2.30                     | 0.63              |
| 1:A:534:SER:O    | 1:A:537:THR:OG1  | 2.12                     | 0.63              |
| 1:A:585:ARG:NH1  | 2:B:543:SER:OG   | 2.30                     | 0.63              |
| 1:A:615:LYS:O    | 1:A:618:LYS:HG2  | 1.99                     | 0.63              |
| 2:B:501:GLU:OE1  | 2:B:501:GLU:N    | 2.30                     | 0.63              |
| 3:M:161:TRP:NE1  | 3:M:277:ILE:O    | 2.32                     | 0.63              |
| 1:A:285:GLU:OE2  | 1:A:329:ARG:NH1  | 2.31                     | 0.63              |
| 1:A:502:TYR:O    | 1:A:547:LYS:NZ   | 2.32                     | 0.63              |
| 1:A:564:ARG:HE   | 1:A:588:THR:HG1  | 1.44                     | 0.63              |
| 4:S:7:ILE:HG13   | 4:S:67:PHE:HA    | 1.80                     | 0.63              |
| 4:S:10:ARG:N     | 4:S:64:GLY:O     | 2.32                     | 0.63              |
| 4:S:93:GLU:O     | 4:S:96:HIS:ND1   | 2.31                     | 0.63              |
| 1:A:339:GLN:O    | 1:A:341:ARG:NH1  | 2.31                     | 0.63              |
| 3:M:74:ASN:OD1   | 3:M:77:MET:N     | 2.24                     | 0.63              |
| 3:M:405:PHE:N    | 3:M:437:GLY:H    | 1.96                     | 0.63              |
| 1:A:137:ASN:OD1  | 1:A:138:VAL:N    | 2.32                     | 0.62              |
| 3:M:18:ARG:HG3   | 3:M:20:TYR:CE2   | 2.34                     | 0.62              |
| 2:B:11:LYS:HB3   | 2:B:12:LYS:HZ3   | 1.64                     | 0.62              |
| 3:M:336:PRO:O    | 3:M:445:ARG:NH1  | 2.32                     | 0.62              |
| 4:S:134:GLN:HG3  | 4:S:137:MET:HE2  | 1.81                     | 0.62              |
| 1:A:518:SER:N    | 1:A:522:GLN:HE22 | 1.96                     | 0.62              |
| 2:B:416:ASP:HA   | 2:B:419:ARG:HD3  | 1.80                     | 0.62              |
| 2:B:453:GLY:O    | 2:B:494:LYS:NZ   | 2.28                     | 0.62              |
| 2:B:212:ASN:O    | 3:M:264:ARG:NH1  | 2.28                     | 0.62              |
| 1:A:382:ASP:O    | 1:A:386:ARG:NH1  | 2.32                     | 0.62              |
| 1:A:343:THR:HG23 | 4:S:45:LYS:HE3   | 1.81                     | 0.62              |
| 1:A:572:ALA:O    | 2:B:419:ARG:NH2  | 2.24                     | 0.62              |
| 3:M:59:LYS:HA    | 3:M:64:TRP:HA    | 1.82                     | 0.62              |
| 3:M:170:ARG:NH1  | 3:M:171:ASN:H    | 1.98                     | 0.62              |
| 4:S:84:ILE:O     | 4:S:88:VAL:HG23  | 2.00                     | 0.62              |
| 3:M:306:GLU:OE1  | 3:M:309:ARG:NE   | 2.33                     | 0.62              |
| 4:S:7:ILE:O      | 4:S:15:ARG:N     | 2.33                     | 0.62              |
| 1:A:357:ALA:HB2  | 1:A:392:LEU:HD12 | 1.81                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:465:LEU:O    | 2:B:468:SER:OG   | 2.13                     | 0.62              |
| 1:A:87:ARG:N     | 1:A:90:GLU:OE1   | 2.32                     | 0.62              |
| 2:B:74:MET:HE3   | 2:B:109:THR:HG23 | 1.82                     | 0.62              |
| 2:B:211:LEU:HD21 | 2:B:247:ARG:HD2  | 1.80                     | 0.62              |
| 2:B:333:TYR:HA   | 2:B:336:LEU:HD12 | 1.80                     | 0.62              |
| 2:B:563:LEU:HD13 | 2:B:572:SER:HA   | 1.81                     | 0.62              |
| 3:M:130:LYS:H    | 3:M:162:ARG:HH22 | 1.47                     | 0.62              |
| 1:A:96:LEU:O     | 1:A:100:VAL:N    | 2.28                     | 0.62              |
| 3:M:221:VAL:HG23 | 3:M:247:LEU:HA   | 1.82                     | 0.62              |
| 1:A:549:VAL:HG13 | 1:A:556:LYS:HB2  | 1.82                     | 0.61              |
| 2:B:524:TYR:HA   | 2:B:527:TRP:NE1  | 2.15                     | 0.61              |
| 3:M:8:TYR:HE1    | 3:M:33:ARG:HH21  | 1.48                     | 0.61              |
| 1:A:498:LYS:HD3  | 1:A:537:THR:HG22 | 1.82                     | 0.61              |
| 2:B:90:SER:HA    | 2:B:93:LYS:HD2   | 1.82                     | 0.61              |
| 3:M:69:THR:OG1   | 3:M:71:GLN:OE1   | 2.18                     | 0.61              |
| 1:A:326:LEU:HD13 | 1:A:329:ARG:HD3  | 1.82                     | 0.61              |
| 2:B:99:ASN:ND2   | 3:M:143:GLN:OE1  | 2.34                     | 0.61              |
| 1:A:571:ASN:OD1  | 1:A:577:GLN:NE2  | 2.33                     | 0.61              |
| 2:B:327:LYS:N    | 2:B:330:ASP:OD2  | 2.33                     | 0.61              |
| 1:A:585:ARG:HD3  | 2:B:540:VAL:HG13 | 1.83                     | 0.61              |
| 3:M:200:VAL:N    | 3:M:284:GLU:OE2  | 2.34                     | 0.61              |
| 4:S:42:ARG:NH1   | 4:S:46:HIS:HB3   | 2.16                     | 0.61              |
| 1:A:462:TRP:HA   | 1:A:465:VAL:HG12 | 1.81                     | 0.61              |
| 2:B:344:ARG:HH12 | 2:B:552:THR:HB   | 1.64                     | 0.61              |
| 2:B:53:ASP:HA    | 2:B:56:ASN:HD21  | 1.65                     | 0.61              |
| 2:B:263:LEU:O    | 2:B:267:LEU:N    | 2.34                     | 0.61              |
| 2:B:398:LEU:HA   | 2:B:401:THR:HG23 | 1.83                     | 0.61              |
| 2:B:412:VAL:HG13 | 2:B:415:ARG:HH21 | 1.66                     | 0.61              |
| 2:B:481:GLN:OE1  | 2:B:481:GLN:N    | 2.33                     | 0.61              |
| 1:A:347:TYR:OH   | 1:A:388:ARG:NH2  | 2.34                     | 0.61              |
| 2:B:249:SER:HB3  | 3:M:259:PHE:HD2  | 1.65                     | 0.61              |
| 2:B:362:ALA:O    | 3:M:390:LYS:NZ   | 2.33                     | 0.61              |
| 3:M:223:GLU:HG2  | 3:M:246:ASP:HA   | 1.83                     | 0.61              |
| 1:A:299:LYS:HB2  | 1:A:302:HIS:CD2  | 2.35                     | 0.61              |
| 1:A:468:ILE:O    | 1:A:472:ARG:N    | 2.34                     | 0.61              |
| 2:B:348:GLN:N    | 2:B:348:GLN:OE1  | 2.32                     | 0.61              |
| 2:B:493:LEU:HB3  | 2:B:542:LEU:HD11 | 1.82                     | 0.61              |
| 3:M:58:VAL:O     | 3:M:65:LEU:N     | 2.34                     | 0.61              |
| 3:M:126:THR:OG1  | 3:M:162:ARG:NH2  | 2.30                     | 0.61              |
| 4:S:58:ILE:N     | 4:S:69:ILE:O     | 2.34                     | 0.60              |
| 1:A:460:GLU:N    | 1:A:460:GLU:OE1  | 2.32                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:573:ASP:OD2  | 1:A:576:LEU:N    | 2.27                     | 0.60              |
| 2:B:267:LEU:O    | 2:B:313:ARG:NH2  | 2.34                     | 0.60              |
| 1:A:25:SER:O     | 1:A:28:ALA:N     | 2.33                     | 0.60              |
| 1:A:567:SER:OG   | 1:A:568:GLN:OE1  | 2.19                     | 0.60              |
| 3:M:48:THR:O     | 3:M:55:PHE:N     | 2.35                     | 0.60              |
| 4:S:52:PHE:CE1   | 4:S:57:ILE:HG23  | 2.36                     | 0.60              |
| 1:A:99:SER:OG    | 1:A:134:CYS:SG   | 2.59                     | 0.60              |
| 3:M:213:LYS:N    | 3:M:416:LYS:O    | 2.31                     | 0.60              |
| 2:B:398:LEU:O    | 2:B:401:THR:OG1  | 2.12                     | 0.60              |
| 2:B:407:VAL:O    | 2:B:411:ILE:HG13 | 2.01                     | 0.60              |
| 3:M:199:ARG:HA   | 3:M:287:ARG:HA   | 1.81                     | 0.60              |
| 4:S:10:ARG:HB2   | 4:S:64:GLY:HA2   | 1.82                     | 0.60              |
| 2:B:411:ILE:HG22 | 2:B:447:ALA:HB3  | 1.83                     | 0.60              |
| 1:A:27:GLU:HG2   | 1:A:31:LYS:HE2   | 1.81                     | 0.60              |
| 1:A:548:PHE:O    | 1:A:552:PHE:N    | 2.34                     | 0.60              |
| 3:M:126:THR:O    | 3:M:162:ARG:NE   | 2.34                     | 0.60              |
| 3:M:238:GLU:OE2  | 3:M:240:LYS:N    | 2.34                     | 0.60              |
| 1:A:124:ASN:HD21 | 1:A:127:PHE:H    | 1.48                     | 0.59              |
| 1:A:430:ILE:HG12 | 1:A:434:LYS:HE3  | 1.84                     | 0.59              |
| 2:B:199:LEU:HD12 | 2:B:229:TYR:HD1  | 1.67                     | 0.59              |
| 3:M:161:TRP:HE1  | 3:M:277:ILE:HG22 | 1.66                     | 0.59              |
| 1:A:360:GLU:HA   | 1:A:363:HIS:CD2  | 2.37                     | 0.59              |
| 2:B:207:LEU:HD13 | 2:B:222:ILE:HG23 | 1.84                     | 0.59              |
| 2:B:556:GLU:HB3  | 2:B:559:LEU:HB3  | 1.85                     | 0.59              |
| 1:A:159:ASP:HA   | 1:A:165:LYS:HE3  | 1.83                     | 0.59              |
| 1:A:444:ASP:OD1  | 1:A:478:TYR:OH   | 2.10                     | 0.59              |
| 2:B:487:ALA:HA   | 2:B:490:LYS:HE2  | 1.84                     | 0.59              |
| 2:B:32:GLU:O     | 2:B:36:LYS:HG3   | 2.02                     | 0.59              |
| 2:B:105:LEU:HD12 | 2:B:108:ARG:HD2  | 1.84                     | 0.59              |
| 1:A:525:LEU:O    | 1:A:528:SER:OG   | 2.17                     | 0.59              |
| 3:M:217:ASN:ND2  | 3:M:244:GLU:OE2  | 2.31                     | 0.59              |
| 3:M:268:PHE:HA   | 3:M:273:SER:N    | 2.17                     | 0.59              |
| 2:B:412:VAL:HG21 | 2:B:443:ASP:HB2  | 1.83                     | 0.59              |
| 2:B:415:ARG:NH2  | 2:B:443:ASP:O    | 2.36                     | 0.59              |
| 1:A:32:ARG:HD2   | 1:A:35:LYS:HE3   | 1.84                     | 0.59              |
| 2:B:7:PHE:HZ     | 2:B:32:GLU:HG3   | 1.68                     | 0.59              |
| 2:B:556:GLU:OE1  | 2:B:559:LEU:N    | 2.25                     | 0.59              |
| 3:M:329:GLN:HA   | 3:M:368:ARG:HA   | 1.85                     | 0.59              |
| 3:M:336:PRO:HA   | 3:M:361:ALA:HA   | 1.83                     | 0.59              |
| 4:S:47:THR:HG23  | 4:S:49:PHE:H     | 1.67                     | 0.59              |
| 2:B:139:LYS:O    | 2:B:179:ASN:ND2  | 2.36                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:308:LEU:HD21 | 2:B:575:HIS:HD1  | 1.67                     | 0.58              |
| 2:B:312:LYS:HZ3  | 2:B:564:ILE:HD12 | 1.68                     | 0.58              |
| 3:M:95:LYS:NZ    | 3:M:100:ASN:OD1  | 2.32                     | 0.58              |
| 3:M:335:ILE:HB   | 3:M:362:ILE:HB   | 1.84                     | 0.58              |
| 2:B:213:GLU:HA   | 3:M:264:ARG:HH22 | 1.68                     | 0.58              |
| 1:A:390:VAL:O    | 1:A:394:TYR:HB2  | 2.03                     | 0.58              |
| 1:A:154:ILE:O    | 1:A:165:LYS:NZ   | 2.36                     | 0.58              |
| 1:A:564:ARG:HH21 | 1:A:588:THR:HA   | 1.68                     | 0.58              |
| 3:M:331:ILE:N    | 3:M:366:ILE:O    | 2.35                     | 0.58              |
| 1:A:105:ASN:HD22 | 1:A:108:LEU:HD12 | 1.69                     | 0.58              |
| 1:A:542:LEU:HB3  | 1:A:583:TYR:CE2  | 2.38                     | 0.58              |
| 2:B:70:TYR:OH    | 2:B:94:ASP:OD2   | 2.21                     | 0.58              |
| 2:B:110:MET:O    | 2:B:113:ILE:HG12 | 2.01                     | 0.58              |
| 3:M:117:ASP:N    | 3:M:122:GLN:HE22 | 2.00                     | 0.58              |
| 1:A:212:THR:HG22 | 1:A:216:GLN:HE21 | 1.67                     | 0.58              |
| 1:A:354:CYS:HA   | 1:A:357:ALA:HB2  | 1.85                     | 0.58              |
| 3:M:298:PHE:HD2  | 3:M:442:TYR:CZ   | 2.21                     | 0.58              |
| 1:A:360:GLU:HA   | 1:A:363:HIS:HD2  | 1.68                     | 0.58              |
| 2:B:524:TYR:HB3  | 2:B:528:ARG:CZ   | 2.34                     | 0.58              |
| 1:A:542:LEU:HB3  | 1:A:583:TYR:HE2  | 1.69                     | 0.58              |
| 1:A:273:ASP:OD1  | 1:A:276:VAL:N    | 2.37                     | 0.57              |
| 1:A:459:GLU:HA   | 1:A:462:TRP:NE1  | 2.19                     | 0.57              |
| 1:A:608:ARG:NH2  | 2:B:512:GLN:O    | 2.37                     | 0.57              |
| 2:B:175:MET:SD   | 2:B:175:MET:N    | 2.77                     | 0.57              |
| 1:A:314:ILE:O    | 1:A:318:ILE:N    | 2.35                     | 0.57              |
| 2:B:88:VAL:HG12  | 2:B:118:ILE:HD13 | 1.86                     | 0.57              |
| 2:B:457:GLU:HB3  | 2:B:494:LYS:HD3  | 1.84                     | 0.57              |
| 2:B:486:THR:OG1  | 2:B:490:LYS:NZ   | 2.36                     | 0.57              |
| 1:A:205:THR:HG22 | 1:A:257:LEU:HB2  | 1.85                     | 0.57              |
| 1:A:394:TYR:CZ   | 1:A:431:LEU:HG   | 2.39                     | 0.57              |
| 4:S:36:HIS:O     | 4:S:40:THR:HG23  | 2.04                     | 0.57              |
| 1:A:235:ARG:NH1  | 1:A:238:THR:OG1  | 2.37                     | 0.57              |
| 2:B:386:GLN:O    | 2:B:390:ARG:NH1  | 2.38                     | 0.57              |
| 3:M:214:PHE:HE2  | 3:M:216:MET:HB2  | 1.69                     | 0.57              |
| 1:A:303:SER:O    | 1:A:307:ASN:ND2  | 2.38                     | 0.57              |
| 1:A:353:MET:HE2  | 1:A:366:VAL:HG13 | 1.86                     | 0.57              |
| 2:B:249:SER:HA   | 2:B:252:ASN:ND2  | 2.20                     | 0.57              |
| 1:A:606:PRO:HB2  | 1:A:608:ARG:HH12 | 1.68                     | 0.57              |
| 2:B:240:ILE:O    | 2:B:244:VAL:HG23 | 2.04                     | 0.57              |
| 3:M:186:SER:HB3  | 3:M:192:LEU:HD21 | 1.85                     | 0.57              |
| 3:M:116:LEU:HD12 | 3:M:121:PRO:HB3  | 1.87                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:292:LYS:NZ   | 3:M:293:ASP:OD1  | 2.29                     | 0.57              |
| 2:B:396:LEU:HA   | 2:B:399:ILE:HD12 | 1.86                     | 0.57              |
| 3:M:174:PHE:HD2  | 3:M:434:ARG:HH12 | 1.53                     | 0.57              |
| 3:M:397:ILE:H    | 3:M:445:ARG:HB2  | 1.69                     | 0.57              |
| 4:S:3:ARG:N      | 4:S:70:CYS:O     | 2.34                     | 0.57              |
| 1:A:526:LEU:O    | 1:A:530:PHE:N    | 2.38                     | 0.57              |
| 2:B:296:PRO:O    | 2:B:300:TYR:HB2  | 2.05                     | 0.57              |
| 2:B:368:ASP:O    | 2:B:372:LYS:HG2  | 2.05                     | 0.57              |
| 3:M:222:ILE:HG12 | 3:M:249:LYS:N    | 2.20                     | 0.57              |
| 3:M:405:PHE:H    | 3:M:437:GLY:H    | 1.52                     | 0.57              |
| 1:A:38:ALA:O     | 1:A:42:SER:OG    | 2.17                     | 0.56              |
| 1:A:341:ARG:O    | 1:A:346:ARG:NH2  | 2.38                     | 0.56              |
| 1:A:431:LEU:HD23 | 1:A:434:LYS:HD2  | 1.87                     | 0.56              |
| 2:B:192:PRO:HD2  | 2:B:195:ASN:HD21 | 1.70                     | 0.56              |
| 2:B:375:ARG:HD2  | 2:B:413:VAL:HG22 | 1.86                     | 0.56              |
| 3:M:188:GLN:HG3  | 3:M:303:LEU:HD11 | 1.85                     | 0.56              |
| 1:A:136:ALA:O    | 1:A:174:ARG:NE   | 2.39                     | 0.56              |
| 2:B:146:ALA:HA   | 2:B:149:HIS:CD2  | 2.41                     | 0.56              |
| 2:B:463:ASP:OD1  | 2:B:463:ASP:N    | 2.35                     | 0.56              |
| 3:M:337:THR:H    | 3:M:361:ALA:HA   | 1.69                     | 0.56              |
| 2:B:82:ASP:OD1   | 2:B:82:ASP:N     | 2.38                     | 0.56              |
| 2:B:28:GLU:HA    | 2:B:31:LYS:HE2   | 1.88                     | 0.56              |
| 2:B:118:ILE:HD12 | 2:B:121:TYR:HB2  | 1.86                     | 0.56              |
| 2:B:481:GLN:O    | 2:B:485:LEU:HG   | 2.04                     | 0.56              |
| 2:B:501:GLU:O    | 2:B:504:GLN:HG2  | 2.05                     | 0.56              |
| 3:M:56:PHE:HB2   | 3:M:67:ALA:HB3   | 1.87                     | 0.56              |
| 2:B:366:ASP:HB3  | 2:B:369:PHE:CD1  | 2.40                     | 0.56              |
| 3:M:78:VAL:O     | 3:M:82:LEU:HG    | 2.05                     | 0.56              |
| 2:B:33:ALA:O     | 2:B:37:VAL:HG23  | 2.05                     | 0.56              |
| 2:B:302:ALA:O    | 2:B:306:ILE:HG12 | 2.05                     | 0.56              |
| 3:M:394:ARG:HB3  | 3:M:446:CYS:HB3  | 1.86                     | 0.56              |
| 4:S:91:LEU:HD22  | 4:S:95:PHE:HE2   | 1.69                     | 0.56              |
| 1:A:34:ASN:HA    | 1:A:37:LEU:HD12  | 1.87                     | 0.56              |
| 1:A:402:ALA:HA   | 1:A:405:ILE:HB   | 1.87                     | 0.56              |
| 1:A:471:ASN:HA   | 1:A:604:PRO:HB3  | 1.87                     | 0.56              |
| 2:B:18:LEU:HD21  | 2:B:50:LEU:HD11  | 1.87                     | 0.56              |
| 1:A:214:LEU:O    | 1:A:218:ASN:N    | 2.38                     | 0.56              |
| 2:B:127:ARG:NH2  | 2:B:157:GLU:OE1  | 2.38                     | 0.56              |
| 2:B:279:MET:HA   | 2:B:282:LYS:HE3  | 1.87                     | 0.56              |
| 1:A:560:GLN:O    | 1:A:564:ARG:HD3  | 2.06                     | 0.56              |
| 2:B:443:ASP:OD1  | 2:B:444:ALA:N    | 2.39                     | 0.56              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:99:SER:HB3  | 1:A:137:ASN:ND2  | 2.20                     | 0.56              |
| 1:A:106:SER:O   | 1:A:110:ARG:N    | 2.34                     | 0.56              |
| 1:A:176:TYR:HD1 | 1:A:183:VAL:HG21 | 1.70                     | 0.56              |
| 2:B:21:GLU:OE2  | 2:B:36:LYS:NZ    | 2.39                     | 0.56              |
| 1:A:176:TYR:OH  | 1:A:217:LYS:HG3  | 2.06                     | 0.55              |
| 1:A:380:GLU:C   | 1:A:381:ARG:HD2  | 2.31                     | 0.55              |
| 1:A:465:VAL:HA  | 1:A:468:ILE:HD12 | 1.87                     | 0.55              |
| 2:B:11:LYS:HG2  | 2:B:12:LYS:HG3   | 1.87                     | 0.55              |
| 2:B:491:LEU:O   | 2:B:495:LYS:N    | 2.27                     | 0.55              |
| 3:M:170:ARG:NH2 | 3:M:430:ILE:HG12 | 2.13                     | 0.55              |
| 4:S:100:GLU:O   | 4:S:104:VAL:HG23 | 2.06                     | 0.55              |
| 2:B:21:GLU:HB2  | 2:B:29:LYS:HB3   | 1.88                     | 0.55              |
| 3:M:209:MET:HB2 | 3:M:421:LYS:HZ2  | 1.71                     | 0.55              |
| 3:M:209:MET:HB2 | 3:M:421:LYS:NZ   | 2.21                     | 0.55              |
| 4:S:39:VAL:HG13 | 4:S:61:ARG:HD3   | 1.88                     | 0.55              |
| 1:A:273:ASP:OD1 | 1:A:277:ARG:N    | 2.38                     | 0.55              |
| 1:A:337:PHE:HA  | 1:A:340:HIS:NE2  | 2.21                     | 0.55              |
| 1:A:602:MET:HE3 | 1:A:603:PRO:HD2  | 1.87                     | 0.55              |
| 2:B:360:GLU:O   | 2:B:363:THR:OG1  | 2.18                     | 0.55              |
| 3:M:172:GLU:HG2 | 3:M:430:ILE:HB   | 1.88                     | 0.55              |
| 3:M:186:SER:N   | 3:M:190:GLN:O    | 2.32                     | 0.55              |
| 4:S:135:LEU:O   | 4:S:139:GLN:N    | 2.40                     | 0.55              |
| 1:A:63:LEU:O    | 1:A:67:LEU:HG    | 2.07                     | 0.55              |
| 2:B:418:PHE:HB3 | 2:B:450:TRP:HH2  | 1.71                     | 0.55              |
| 1:A:341:ARG:H   | 1:A:341:ARG:HD2  | 1.70                     | 0.55              |
| 1:A:564:ARG:NE  | 1:A:588:THR:OG1  | 2.25                     | 0.55              |
| 2:B:361:TYR:HB3 | 2:B:369:PHE:HE2  | 1.71                     | 0.55              |
| 3:M:216:MET:O   | 3:M:413:ARG:NH2  | 2.40                     | 0.55              |
| 4:S:32:ILE:O    | 4:S:36:HIS:ND1   | 2.40                     | 0.55              |
| 4:S:116:GLU:CD  | 4:S:124:ARG:HH12 | 2.14                     | 0.55              |
| 1:A:147:PHE:HA  | 1:A:150:GLU:HB3  | 1.88                     | 0.55              |
| 1:A:341:ARG:HD2 | 1:A:341:ARG:N    | 2.20                     | 0.55              |
| 1:A:460:GLU:HA  | 1:A:463:TYR:HB2  | 1.89                     | 0.55              |
| 2:B:7:PHE:HD2   | 2:B:36:LYS:HG2   | 1.69                     | 0.55              |
| 2:B:324:PHE:HA  | 2:B:338:LYS:HG2  | 1.88                     | 0.55              |
| 3:M:10:HIS:NE2  | 3:M:62:ASN:HB2   | 2.21                     | 0.55              |
| 1:A:112:ILE:O   | 1:A:116:ILE:HG12 | 2.06                     | 0.55              |
| 1:A:560:GLN:O   | 1:A:563:LEU:HD23 | 2.06                     | 0.55              |
| 2:B:213:GLU:O   | 3:M:158:GLN:NE2  | 2.40                     | 0.55              |
| 2:B:421:TYR:HB3 | 2:B:424:LYS:HD2  | 1.89                     | 0.55              |
| 3:M:129:LEU:HA  | 3:M:132:PHE:CE1  | 2.42                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:151:ILE:O    | 3:M:154:GLN:HG2  | 2.07                     | 0.55              |
| 3:M:184:LEU:H    | 3:M:193:SER:HB3  | 1.72                     | 0.55              |
| 4:S:118:PHE:HD1  | 4:S:123:ILE:HA   | 1.71                     | 0.55              |
| 1:A:75:GLY:O     | 1:A:79:ALA:N     | 2.39                     | 0.55              |
| 2:B:301:VAL:HG13 | 2:B:573:VAL:HG11 | 1.88                     | 0.55              |
| 3:M:178:LEU:HA   | 3:M:436:ILE:HG13 | 1.88                     | 0.55              |
| 3:M:396:PRO:HA   | 3:M:445:ARG:N    | 2.22                     | 0.55              |
| 4:S:59:TYR:HA    | 4:S:68:CYS:HA    | 1.89                     | 0.55              |
| 4:S:124:ARG:NH1  | 4:S:125:GLU:OE1  | 2.39                     | 0.55              |
| 1:A:163:SER:HA   | 1:A:166:GLN:NE2  | 2.22                     | 0.55              |
| 1:A:398:ASP:H    | 1:A:401:ASN:ND2  | 2.05                     | 0.55              |
| 2:B:202:GLN:O    | 2:B:206:LYS:HE3  | 2.07                     | 0.55              |
| 2:B:386:GLN:CD   | 2:B:386:GLN:H    | 2.15                     | 0.55              |
| 3:M:49:ASN:HA    | 3:M:53:THR:O     | 2.06                     | 0.55              |
| 4:S:1:MET:N      | 4:S:3:ARG:HH21   | 2.05                     | 0.55              |
| 1:A:459:GLU:HA   | 1:A:462:TRP:CE2  | 2.42                     | 0.55              |
| 2:B:307:ASN:OD1  | 2:B:308:LEU:N    | 2.39                     | 0.55              |
| 2:B:357:GLU:O    | 2:B:360:GLU:HB3  | 2.07                     | 0.55              |
| 3:M:338:PRO:HD2  | 3:M:381:ILE:HG13 | 1.89                     | 0.55              |
| 1:A:244:LEU:HD13 | 1:A:247:TYR:CD2  | 2.42                     | 0.54              |
| 1:A:252:VAL:HG23 | 1:A:255:PRO:HD3  | 1.89                     | 0.54              |
| 1:A:279:ARG:HA   | 1:A:282:GLU:CD   | 2.32                     | 0.54              |
| 2:B:61:ASP:OD1   | 2:B:61:ASP:N     | 2.38                     | 0.54              |
| 3:M:201:VAL:HA   | 3:M:284:GLU:HA   | 1.90                     | 0.54              |
| 2:B:341:ILE:O    | 2:B:345:LEU:N    | 2.35                     | 0.54              |
| 2:B:450:TRP:NE1  | 2:B:454:GLU:OE2  | 2.40                     | 0.54              |
| 3:M:99:GLU:HA    | 3:M:102:LYS:HD2  | 1.88                     | 0.54              |
| 3:M:117:ASP:H    | 3:M:122:GLN:HE22 | 1.56                     | 0.54              |
| 3:M:214:PHE:CE2  | 3:M:216:MET:HB2  | 2.42                     | 0.54              |
| 1:A:116:ILE:O    | 1:A:120:LEU:HG   | 2.07                     | 0.54              |
| 2:B:118:ILE:HA   | 2:B:121:TYR:CD2  | 2.42                     | 0.54              |
| 2:B:127:ARG:O    | 2:B:131:LYS:N    | 2.32                     | 0.54              |
| 2:B:287:PRO:O    | 2:B:290:THR:OG1  | 2.21                     | 0.54              |
| 2:B:371:ARG:NH2  | 2:B:405:TYR:O    | 2.41                     | 0.54              |
| 4:S:8:GLN:HA     | 4:S:15:ARG:H     | 1.72                     | 0.54              |
| 2:B:51:PHE:HE1   | 2:B:73:LEU:HD12  | 1.73                     | 0.54              |
| 2:B:239:SER:O    | 2:B:243:ARG:HG2  | 2.07                     | 0.54              |
| 2:B:330:ASP:OD2  | 2:B:338:LYS:NZ   | 2.37                     | 0.54              |
| 3:M:203:LYS:NZ   | 3:M:204:SER:O    | 2.40                     | 0.54              |
| 3:M:315:LYS:NZ   | 3:M:378:SER:OG   | 2.41                     | 0.54              |
| 1:A:188:TRP:CD1  | 1:A:191:ARG:HH22 | 2.26                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:497:SER:C    | 2:B:500:GLN:HE22 | 2.15                     | 0.54              |
| 2:B:499:THR:HG22 | 2:B:503:VAL:HG13 | 1.90                     | 0.54              |
| 2:B:578:PRO:HA   | 2:B:581:PHE:CZ   | 2.43                     | 0.54              |
| 1:A:466:ILE:HD11 | 1:A:499:VAL:HG22 | 1.88                     | 0.54              |
| 2:B:135:PRO:O    | 2:B:139:LYS:CB   | 2.55                     | 0.54              |
| 2:B:26:LYS:HZ2   | 2:B:27:LYS:HG2   | 1.71                     | 0.54              |
| 2:B:252:ASN:O    | 2:B:255:VAL:N    | 2.40                     | 0.54              |
| 2:B:351:ILE:HA   | 2:B:354:VAL:HB   | 1.90                     | 0.54              |
| 2:B:395:LEU:HA   | 2:B:398:LEU:HD12 | 1.89                     | 0.54              |
| 3:M:411:LYS:HG2  | 3:M:435:TYR:CZ   | 2.42                     | 0.54              |
| 4:S:62:TYR:N     | 4:S:65:LEU:O     | 2.41                     | 0.54              |
| 1:A:359:SER:O    | 1:A:363:HIS:N    | 2.40                     | 0.54              |
| 3:M:129:LEU:HD23 | 3:M:132:PHE:HE1  | 1.73                     | 0.54              |
| 3:M:332:GLU:HB2  | 3:M:365:LYS:HD3  | 1.88                     | 0.54              |
| 1:A:581:VAL:HG11 | 2:B:545:LYS:HE3  | 1.89                     | 0.54              |
| 1:A:585:ARG:NH2  | 2:B:539:GLU:O    | 2.41                     | 0.54              |
| 1:A:324:PRO:HA   | 1:A:327:LEU:HD12 | 1.90                     | 0.53              |
| 1:A:495:ASN:HA   | 1:A:498:LYS:HE2  | 1.90                     | 0.53              |
| 1:A:526:LEU:HA   | 1:A:529:LYS:HD2  | 1.90                     | 0.53              |
| 2:B:479:GLN:HA   | 2:B:482:LEU:HD12 | 1.90                     | 0.53              |
| 1:A:10:MET:HE1   | 1:A:56:LYS:HE2   | 1.88                     | 0.53              |
| 1:A:244:LEU:HD13 | 1:A:247:TYR:HD2  | 1.74                     | 0.53              |
| 1:A:563:LEU:C    | 1:A:568:GLN:HE21 | 2.17                     | 0.53              |
| 2:B:226:LEU:O    | 2:B:265:LYS:NZ   | 2.39                     | 0.53              |
| 2:B:521:ASP:OD1  | 2:B:528:ARG:NH2  | 2.42                     | 0.53              |
| 3:M:41:GLN:HE22  | 3:M:43:VAL:HG23  | 1.74                     | 0.53              |
| 1:A:30:ILE:HG22  | 1:A:34:ASN:HD21  | 1.74                     | 0.53              |
| 2:B:201:PRO:HA   | 2:B:204:ILE:HD12 | 1.90                     | 0.53              |
| 2:B:166:ARG:HH12 | 2:B:197:LEU:N    | 2.05                     | 0.53              |
| 3:M:268:PHE:HB2  | 3:M:274:ILE:HG23 | 1.91                     | 0.53              |
| 4:S:78:LEU:O     | 4:S:82:GLU:HG2   | 2.08                     | 0.53              |
| 2:B:485:LEU:HB2  | 2:B:522:ARG:NH2  | 2.20                     | 0.53              |
| 3:M:126:THR:HG1  | 3:M:162:ARG:HH21 | 1.57                     | 0.53              |
| 3:M:215:GLY:O    | 3:M:413:ARG:N    | 2.41                     | 0.53              |
| 3:M:296:LEU:HB2  | 3:M:299:ARG:CZ   | 2.39                     | 0.53              |
| 3:M:311:LYS:HA   | 3:M:382:GLU:HA   | 1.91                     | 0.53              |
| 4:S:25:ASP:OD1   | 4:S:25:ASP:N     | 2.40                     | 0.53              |
| 1:A:362:SER:O    | 1:A:366:VAL:HG23 | 2.09                     | 0.53              |
| 3:M:221:VAL:HA   | 3:M:251:SER:HB3  | 1.90                     | 0.53              |
| 3:M:307:VAL:HB   | 3:M:311:LYS:HB3  | 1.90                     | 0.53              |
| 4:S:1:MET:HG2    | 4:S:3:ARG:NH2    | 2.23                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:276:VAL:HG13 | 1:A:279:ARG:NH2  | 2.24                     | 0.53              |
| 2:B:159:GLN:HA   | 2:B:162:LEU:HD12 | 1.91                     | 0.53              |
| 2:B:264:MET:HG3  | 2:B:312:LYS:HZ1  | 1.73                     | 0.53              |
| 3:M:59:LYS:HG2   | 3:M:64:TRP:CG    | 2.43                     | 0.53              |
| 3:M:167:LYS:HA   | 3:M:207:SER:HB3  | 1.90                     | 0.53              |
| 3:M:299:ARG:HH11 | 3:M:321:ASN:HB2  | 1.74                     | 0.53              |
| 4:S:52:PHE:O     | 4:S:53:ARG:HG2   | 2.09                     | 0.53              |
| 4:S:99:CYS:N     | 4:S:102:ASP:OD2  | 2.41                     | 0.53              |
| 1:A:103:ASN:ND2  | 1:A:109:ILE:HG12 | 2.24                     | 0.53              |
| 1:A:259:VAL:HA   | 1:A:312:GLU:HG2  | 1.91                     | 0.53              |
| 1:A:472:ARG:HB2  | 1:A:476:GLN:HE22 | 1.74                     | 0.53              |
| 1:A:518:SER:H    | 1:A:522:GLN:NE2  | 2.01                     | 0.53              |
| 3:M:55:PHE:HB3   | 3:M:57:HIS:NE2   | 2.22                     | 0.53              |
| 3:M:299:ARG:N    | 3:M:319:LYS:O    | 2.25                     | 0.53              |
| 1:A:32:ARG:NH1   | 1:A:36:GLU:HG2   | 2.23                     | 0.52              |
| 2:B:10:ASN:ND2   | 2:B:40:ALA:HA    | 2.24                     | 0.52              |
| 4:S:26:ASP:N     | 4:S:26:ASP:OD1   | 2.41                     | 0.52              |
| 4:S:98:VAL:HG23  | 4:S:102:ASP:HB2  | 1.92                     | 0.52              |
| 1:A:325:ASN:O    | 1:A:329:ARG:HG3  | 2.09                     | 0.52              |
| 3:M:213:LYS:HE3  | 3:M:275:SER:HA   | 1.91                     | 0.52              |
| 3:M:218:ASP:HB3  | 3:M:219:LYS:HD2  | 1.90                     | 0.52              |
| 3:M:254:ILE:HD11 | 3:M:288:TYR:HB2  | 1.91                     | 0.52              |
| 4:S:5:ILE:HG23   | 4:S:69:ILE:HG12  | 1.91                     | 0.52              |
| 4:S:55:PHE:HB2   | 4:S:72:ASP:HA    | 1.91                     | 0.52              |
| 2:B:518:ASP:O    | 2:B:522:ARG:HB2  | 2.08                     | 0.52              |
| 3:M:299:ARG:O    | 3:M:319:LYS:HB3  | 2.09                     | 0.52              |
| 1:A:51:ASP:O     | 1:A:55:LYS:HB2   | 2.09                     | 0.52              |
| 2:B:175:MET:HE1  | 3:M:156:THR:HA   | 1.92                     | 0.52              |
| 2:B:261:LYS:HE3  | 2:B:567:ILE:O    | 2.10                     | 0.52              |
| 2:B:426:GLU:OE1  | 2:B:426:GLU:N    | 2.37                     | 0.52              |
| 2:B:525:ILE:HG13 | 2:B:528:ARG:HH21 | 1.75                     | 0.52              |
| 3:M:125:GLU:OE2  | 3:M:161:TRP:N    | 2.25                     | 0.52              |
| 3:M:172:GLU:HB3  | 3:M:432:TRP:HZ3  | 1.75                     | 0.52              |
| 1:A:75:GLY:HA2   | 1:A:78:GLU:HB2   | 1.92                     | 0.52              |
| 1:A:210:LEU:O    | 1:A:214:LEU:HG   | 2.09                     | 0.52              |
| 1:A:213:THR:O    | 1:A:217:LYS:HG2  | 2.10                     | 0.52              |
| 1:A:463:TYR:CE1  | 2:B:516:ASN:HA   | 2.44                     | 0.52              |
| 3:M:251:SER:HB2  | 3:M:410:LEU:HD13 | 1.92                     | 0.52              |
| 1:A:170:LEU:HD12 | 4:S:119:LEU:HB3  | 1.90                     | 0.52              |
| 2:B:175:MET:HE3  | 3:M:155:VAL:HG12 | 1.91                     | 0.52              |
| 2:B:211:LEU:HG   | 2:B:219:GLN:HG2  | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:524:TYR:HA   | 2:B:527:TRP:CD1  | 2.44                     | 0.52              |
| 3:M:249:LYS:HZ3  | 3:M:409:GLY:HA3  | 1.74                     | 0.52              |
| 3:M:260:HIS:CD2  | 3:M:286:MET:HA   | 2.45                     | 0.52              |
| 3:M:304:VAL:HB   | 3:M:394:ARG:NH2  | 2.25                     | 0.52              |
| 1:A:280:LEU:O    | 1:A:284:LEU:HG   | 2.10                     | 0.52              |
| 3:M:144:THR:O    | 3:M:148:GLN:N    | 2.31                     | 0.52              |
| 3:M:329:GLN:N    | 3:M:402:GLU:OE2  | 2.43                     | 0.52              |
| 1:A:150:GLU:HA   | 1:A:153:LYS:HE2  | 1.91                     | 0.52              |
| 1:A:13:LEU:HB2   | 1:A:57:LYS:HG3   | 1.92                     | 0.52              |
| 1:A:81:ASN:O     | 1:A:85:SER:HB2   | 2.09                     | 0.52              |
| 2:B:296:PRO:HA   | 2:B:299:GLN:HE21 | 1.74                     | 0.52              |
| 1:A:181:ASP:OD1  | 1:A:182:LEU:N    | 2.43                     | 0.52              |
| 1:A:303:SER:HA   | 1:A:306:LYS:HE3  | 1.92                     | 0.52              |
| 1:A:417:ASP:HB3  | 1:A:420:ILE:HG12 | 1.92                     | 0.52              |
| 3:M:9:ASN:HD21   | 3:M:13:GLU:HG2   | 1.73                     | 0.52              |
| 3:M:177:VAL:N    | 3:M:434:ARG:O    | 2.37                     | 0.52              |
| 4:S:138:LEU:HD22 | 4:S:141:LEU:HD11 | 1.92                     | 0.52              |
| 1:A:105:ASN:O    | 1:A:108:LEU:N    | 2.42                     | 0.51              |
| 2:B:382:ILE:HA   | 2:B:421:TYR:HE2  | 1.75                     | 0.51              |
| 4:S:49:PHE:HA    | 4:S:57:ILE:O     | 2.11                     | 0.51              |
| 1:A:472:ARG:HB3  | 1:A:474:ASP:OD1  | 2.11                     | 0.51              |
| 1:A:579:ARG:NH2  | 1:A:583:TYR:OH   | 2.42                     | 0.51              |
| 3:M:170:ARG:HH22 | 3:M:428:ASP:C    | 2.18                     | 0.51              |
| 3:M:184:LEU:HB3  | 3:M:193:SER:HB3  | 1.93                     | 0.51              |
| 3:M:203:LYS:HA   | 3:M:282:GLU:HA   | 1.92                     | 0.51              |
| 2:B:199:LEU:HD23 | 2:B:199:LEU:H    | 1.75                     | 0.51              |
| 3:M:426:ASP:OD1  | 3:M:426:ASP:N    | 2.42                     | 0.51              |
| 1:A:430:ILE:O    | 1:A:433:GLU:HG3  | 2.10                     | 0.51              |
| 1:A:444:ASP:HA   | 1:A:447:LEU:HD12 | 1.91                     | 0.51              |
| 1:A:544:THR:HA   | 1:A:547:LYS:HE3  | 1.92                     | 0.51              |
| 2:B:135:PRO:N    | 2:B:138:ARG:HH21 | 2.08                     | 0.51              |
| 2:B:189:GLU:OE1  | 2:B:189:GLU:N    | 2.43                     | 0.51              |
| 1:A:475:VAL:O    | 1:A:479:ALA:N    | 2.29                     | 0.51              |
| 4:S:23:PHE:HB2   | 4:S:28:LYS:NZ    | 2.26                     | 0.51              |
| 4:S:43:ASP:OD1   | 4:S:46:HIS:NE2   | 2.43                     | 0.51              |
| 4:S:75:ASP:HB3   | 4:S:80:TYR:CE2   | 2.46                     | 0.51              |
| 1:A:443:VAL:O    | 1:A:447:LEU:HG   | 2.10                     | 0.51              |
| 1:A:566:ASP:O    | 1:A:570:LYS:N    | 2.43                     | 0.51              |
| 2:B:277:TYR:O    | 2:B:281:LEU:HG   | 2.11                     | 0.51              |
| 2:B:357:GLU:HB3  | 2:B:361:TYR:CZ   | 2.45                     | 0.51              |
| 3:M:262:CYS:O    | 3:M:276:PHE:HA   | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:S:13:LYS:HB2   | 4:S:15:ARG:NH2   | 2.19                     | 0.51              |
| 1:A:109:ILE:HA   | 1:A:112:ILE:HD12 | 1.93                     | 0.51              |
| 1:A:605:PHE:CD1  | 1:A:606:PRO:HD2  | 2.46                     | 0.51              |
| 2:B:62:ASN:HB3   | 2:B:65:LEU:HB3   | 1.91                     | 0.51              |
| 2:B:166:ARG:HH22 | 2:B:197:LEU:HB2  | 1.75                     | 0.51              |
| 2:B:341:ILE:HG22 | 2:B:345:LEU:HG   | 1.93                     | 0.51              |
| 2:B:404:ASN:HB2  | 2:B:408:GLN:HE21 | 1.76                     | 0.51              |
| 2:B:581:PHE:HA   | 3:M:52:ARG:NE    | 2.26                     | 0.51              |
| 3:M:405:PHE:N    | 3:M:435:TYR:O    | 2.43                     | 0.51              |
| 4:S:56:LYS:HG3   | 4:S:71:VAL:HG23  | 1.92                     | 0.51              |
| 4:S:60:ARG:O     | 4:S:67:PHE:N     | 2.39                     | 0.51              |
| 2:B:74:MET:O     | 2:B:78:LYS:HG2   | 2.11                     | 0.51              |
| 2:B:456:ALA:HB1  | 2:B:491:LEU:HD13 | 1.92                     | 0.51              |
| 2:B:510:ALA:O    | 2:B:514:SER:HB2  | 2.10                     | 0.51              |
| 3:M:75:ALA:HB1   | 3:M:79:PHE:CZ    | 2.46                     | 0.51              |
| 3:M:128:ALA:HB3  | 3:M:154:GLN:NE2  | 2.26                     | 0.51              |
| 3:M:185:MET:HA   | 3:M:191:VAL:HA   | 1.92                     | 0.51              |
| 3:M:254:ILE:HG21 | 3:M:257:CYS:HB3  | 1.93                     | 0.51              |
| 4:S:123:ILE:HG21 | 4:S:126:THR:HG23 | 1.92                     | 0.51              |
| 1:A:233:LEU:O    | 1:A:237:VAL:HG23 | 2.11                     | 0.51              |
| 1:A:250:TYR:CE2  | 1:A:301:GLN:HG3  | 2.46                     | 0.51              |
| 1:A:360:GLU:OE1  | 1:A:360:GLU:N    | 2.38                     | 0.51              |
| 2:B:315:GLU:O    | 2:B:317:LEU:N    | 2.44                     | 0.51              |
| 2:B:318:LYS:NZ   | 2:B:346:ALA:O    | 2.34                     | 0.51              |
| 2:B:436:LEU:HD22 | 2:B:469:PHE:HZ   | 1.76                     | 0.51              |
| 2:B:521:ASP:O    | 2:B:524:TYR:HB2  | 2.10                     | 0.51              |
| 3:M:27:ASN:OD1   | 3:M:28:ALA:N     | 2.44                     | 0.51              |
| 3:M:350:LYS:H    | 3:M:364:TRP:HZ2  | 1.59                     | 0.51              |
| 1:A:64:PHE:HA    | 1:A:67:LEU:HD12  | 1.93                     | 0.50              |
| 1:A:65:ILE:HG22  | 1:A:70:HIS:HB2   | 1.93                     | 0.50              |
| 1:A:225:SER:O    | 1:A:228:LEU:HG   | 2.11                     | 0.50              |
| 1:A:243:ASP:HA   | 1:A:245:GLN:NE2  | 2.26                     | 0.50              |
| 1:A:565:SER:OG   | 1:A:567:SER:OG   | 2.28                     | 0.50              |
| 2:B:5:LYS:HD2    | 2:B:6:TYR:O      | 2.12                     | 0.50              |
| 2:B:287:PRO:O    | 2:B:291:LEU:HG   | 2.11                     | 0.50              |
| 2:B:297:GLU:O    | 2:B:301:VAL:HG23 | 2.11                     | 0.50              |
| 2:B:375:ARG:HH21 | 2:B:379:ARG:N    | 2.10                     | 0.50              |
| 2:B:574:TYR:CD2  | 2:B:576:LYS:HB2  | 2.46                     | 0.50              |
| 3:M:26:ARG:HH12  | 3:M:30:ASP:N     | 2.09                     | 0.50              |
| 1:A:15:VAL:O     | 1:A:18:SER:OG    | 2.23                     | 0.50              |
| 1:A:79:ALA:O     | 1:A:83:LEU:HG    | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:414:GLU:OE1  | 1:A:415:THR:HG23 | 2.11                     | 0.50              |
| 2:B:354:VAL:O    | 2:B:358:LEU:HG   | 2.12                     | 0.50              |
| 3:M:102:LYS:HA   | 3:M:105:PHE:CZ   | 2.46                     | 0.50              |
| 3:M:209:MET:HE3  | 3:M:421:LYS:HZ2  | 1.76                     | 0.50              |
| 3:M:209:MET:HE3  | 3:M:421:LYS:NZ   | 2.26                     | 0.50              |
| 1:A:132:LEU:HD22 | 1:A:168:ALA:HA   | 1.93                     | 0.50              |
| 2:B:206:LYS:O    | 2:B:209:THR:OG1  | 2.28                     | 0.50              |
| 1:A:167:SER:OG   | 4:S:124:ARG:NE   | 2.37                     | 0.50              |
| 2:B:125:PRO:HA   | 2:B:128:LYS:HD2  | 1.94                     | 0.50              |
| 2:B:135:PRO:HB3  | 2:B:173:ASN:ND2  | 2.26                     | 0.50              |
| 2:B:261:LYS:HB2  | 2:B:567:ILE:HG23 | 1.93                     | 0.50              |
| 3:M:10:HIS:HA    | 3:M:64:TRP:CZ2   | 2.46                     | 0.50              |
| 3:M:80:GLU:HB3   | 3:M:84:LYS:NZ    | 2.25                     | 0.50              |
| 3:M:212:CYS:HB2  | 3:M:276:PHE:CE2  | 2.46                     | 0.50              |
| 3:M:357:ALA:C    | 3:M:359:GLU:H    | 2.18                     | 0.50              |
| 3:M:364:TRP:HB2  | 3:M:377:ILE:HD13 | 1.94                     | 0.50              |
| 1:A:299:LYS:HB3  | 1:A:301:GLN:CD   | 2.37                     | 0.50              |
| 1:A:612:ILE:HA   | 1:A:615:LYS:HE3  | 1.93                     | 0.50              |
| 2:B:28:GLU:HG2   | 2:B:29:LYS:N     | 2.25                     | 0.50              |
| 2:B:289:VAL:O    | 2:B:293:SER:N    | 2.45                     | 0.50              |
| 2:B:312:LYS:HG2  | 2:B:313:ARG:HG2  | 1.94                     | 0.50              |
| 1:A:342:GLU:HA   | 4:S:45:LYS:NZ    | 2.26                     | 0.50              |
| 1:A:369:HIS:O    | 1:A:373:VAL:HG23 | 2.12                     | 0.50              |
| 2:B:99:ASN:ND2   | 3:M:148:GLN:HE22 | 2.10                     | 0.50              |
| 2:B:290:THR:HA   | 2:B:293:SER:HB2  | 1.93                     | 0.50              |
| 2:B:350:ASN:HB3  | 2:B:354:VAL:HG23 | 1.93                     | 0.50              |
| 3:M:218:ASP:HB2  | 3:M:413:ARG:HH12 | 1.77                     | 0.50              |
| 3:M:327:LEU:O    | 3:M:329:GLN:NE2  | 2.38                     | 0.50              |
| 1:A:43:LYS:HG2   | 1:A:58:TYR:HE2   | 1.76                     | 0.50              |
| 1:A:91:LYS:HE2   | 1:A:127:PHE:CZ   | 2.47                     | 0.50              |
| 1:A:115:ALA:HA   | 1:A:118:ASN:HD22 | 1.77                     | 0.50              |
| 1:A:387:GLN:HB2  | 1:A:388:ARG:NH1  | 2.25                     | 0.50              |
| 1:A:484:PHE:HB3  | 1:A:516:ARG:NH2  | 2.27                     | 0.50              |
| 2:B:417:ILE:O    | 2:B:421:TYR:N    | 2.45                     | 0.50              |
| 3:M:161:TRP:HZ2  | 3:M:277:ILE:HB   | 1.76                     | 0.50              |
| 3:M:257:CYS:HB2  | 3:M:286:MET:HE1  | 1.93                     | 0.50              |
| 3:M:310:THR:O    | 3:M:383:LEU:N    | 2.24                     | 0.50              |
| 2:B:6:TYR:HB3    | 3:M:102:LYS:CG   | 2.42                     | 0.50              |
| 2:B:461:ASN:OD1  | 2:B:461:ASN:N    | 2.45                     | 0.50              |
| 1:A:58:TYR:O     | 1:A:62:LEU:HG    | 2.11                     | 0.50              |
| 1:A:156:VAL:HG11 | 1:A:191:ARG:HE   | 1.77                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:616:LEU:HA   | 1:A:619:LYS:HD3  | 1.94                     | 0.50              |
| 3:M:181:VAL:O    | 3:M:441:ILE:HB   | 2.12                     | 0.50              |
| 3:M:211:GLU:OE2  | 3:M:276:PHE:N    | 2.45                     | 0.50              |
| 1:A:402:ALA:O    | 1:A:406:VAL:HG23 | 2.12                     | 0.49              |
| 2:B:22:LEU:C     | 2:B:24:ASN:H     | 2.20                     | 0.49              |
| 2:B:355:LEU:HD12 | 2:B:358:LEU:HB2  | 1.93                     | 0.49              |
| 2:B:527:TRP:O    | 2:B:531:SER:N    | 2.39                     | 0.49              |
| 1:A:196:LEU:O    | 1:A:232:ARG:NE   | 2.46                     | 0.49              |
| 1:A:413:LEU:HD21 | 1:A:424:ILE:HG21 | 1.94                     | 0.49              |
| 1:A:430:ILE:HA   | 1:A:433:GLU:HG3  | 1.94                     | 0.49              |
| 1:A:482:THR:HA   | 1:A:485:GLU:CD   | 2.36                     | 0.49              |
| 2:B:67:LYS:HD3   | 2:B:105:LEU:HD21 | 1.94                     | 0.49              |
| 2:B:249:SER:HB3  | 3:M:259:PHE:CD2  | 2.46                     | 0.49              |
| 2:B:297:GLU:OE1  | 2:B:297:GLU:N    | 2.31                     | 0.49              |
| 2:B:324:PHE:HD1  | 2:B:338:LYS:HA   | 1.77                     | 0.49              |
| 3:M:202:MET:N    | 3:M:283:PHE:O    | 2.29                     | 0.49              |
| 1:A:161:MET:SD   | 1:A:163:SER:N    | 2.86                     | 0.49              |
| 1:A:353:MET:O    | 1:A:357:ALA:N    | 2.45                     | 0.49              |
| 2:B:53:ASP:HA    | 2:B:56:ASN:ND2   | 2.26                     | 0.49              |
| 2:B:132:ASP:O    | 2:B:138:ARG:HD3  | 2.12                     | 0.49              |
| 2:B:581:PHE:HA   | 3:M:52:ARG:HE    | 1.77                     | 0.49              |
| 3:M:215:GLY:HA3  | 3:M:414:TYR:CD2  | 2.47                     | 0.49              |
| 3:M:322:PHE:HB3  | 3:M:326:LEU:HD12 | 1.95                     | 0.49              |
| 1:A:99:SER:HB3   | 1:A:137:ASN:HD21 | 1.76                     | 0.49              |
| 1:A:124:ASN:ND2  | 1:A:127:PHE:H    | 2.11                     | 0.49              |
| 1:A:381:ARG:H    | 1:A:386:ARG:NH2  | 2.09                     | 0.49              |
| 2:B:7:PHE:O      | 2:B:9:THR:HG23   | 2.12                     | 0.49              |
| 2:B:52:PRO:O     | 2:B:56:ASN:ND2   | 2.45                     | 0.49              |
| 2:B:54:VAL:O     | 2:B:58:MET:CB    | 2.53                     | 0.49              |
| 2:B:564:ILE:O    | 2:B:567:ILE:HG22 | 2.12                     | 0.49              |
| 3:M:146:GLU:O    | 3:M:150:GLN:HB2  | 2.12                     | 0.49              |
| 3:M:221:VAL:HG12 | 3:M:251:SER:H    | 1.78                     | 0.49              |
| 1:A:523:PHE:CZ   | 1:A:559:ILE:HG12 | 2.48                     | 0.49              |
| 2:B:258:SER:O    | 2:B:262:VAL:HG23 | 2.12                     | 0.49              |
| 1:A:57:LYS:HG2   | 1:A:58:TYR:CD1   | 2.48                     | 0.49              |
| 1:A:171:CYS:O    | 1:A:175:LEU:HG   | 2.13                     | 0.49              |
| 1:A:343:THR:HA   | 1:A:346:ARG:HH21 | 1.77                     | 0.49              |
| 2:B:94:ASP:OD2   | 2:B:106:ALA:HB2  | 2.11                     | 0.49              |
| 3:M:13:GLU:HA    | 3:M:33:ARG:CZ    | 2.42                     | 0.49              |
| 3:M:188:GLN:CD   | 3:M:188:GLN:H    | 2.21                     | 0.49              |
| 3:M:322:PHE:O    | 3:M:372:MET:HG2  | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:325:ASN:OD1  | 1:A:326:LEU:N    | 2.44                     | 0.49              |
| 2:B:187:ILE:O    | 2:B:190:SER:OG   | 2.18                     | 0.49              |
| 3:M:354:LYS:HD3  | 3:M:363:VAL:HG11 | 1.93                     | 0.49              |
| 4:S:19:TRP:HB3   | 4:S:23:PHE:CD2   | 2.46                     | 0.49              |
| 4:S:49:PHE:CE1   | 4:S:58:ILE:HG23  | 2.48                     | 0.49              |
| 4:S:86:ASN:HA    | 4:S:89:GLU:CD    | 2.38                     | 0.49              |
| 4:S:20:TYR:CD2   | 4:S:121:GLY:HA2  | 2.48                     | 0.49              |
| 1:A:380:GLU:HB3  | 1:A:386:ARG:NH2  | 2.27                     | 0.49              |
| 2:B:285:ALA:HB3  | 2:B:286:PRO:HD3  | 1.95                     | 0.49              |
| 2:B:428:ILE:O    | 2:B:432:LEU:HG   | 2.13                     | 0.49              |
| 3:M:305:ARG:HD3  | 3:M:313:GLU:O    | 2.13                     | 0.49              |
| 1:A:52:GLY:HA2   | 1:A:90:GLU:OE2   | 2.13                     | 0.49              |
| 1:A:166:GLN:NE2  | 4:S:125:GLU:OE2  | 2.44                     | 0.49              |
| 1:A:397:CYS:SG   | 1:A:398:ASP:N    | 2.86                     | 0.49              |
| 1:A:20:ILE:HA    | 1:A:23:CYS:SG    | 2.53                     | 0.48              |
| 1:A:88:TYR:CD2   | 4:S:141:LEU:HB3  | 2.48                     | 0.48              |
| 1:A:156:VAL:HG21 | 1:A:191:ARG:HH21 | 1.77                     | 0.48              |
| 1:A:277:ARG:HA   | 1:A:280:LEU:HB3  | 1.94                     | 0.48              |
| 1:A:384:SER:O    | 1:A:388:ARG:HG2  | 2.13                     | 0.48              |
| 1:A:547:LYS:HA   | 1:A:599:LEU:HD21 | 1.95                     | 0.48              |
| 2:B:73:LEU:HD11  | 2:B:87:ALA:HB2   | 1.95                     | 0.48              |
| 4:S:103:LEU:C    | 4:S:106:ASN:H    | 2.21                     | 0.48              |
| 1:A:450:ILE:HG21 | 1:A:496:LEU:HB2  | 1.95                     | 0.48              |
| 2:B:441:GLU:O    | 2:B:445:ARG:HG3  | 2.13                     | 0.48              |
| 3:M:200:VAL:O    | 3:M:285:LEU:N    | 2.39                     | 0.48              |
| 1:A:18:SER:O     | 1:A:22:ASN:ND2   | 2.47                     | 0.48              |
| 1:A:380:GLU:HG3  | 1:A:382:ASP:N    | 2.27                     | 0.48              |
| 1:A:535:VAL:HG13 | 1:A:576:LEU:HD11 | 1.95                     | 0.48              |
| 1:A:573:ASP:OD1  | 1:A:576:LEU:HB2  | 2.13                     | 0.48              |
| 2:B:306:ILE:O    | 2:B:310:VAL:HG23 | 2.12                     | 0.48              |
| 3:M:143:GLN:NE2  | 3:M:148:GLN:HA   | 2.28                     | 0.48              |
| 3:M:321:ASN:HA   | 3:M:372:MET:HA   | 1.95                     | 0.48              |
| 4:S:95:PHE:HB3   | 4:S:98:VAL:HB    | 1.94                     | 0.48              |
| 1:A:333:GLN:HB3  | 1:A:337:PHE:CZ   | 2.49                     | 0.48              |
| 1:A:612:ILE:HG23 | 1:A:615:LYS:NZ   | 2.28                     | 0.48              |
| 2:B:442:PRO:HG3  | 2:B:445:ARG:HH22 | 1.78                     | 0.48              |
| 4:S:1:MET:HE2    | 4:S:21:MET:SD    | 2.54                     | 0.48              |
| 2:B:46:ASP:HA    | 2:B:76:TYR:CE1   | 2.48                     | 0.48              |
| 2:B:456:ALA:HB3  | 2:B:494:LYS:HD2  | 1.94                     | 0.48              |
| 3:M:97:SER:N     | 3:M:100:ASN:OD1  | 2.46                     | 0.48              |
| 1:A:199:GLN:N    | 1:A:199:GLN:OE1  | 2.47                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:304:ASN:ND2  | 4:S:82:GLU:OE2   | 2.45                     | 0.48              |
| 1:A:565:SER:O    | 1:A:569:LEU:HG   | 2.13                     | 0.48              |
| 4:S:8:GLN:HB3    | 4:S:14:THR:HA    | 1.96                     | 0.48              |
| 1:A:10:MET:HB2   | 1:A:57:LYS:HB2   | 1.95                     | 0.48              |
| 1:A:330:ALA:HA   | 1:A:333:GLN:HE21 | 1.79                     | 0.48              |
| 2:B:234:ASP:HB2  | 2:B:238:GLN:HE21 | 1.77                     | 0.48              |
| 2:B:333:TYR:O    | 2:B:336:LEU:HB2  | 2.14                     | 0.48              |
| 2:B:415:ARG:HA   | 2:B:450:TRP:CZ3  | 2.49                     | 0.48              |
| 3:M:166:ILE:O    | 3:M:208:GLY:N    | 2.26                     | 0.48              |
| 3:M:345:GLN:OE1  | 3:M:380:GLU:HB2  | 2.13                     | 0.48              |
| 1:A:330:ALA:HA   | 1:A:333:GLN:NE2  | 2.28                     | 0.48              |
| 1:A:363:HIS:O    | 1:A:367:LYS:HG3  | 2.13                     | 0.48              |
| 1:A:383:VAL:HB   | 1:A:387:GLN:NE2  | 2.26                     | 0.48              |
| 1:A:384:SER:OG   | 1:A:385:VAL:N    | 2.46                     | 0.48              |
| 2:B:6:TYR:CD1    | 3:M:102:LYS:HD3  | 2.49                     | 0.48              |
| 2:B:403:VAL:HB   | 2:B:405:TYR:CZ   | 2.48                     | 0.48              |
| 2:B:468:SER:OG   | 2:B:469:PHE:N    | 2.46                     | 0.48              |
| 2:B:541:VAL:O    | 2:B:545:LYS:NZ   | 2.36                     | 0.48              |
| 2:B:579:ASN:O    | 3:M:52:ARG:NH2   | 2.47                     | 0.48              |
| 2:B:582:VAL:HB   | 3:M:52:ARG:NH1   | 2.28                     | 0.48              |
| 3:M:223:GLU:HG2  | 3:M:247:LEU:H    | 1.78                     | 0.48              |
| 1:A:97:PHE:O     | 1:A:101:LEU:N    | 2.31                     | 0.48              |
| 1:A:156:VAL:HG21 | 1:A:191:ARG:NH2  | 2.29                     | 0.48              |
| 1:A:371:GLU:HA   | 1:A:374:ILE:HD12 | 1.95                     | 0.48              |
| 1:A:445:THR:O    | 1:A:449:LEU:HG   | 2.14                     | 0.48              |
| 3:M:50:ILE:HB    | 3:M:55:PHE:CE2   | 2.49                     | 0.48              |
| 3:M:171:ASN:O    | 3:M:429:VAL:HA   | 2.14                     | 0.48              |
| 4:S:67:PHE:CE2   | 4:S:88:VAL:HG22  | 2.49                     | 0.48              |
| 1:A:87:ARG:HB2   | 1:A:90:GLU:HG3   | 1.94                     | 0.48              |
| 1:A:246:ASP:HB3  | 4:S:130:LYS:NZ   | 2.28                     | 0.48              |
| 1:A:381:ARG:H    | 1:A:386:ARG:HH22 | 1.62                     | 0.48              |
| 1:A:476:GLN:N    | 1:A:476:GLN:OE1  | 2.47                     | 0.48              |
| 2:B:182:ALA:HB2  | 2:B:221:PHE:CE2  | 2.49                     | 0.48              |
| 2:B:114:ARG:HH21 | 2:B:150:ASP:CG   | 2.21                     | 0.47              |
| 3:M:25:GLY:O     | 3:M:29:VAL:HG23  | 2.14                     | 0.47              |
| 3:M:311:LYS:HE2  | 3:M:380:GLU:HB3  | 1.96                     | 0.47              |
| 3:M:211:GLU:HG2  | 3:M:277:ILE:HG13 | 1.95                     | 0.47              |
| 3:M:264:ARG:HB2  | 3:M:275:SER:H    | 1.78                     | 0.47              |
| 3:M:405:PHE:CE2  | 3:M:407:PRO:HA   | 2.49                     | 0.47              |
| 1:A:423:GLU:HG3  | 1:A:619:LYS:HZ3  | 1.79                     | 0.47              |
| 1:A:558:THR:O    | 1:A:562:VAL:HG13 | 2.13                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:104:ALA:O    | 2:B:140:THR:HG21 | 2.15                     | 0.47              |
| 1:A:244:LEU:HB3  | 1:A:247:TYR:HB2  | 1.97                     | 0.47              |
| 1:A:249:TYR:O    | 1:A:252:VAL:HG22 | 2.14                     | 0.47              |
| 1:A:503:ILE:HG23 | 1:A:507:PHE:HD2  | 1.80                     | 0.47              |
| 1:A:563:LEU:HD11 | 1:A:584:LEU:HA   | 1.96                     | 0.47              |
| 4:S:54:ASN:N     | 4:S:54:ASN:OD1   | 2.47                     | 0.47              |
| 2:B:66:LYS:NZ    | 2:B:102:ILE:HG23 | 2.29                     | 0.47              |
| 3:M:81:PHE:HZ    | 3:M:115:ILE:HG23 | 1.79                     | 0.47              |
| 3:M:97:SER:O     | 3:M:101:ILE:HG12 | 2.14                     | 0.47              |
| 3:M:171:ASN:HB3  | 3:M:206:LEU:HG   | 1.97                     | 0.47              |
| 1:A:483:VAL:O    | 1:A:487:LEU:HG   | 2.15                     | 0.47              |
| 1:A:543:SER:O    | 1:A:546:ILE:HG22 | 2.15                     | 0.47              |
| 2:B:99:ASN:HD22  | 3:M:148:GLN:HE22 | 1.63                     | 0.47              |
| 2:B:199:LEU:HD12 | 2:B:229:TYR:CD1  | 2.48                     | 0.47              |
| 2:B:408:GLN:HB3  | 2:B:441:GLU:CD   | 2.40                     | 0.47              |
| 3:M:9:ASN:HB3    | 3:M:15:LEU:HD21  | 1.96                     | 0.47              |
| 1:A:163:SER:OG   | 4:S:124:ARG:NH2  | 2.47                     | 0.47              |
| 1:A:276:VAL:O    | 1:A:279:ARG:HG2  | 2.14                     | 0.47              |
| 1:A:303:SER:HA   | 1:A:306:LYS:HG2  | 1.97                     | 0.47              |
| 1:A:314:ILE:O    | 1:A:318:ILE:HG12 | 2.15                     | 0.47              |
| 1:A:418:TYR:O    | 1:A:421:ARG:HB3  | 2.14                     | 0.47              |
| 1:A:519:PRO:O    | 1:A:523:PHE:HB3  | 2.15                     | 0.47              |
| 1:A:544:THR:HG22 | 1:A:548:PHE:CE1  | 2.49                     | 0.47              |
| 2:B:135:PRO:HD2  | 3:M:152:THR:HG23 | 1.96                     | 0.47              |
| 2:B:166:ARG:NH1  | 2:B:198:ASP:OD1  | 2.48                     | 0.47              |
| 2:B:404:ASN:OD1  | 2:B:404:ASN:N    | 2.46                     | 0.47              |
| 3:M:116:LEU:HA   | 3:M:121:PRO:HA   | 1.95                     | 0.47              |
| 3:M:170:ARG:HH11 | 3:M:171:ASN:H    | 1.63                     | 0.47              |
| 3:M:184:LEU:N    | 3:M:193:SER:HB3  | 2.30                     | 0.47              |
| 3:M:338:PRO:HB3  | 3:M:383:LEU:HD21 | 1.97                     | 0.47              |
| 3:M:397:ILE:HG13 | 3:M:445:ARG:HE   | 1.79                     | 0.47              |
| 1:A:299:LYS:HB2  | 1:A:302:HIS:HD2  | 1.77                     | 0.47              |
| 1:A:380:GLU:CD   | 1:A:385:VAL:HG21 | 2.40                     | 0.47              |
| 1:A:552:PHE:HB3  | 1:A:554:GLU:OE2  | 2.15                     | 0.47              |
| 1:A:598:VAL:HG22 | 2:B:528:ARG:HG3  | 1.97                     | 0.47              |
| 2:B:177:VAL:O    | 2:B:181:VAL:HG23 | 2.15                     | 0.47              |
| 2:B:415:ARG:HD3  | 2:B:447:ALA:HA   | 1.96                     | 0.47              |
| 3:M:50:ILE:HB    | 3:M:55:PHE:HE2   | 1.78                     | 0.47              |
| 4:S:19:TRP:HB3   | 4:S:23:PHE:CE2   | 2.49                     | 0.47              |
| 4:S:48:ASN:ND2   | 4:S:60:ARG:HA    | 2.30                     | 0.47              |
| 1:A:139:GLY:HA3  | 1:A:174:ARG:NH2  | 2.30                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:364:GLU:O    | 1:A:368:THR:HG23 | 2.14                     | 0.47              |
| 1:A:474:ASP:N    | 1:A:476:GLN:OE1  | 2.48                     | 0.47              |
| 2:B:26:LYS:NZ    | 2:B:27:LYS:HG2   | 2.29                     | 0.47              |
| 2:B:375:ARG:NH1  | 2:B:413:VAL:HA   | 2.30                     | 0.47              |
| 3:M:20:TYR:HB3   | 3:M:118:PHE:HA   | 1.97                     | 0.47              |
| 3:M:214:PHE:HZ   | 3:M:216:MET:HE3  | 1.80                     | 0.47              |
| 3:M:258:THR:OG1  | 3:M:287:ARG:HB3  | 2.15                     | 0.47              |
| 3:M:396:PRO:HB2  | 3:M:443:GLU:HB2  | 1.95                     | 0.47              |
| 1:A:149:GLY:HA2  | 1:A:152:PRO:HG2  | 1.97                     | 0.47              |
| 1:A:342:GLU:HB3  | 1:A:345:LEU:HG   | 1.95                     | 0.47              |
| 1:A:481:LYS:HG2  | 1:A:516:ARG:HH21 | 1.80                     | 0.47              |
| 2:B:203:ASN:O    | 2:B:206:LYS:HG2  | 2.14                     | 0.47              |
| 2:B:241:CYS:O    | 2:B:276:TYR:OH   | 2.32                     | 0.47              |
| 2:B:304:ARG:CZ   | 2:B:575:HIS:HD2  | 2.28                     | 0.47              |
| 2:B:382:ILE:HG22 | 2:B:550:GLU:OE1  | 2.15                     | 0.47              |
| 3:M:320:SER:O    | 3:M:373:LYS:N    | 2.48                     | 0.47              |
| 3:M:347:ILE:HG13 | 3:M:378:SER:HB2  | 1.96                     | 0.47              |
| 1:A:13:LEU:O     | 1:A:17:ILE:HG12  | 2.16                     | 0.46              |
| 1:A:394:TYR:OH   | 1:A:427:LYS:O    | 2.27                     | 0.46              |
| 1:A:574:VAL:O    | 1:A:577:GLN:HB2  | 2.15                     | 0.46              |
| 2:B:108:ARG:HA   | 2:B:144:CYS:SG   | 2.55                     | 0.46              |
| 2:B:186:GLU:O    | 2:B:189:GLU:HB2  | 2.15                     | 0.46              |
| 2:B:500:GLN:H    | 2:B:500:GLN:CD   | 2.23                     | 0.46              |
| 2:B:555:ILE:HG21 | 2:B:560:LEU:HD13 | 1.96                     | 0.46              |
| 2:B:570:LEU:HD12 | 3:M:72:ASN:HA    | 1.97                     | 0.46              |
| 3:M:34:VAL:HA    | 3:M:38:HIS:HD2   | 1.78                     | 0.46              |
| 3:M:411:LYS:HG2  | 3:M:435:TYR:CE2  | 2.50                     | 0.46              |
| 1:A:399:ARG:O    | 1:A:403:GLN:NE2  | 2.31                     | 0.46              |
| 2:B:66:LYS:HZ3   | 2:B:102:ILE:HG23 | 1.80                     | 0.46              |
| 2:B:575:HIS:O    | 2:B:576:LYS:HD3  | 2.15                     | 0.46              |
| 3:M:101:ILE:HG22 | 3:M:105:PHE:CE1  | 2.50                     | 0.46              |
| 3:M:101:ILE:HG22 | 3:M:105:PHE:HE1  | 1.79                     | 0.46              |
| 4:S:65:LEU:HB3   | 4:S:67:PHE:CE1   | 2.50                     | 0.46              |
| 1:A:417:ASP:HB3  | 1:A:420:ILE:CG1  | 2.45                     | 0.46              |
| 1:A:430:ILE:HG23 | 1:A:434:LYS:NZ   | 2.31                     | 0.46              |
| 1:A:442:TYR:O    | 1:A:446:ILE:HG12 | 2.15                     | 0.46              |
| 2:B:339:LEU:O    | 2:B:343:ILE:HG12 | 2.16                     | 0.46              |
| 4:S:127:SER:O    | 4:S:131:VAL:HG23 | 2.16                     | 0.46              |
| 2:B:221:PHE:HA   | 2:B:224:ASP:OD2  | 2.16                     | 0.46              |
| 2:B:304:ARG:NE   | 2:B:573:VAL:O    | 2.48                     | 0.46              |
| 3:M:270:SER:O    | 3:M:272:ARG:NH1  | 2.48                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:298:PHE:HD1  | 3:M:320:SER:HA   | 1.81                     | 0.46              |
| 4:S:28:LYS:HA    | 4:S:31:LEU:HD12  | 1.97                     | 0.46              |
| 1:A:26:LYS:HA    | 1:A:26:LYS:HD3   | 1.73                     | 0.46              |
| 1:A:138:VAL:HB   | 1:A:143:MET:HE1  | 1.97                     | 0.46              |
| 1:A:272:GLU:H    | 1:A:277:ARG:CD   | 2.27                     | 0.46              |
| 1:A:485:GLU:HA   | 1:A:488:GLN:NE2  | 2.30                     | 0.46              |
| 1:A:527:HIS:NE2  | 1:A:545:TYR:HE2  | 2.14                     | 0.46              |
| 2:B:189:GLU:HA   | 2:B:191:HIS:CE1  | 2.51                     | 0.46              |
| 2:B:374:VAL:HG13 | 2:B:395:LEU:HD22 | 1.98                     | 0.46              |
| 3:M:64:TRP:N     | 3:M:64:TRP:CD1   | 2.80                     | 0.46              |
| 3:M:116:LEU:HD21 | 3:M:119:GLY:HA2  | 1.97                     | 0.46              |
| 4:S:32:ILE:HG23  | 4:S:36:HIS:CE1   | 2.51                     | 0.46              |
| 4:S:119:LEU:HB2  | 4:S:124:ARG:HB2  | 1.96                     | 0.46              |
| 1:A:142:GLU:HA   | 1:A:145:GLU:CD   | 2.40                     | 0.46              |
| 2:B:400:GLN:HA   | 2:B:402:LYS:NZ   | 2.31                     | 0.46              |
| 3:M:245:GLU:OE1  | 3:M:245:GLU:N    | 2.49                     | 0.46              |
| 3:M:287:ARG:HH12 | 3:M:289:ARG:HB3  | 1.80                     | 0.46              |
| 3:M:372:MET:O    | 3:M:373:LYS:HD3  | 2.16                     | 0.46              |
| 4:S:138:LEU:C    | 4:S:140:SER:H    | 2.24                     | 0.46              |
| 1:A:216:GLN:HB2  | 1:A:217:LYS:HZ2  | 1.81                     | 0.46              |
| 1:A:426:LEU:HD23 | 1:A:615:LYS:NZ   | 2.30                     | 0.46              |
| 2:B:134:ASP:C    | 2:B:138:ARG:HE   | 2.22                     | 0.46              |
| 3:M:18:ARG:HG3   | 3:M:20:TYR:HE2   | 1.76                     | 0.46              |
| 3:M:132:PHE:HE2  | 3:M:154:GLN:HE22 | 1.63                     | 0.46              |
| 3:M:143:GLN:NE2  | 3:M:151:ILE:HD12 | 2.31                     | 0.46              |
| 3:M:244:GLU:OE2  | 3:M:413:ARG:HA   | 2.16                     | 0.46              |
| 4:S:3:ARG:HD3    | 4:S:21:MET:HE1   | 1.98                     | 0.46              |
| 1:A:124:ASN:HD21 | 1:A:127:PHE:HD1  | 1.64                     | 0.46              |
| 1:A:478:TYR:CZ   | 1:A:482:THR:HG21 | 2.51                     | 0.46              |
| 2:B:411:ILE:HD12 | 2:B:444:ALA:HB1  | 1.98                     | 0.46              |
| 3:M:179:GLU:OE2  | 3:M:179:GLU:N    | 2.49                     | 0.46              |
| 3:M:298:PHE:C    | 3:M:299:ARG:HD2  | 2.40                     | 0.46              |
| 3:M:349:MET:HE3  | 3:M:376:GLN:HB3  | 1.97                     | 0.46              |
| 4:S:35:VAL:O     | 4:S:39:VAL:HG23  | 2.15                     | 0.46              |
| 4:S:50:VAL:HG12  | 4:S:59:TYR:CD2   | 2.50                     | 0.46              |
| 1:A:438:ASP:CG   | 1:A:441:TRP:HB3  | 2.41                     | 0.46              |
| 1:A:454:GLY:O    | 1:A:493:HIS:HB3  | 2.16                     | 0.46              |
| 1:A:530:PHE:HB3  | 1:A:531:HIS:CD2  | 2.51                     | 0.46              |
| 2:B:34:VAL:O     | 2:B:38:ILE:HG12  | 2.16                     | 0.46              |
| 2:B:464:GLU:HG2  | 2:B:465:LEU:N    | 2.29                     | 0.46              |
| 2:B:525:ILE:HA   | 2:B:528:ARG:HG2  | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:568:GLY:O    | 3:M:74:ASN:ND2   | 2.49                     | 0.46              |
| 3:M:151:ILE:O    | 3:M:155:VAL:HG23 | 2.16                     | 0.46              |
| 3:M:255:ASP:HB2  | 3:M:290:THR:HA   | 1.98                     | 0.46              |
| 3:M:364:TRP:NE1  | 3:M:375:SER:OG   | 2.43                     | 0.46              |
| 4:S:109:LYS:O    | 4:S:113:VAL:HG13 | 2.16                     | 0.46              |
| 1:A:318:ILE:HD12 | 1:A:356:LEU:HD13 | 1.98                     | 0.46              |
| 2:B:17:GLU:O     | 2:B:21:GLU:HG2   | 2.15                     | 0.46              |
| 2:B:32:GLU:OE1   | 2:B:32:GLU:N     | 2.48                     | 0.46              |
| 2:B:48:SER:OG    | 2:B:80:GLN:HG2   | 2.15                     | 0.46              |
| 2:B:90:SER:N     | 2:B:93:LYS:HZ2   | 2.14                     | 0.46              |
| 4:S:49:PHE:CZ    | 4:S:81:LEU:HB2   | 2.51                     | 0.46              |
| 1:A:192:VAL:HB   | 1:A:211:ILE:HD11 | 1.98                     | 0.45              |
| 2:B:244:VAL:HA   | 2:B:247:ARG:HG2  | 1.97                     | 0.45              |
| 2:B:264:MET:HE1  | 2:B:313:ARG:CZ   | 2.46                     | 0.45              |
| 2:B:284:LEU:O    | 2:B:288:LEU:HG   | 2.17                     | 0.45              |
| 2:B:307:ASN:HD21 | 2:B:575:HIS:CE1  | 2.35                     | 0.45              |
| 2:B:457:GLU:OE2  | 2:B:458:ARG:HG3  | 2.15                     | 0.45              |
| 4:S:92:ASN:HD22  | 4:S:98:VAL:HG12  | 1.81                     | 0.45              |
| 1:A:212:THR:OG1  | 1:A:264:LEU:HD12 | 2.16                     | 0.45              |
| 1:A:480:ALA:O    | 1:A:504:LEU:HD21 | 2.17                     | 0.45              |
| 1:A:610:SER:O    | 1:A:610:SER:OG   | 2.32                     | 0.45              |
| 2:B:491:LEU:HA   | 2:B:494:LYS:HG2  | 1.97                     | 0.45              |
| 3:M:199:ARG:HB2  | 3:M:284:GLU:OE2  | 2.15                     | 0.45              |
| 3:M:214:PHE:HD1  | 3:M:415:LEU:HD13 | 1.81                     | 0.45              |
| 3:M:256:ASP:HB2  | 3:M:289:ARG:HG2  | 1.97                     | 0.45              |
| 3:M:287:ARG:NH1  | 3:M:289:ARG:HB3  | 2.31                     | 0.45              |
| 1:A:566:ASP:OD1  | 1:A:566:ASP:N    | 2.49                     | 0.45              |
| 2:B:28:GLU:OE1   | 2:B:28:GLU:N     | 2.44                     | 0.45              |
| 2:B:128:LYS:HA   | 2:B:131:LYS:HB2  | 1.97                     | 0.45              |
| 2:B:316:ILE:C    | 2:B:318:LYS:H    | 2.23                     | 0.45              |
| 2:B:477:SER:HB3  | 2:B:479:GLN:HE22 | 1.81                     | 0.45              |
| 3:M:1:MET:C      | 3:M:21:ARG:HE    | 2.24                     | 0.45              |
| 3:M:129:LEU:HD23 | 3:M:132:PHE:CE1  | 2.51                     | 0.45              |
| 4:S:47:THR:OG1   | 4:S:48:ASN:N     | 2.48                     | 0.45              |
| 1:A:159:ASP:HA   | 1:A:165:LYS:CE   | 2.47                     | 0.45              |
| 1:A:161:MET:SD   | 1:A:164:VAL:HG22 | 2.56                     | 0.45              |
| 1:A:281:THR:O    | 1:A:285:GLU:HG2  | 2.16                     | 0.45              |
| 1:A:493:HIS:O    | 1:A:497:VAL:HG23 | 2.17                     | 0.45              |
| 2:B:165:LEU:HA   | 2:B:168:LEU:HB2  | 1.98                     | 0.45              |
| 2:B:375:ARG:O    | 2:B:375:ARG:NE   | 2.42                     | 0.45              |
| 2:B:464:GLU:HA   | 2:B:467:GLU:OE1  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:533:ASP:N    | 2:B:533:ASP:OD1  | 2.49                     | 0.45              |
| 2:B:567:ILE:HA   | 2:B:572:SER:OG   | 2.16                     | 0.45              |
| 3:M:107:LEU:HD23 | 3:M:133:ILE:HG22 | 1.98                     | 0.45              |
| 1:A:56:LYS:HD3   | 1:A:87:ARG:HH11  | 1.81                     | 0.45              |
| 1:A:209:SER:HB3  | 1:A:260:LYS:NZ   | 2.32                     | 0.45              |
| 2:B:100:PRO:HD2  | 3:M:148:GLN:OE1  | 2.15                     | 0.45              |
| 2:B:246:PRO:HG2  | 2:B:247:ARG:HE   | 1.81                     | 0.45              |
| 2:B:250:HIS:N    | 2:B:252:ASN:OD1  | 2.49                     | 0.45              |
| 2:B:439:LEU:HB3  | 2:B:445:ARG:HG2  | 1.98                     | 0.45              |
| 2:B:471:GLU:HG2  | 2:B:472:GLY:N    | 2.30                     | 0.45              |
| 3:M:167:LYS:NZ   | 3:M:168:TYR:O    | 2.45                     | 0.45              |
| 1:A:374:ILE:O    | 1:A:377:LEU:HG   | 2.17                     | 0.45              |
| 1:A:377:LEU:O    | 1:A:386:ARG:NE   | 2.41                     | 0.45              |
| 1:A:609:GLU:OE2  | 1:A:611:SER:OG   | 2.29                     | 0.45              |
| 2:B:341:ILE:HA   | 2:B:344:ARG:HB2  | 1.99                     | 0.45              |
| 3:M:7:ILE:HG23   | 3:M:64:TRP:O     | 2.17                     | 0.45              |
| 3:M:21:ARG:HB3   | 3:M:23:ASP:OD1   | 2.17                     | 0.45              |
| 3:M:106:VAL:HG13 | 3:M:107:LEU:HD12 | 1.98                     | 0.45              |
| 3:M:296:LEU:HB2  | 3:M:299:ARG:NH2  | 2.31                     | 0.45              |
| 3:M:322:PHE:HD1  | 3:M:322:PHE:HA   | 1.70                     | 0.45              |
| 3:M:331:ILE:O    | 3:M:366:ILE:N    | 2.26                     | 0.45              |
| 1:A:18:SER:HA    | 1:A:21:ARG:NH2   | 2.30                     | 0.45              |
| 1:A:83:LEU:O     | 1:A:91:LYS:HG2   | 2.16                     | 0.45              |
| 1:A:218:ASN:HB3  | 1:A:221:GLU:HB2  | 1.99                     | 0.45              |
| 1:A:393:LEU:HA   | 1:A:396:MET:HE2  | 1.98                     | 0.45              |
| 1:A:441:TRP:HA   | 1:A:444:ASP:OD2  | 2.17                     | 0.45              |
| 2:B:101:LEU:HD22 | 2:B:136:TYR:HD2  | 1.80                     | 0.45              |
| 2:B:103:ARG:O    | 2:B:107:VAL:HG23 | 2.16                     | 0.45              |
| 3:M:33:ARG:HG3   | 3:M:37:ILE:HD12  | 1.99                     | 0.45              |
| 3:M:127:GLY:O    | 3:M:162:ARG:HD3  | 2.17                     | 0.45              |
| 1:A:65:ILE:HA    | 1:A:68:LEU:HB2   | 1.99                     | 0.45              |
| 1:A:273:ASP:OD1  | 1:A:275:ALA:N    | 2.50                     | 0.45              |
| 1:A:393:LEU:HA   | 1:A:396:MET:HG2  | 1.98                     | 0.45              |
| 1:A:422:GLU:O    | 1:A:426:LEU:HD13 | 2.17                     | 0.45              |
| 2:B:367:VAL:O    | 2:B:371:ARG:HG3  | 2.17                     | 0.45              |
| 3:M:15:LEU:HD12  | 3:M:63:ILE:HG23  | 1.99                     | 0.45              |
| 3:M:26:ARG:NH1   | 3:M:29:VAL:HB    | 2.32                     | 0.45              |
| 3:M:252:ILE:HG12 | 3:M:253:ALA:N    | 2.31                     | 0.45              |
| 1:A:471:ASN:OD1  | 1:A:605:PHE:N    | 2.50                     | 0.45              |
| 2:B:285:ALA:O    | 2:B:289:VAL:HG23 | 2.17                     | 0.45              |
| 2:B:382:ILE:HA   | 2:B:421:TYR:CE2  | 2.52                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:214:PHE:CZ   | 3:M:216:MET:HE3  | 2.51                     | 0.45              |
| 1:A:587:SER:OG   | 1:A:588:THR:N    | 2.50                     | 0.45              |
| 2:B:47:VAL:HG23  | 2:B:72:TYR:CE1   | 2.47                     | 0.45              |
| 2:B:233:ASP:N    | 2:B:236:GLU:OE2  | 2.40                     | 0.45              |
| 2:B:295:GLU:H    | 2:B:298:VAL:CG2  | 2.29                     | 0.45              |
| 2:B:408:GLN:HB3  | 2:B:441:GLU:OE1  | 2.17                     | 0.45              |
| 2:B:545:LYS:N    | 2:B:545:LYS:HD2  | 2.32                     | 0.45              |
| 3:M:71:GLN:O     | 3:M:73:VAL:HG13  | 2.16                     | 0.45              |
| 3:M:215:GLY:C    | 3:M:413:ARG:HB3  | 2.43                     | 0.45              |
| 1:A:13:LEU:HD13  | 1:A:61:LYS:HG3   | 1.99                     | 0.44              |
| 1:A:64:PHE:HD1   | 1:A:67:LEU:HD12  | 1.82                     | 0.44              |
| 1:A:344:ASN:O    | 1:A:348:LEU:HG   | 2.17                     | 0.44              |
| 1:A:550:ASN:HB3  | 1:A:599:LEU:CD2  | 2.46                     | 0.44              |
| 2:B:139:LYS:O    | 2:B:143:VAL:HG23 | 2.17                     | 0.44              |
| 3:M:8:TYR:HB2    | 3:M:64:TRP:HB2   | 1.99                     | 0.44              |
| 4:S:94:TYR:CD2   | 4:S:135:LEU:HD21 | 2.52                     | 0.44              |
| 1:A:13:LEU:HD22  | 1:A:57:LYS:HA    | 1.98                     | 0.44              |
| 1:A:424:ILE:O    | 1:A:427:LYS:HG2  | 2.17                     | 0.44              |
| 1:A:480:ALA:HB2  | 1:A:507:PHE:HB3  | 2.00                     | 0.44              |
| 2:B:54:VAL:HG21  | 2:B:72:TYR:CE2   | 2.52                     | 0.44              |
| 2:B:238:GLN:O    | 2:B:242:GLU:HG2  | 2.16                     | 0.44              |
| 2:B:445:ARG:O    | 2:B:449:ILE:HG12 | 2.17                     | 0.44              |
| 3:M:23:ASP:OD1   | 3:M:24:ILE:N     | 2.49                     | 0.44              |
| 3:M:324:PRO:HA   | 3:M:371:GLY:H    | 1.82                     | 0.44              |
| 1:A:77:MET:N     | 1:A:108:LEU:HD21 | 2.33                     | 0.44              |
| 1:A:133:HIS:HE1  | 1:A:167:SER:HB3  | 1.82                     | 0.44              |
| 1:A:554:GLU:OE1  | 1:A:554:GLU:N    | 2.43                     | 0.44              |
| 2:B:108:ARG:HB3  | 2:B:140:THR:HG23 | 1.98                     | 0.44              |
| 2:B:331:PRO:HG2  | 2:B:334:VAL:HB   | 1.98                     | 0.44              |
| 3:M:7:ILE:HG22   | 3:M:15:LEU:HB2   | 1.99                     | 0.44              |
| 3:M:131:THR:OG1  | 3:M:132:PHE:N    | 2.49                     | 0.44              |
| 3:M:151:ILE:HA   | 3:M:154:GLN:CD   | 2.42                     | 0.44              |
| 3:M:185:MET:HG2  | 3:M:190:GLN:H    | 1.82                     | 0.44              |
| 3:M:336:PRO:HD2  | 3:M:397:ILE:HG12 | 2.00                     | 0.44              |
| 3:M:363:VAL:HG12 | 3:M:365:LYS:HB2  | 1.99                     | 0.44              |
| 4:S:81:LEU:O     | 4:S:85:HIS:HD2   | 2.00                     | 0.44              |
| 1:A:324:PRO:O    | 1:A:328:VAL:HG23 | 2.17                     | 0.44              |
| 1:A:535:VAL:HA   | 1:A:538:ARG:NE   | 2.33                     | 0.44              |
| 2:B:297:GLU:O    | 2:B:300:TYR:HB3  | 2.17                     | 0.44              |
| 2:B:489:VAL:HG21 | 2:B:526:TYR:CE1  | 2.53                     | 0.44              |
| 3:M:188:GLN:HA   | 3:M:301:ILE:HG23 | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:91:LYS:HE2   | 1:A:127:PHE:CE2  | 2.52                     | 0.44              |
| 1:A:358:SER:HA   | 1:A:363:HIS:CE1  | 2.53                     | 0.44              |
| 2:B:10:ASN:ND2   | 2:B:45:LYS:HB2   | 2.32                     | 0.44              |
| 3:M:161:TRP:CZ2  | 3:M:277:ILE:HB   | 2.52                     | 0.44              |
| 3:M:349:MET:HG2  | 3:M:376:GLN:O    | 2.18                     | 0.44              |
| 1:A:216:GLN:HB2  | 1:A:217:LYS:NZ   | 2.31                     | 0.44              |
| 1:A:448:ASN:HA   | 1:A:451:ARG:HE   | 1.81                     | 0.44              |
| 2:B:182:ALA:HB2  | 2:B:221:PHE:CD2  | 2.53                     | 0.44              |
| 2:B:284:LEU:O    | 2:B:287:PRO:HG2  | 2.18                     | 0.44              |
| 2:B:366:ASP:HB3  | 2:B:369:PHE:HD1  | 1.81                     | 0.44              |
| 2:B:380:CYS:HA   | 2:B:383:LYS:HB2  | 1.98                     | 0.44              |
| 2:B:563:LEU:HA   | 2:B:563:LEU:HD23 | 1.80                     | 0.44              |
| 1:A:259:VAL:HG23 | 1:A:309:VAL:HG12 | 1.99                     | 0.44              |
| 1:A:533:CYS:SG   | 1:A:537:THR:OG1  | 2.75                     | 0.44              |
| 1:A:552:PHE:O    | 1:A:555:VAL:HG12 | 2.17                     | 0.44              |
| 3:M:173:LEU:O    | 3:M:432:TRP:HE3  | 2.00                     | 0.44              |
| 1:A:113:ASN:OD1  | 1:A:114:ASN:N    | 2.51                     | 0.44              |
| 1:A:570:LYS:NZ   | 2:B:547:LEU:O    | 2.27                     | 0.44              |
| 2:B:269:LEU:H    | 2:B:269:LEU:HD23 | 1.83                     | 0.44              |
| 3:M:249:LYS:HB3  | 3:M:408:SER:O    | 2.17                     | 0.44              |
| 3:M:311:LYS:HG3  | 3:M:382:GLU:HA   | 2.00                     | 0.44              |
| 3:M:322:PHE:H    | 3:M:372:MET:N    | 2.02                     | 0.44              |
| 1:A:25:SER:O     | 1:A:25:SER:OG    | 2.36                     | 0.44              |
| 1:A:78:GLU:HA    | 1:A:81:ASN:CG    | 2.43                     | 0.44              |
| 1:A:397:CYS:O    | 1:A:435:TYR:OH   | 2.28                     | 0.44              |
| 1:A:521:ILE:HA   | 1:A:524:ASN:ND2  | 2.33                     | 0.44              |
| 2:B:422:PRO:O    | 2:B:424:LYS:HG3  | 2.18                     | 0.44              |
| 3:M:395:PRO:HD2  | 3:M:445:ARG:HD2  | 1.99                     | 0.44              |
| 2:B:217:TRP:CZ2  | 3:M:121:PRO:HB2  | 2.52                     | 0.43              |
| 2:B:524:TYR:HA   | 2:B:527:TRP:HE1  | 1.81                     | 0.43              |
| 3:M:80:GLU:HB3   | 3:M:84:LYS:HZ1   | 1.82                     | 0.43              |
| 3:M:86:CYS:HA    | 3:M:89:MET:SD    | 2.57                     | 0.43              |
| 4:S:129:THR:HG1  | 4:S:130:LYS:N    | 2.15                     | 0.43              |
| 1:A:73:ASP:OD1   | 1:A:74:PHE:HD1   | 2.01                     | 0.43              |
| 1:A:156:VAL:HA   | 1:A:159:ASP:OD1  | 2.18                     | 0.43              |
| 1:A:499:VAL:O    | 1:A:503:ILE:HG12 | 2.18                     | 0.43              |
| 1:A:600:GLU:OE2  | 1:A:603:PRO:HD3  | 2.18                     | 0.43              |
| 2:B:19:LYS:NZ    | 2:B:53:ASP:OD2   | 2.49                     | 0.43              |
| 2:B:459:ILE:HG22 | 2:B:462:ALA:HB2  | 2.00                     | 0.43              |
| 2:B:466:LEU:O    | 2:B:470:LEU:HG   | 2.17                     | 0.43              |
| 3:M:1:MET:HG3    | 3:M:120:TYR:CD1  | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:175:LEU:HB2  | 3:M:433:VAL:HG23 | 1.99                     | 0.43              |
| 3:M:304:VAL:HA   | 3:M:314:VAL:HA   | 2.00                     | 0.43              |
| 4:S:56:LYS:HE3   | 4:S:71:VAL:HG23  | 1.99                     | 0.43              |
| 4:S:108:TYR:CE2  | 4:S:109:LYS:HG3  | 2.52                     | 0.43              |
| 1:A:602:MET:HE1  | 2:B:520:ARG:HD3  | 2.00                     | 0.43              |
| 1:A:612:ILE:HG23 | 1:A:615:LYS:HZ1  | 1.82                     | 0.43              |
| 2:B:243:ARG:O    | 2:B:246:PRO:HD2  | 2.18                     | 0.43              |
| 2:B:275:ASP:O    | 2:B:279:MET:N    | 2.28                     | 0.43              |
| 3:M:260:HIS:O    | 3:M:262:CYS:N    | 2.45                     | 0.43              |
| 1:A:140:SER:N    | 1:A:143:MET:SD   | 2.92                     | 0.43              |
| 1:A:468:ILE:HG22 | 1:A:472:ARG:HG2  | 2.00                     | 0.43              |
| 2:B:49:SER:O     | 2:B:52:PRO:HD2   | 2.18                     | 0.43              |
| 2:B:234:ASP:HA   | 2:B:237:ALA:HB3  | 1.99                     | 0.43              |
| 2:B:379:ARG:O    | 2:B:383:LYS:N    | 2.50                     | 0.43              |
| 3:M:3:GLY:C      | 3:M:20:TYR:H     | 2.27                     | 0.43              |
| 3:M:48:THR:N     | 3:M:55:PHE:O     | 2.51                     | 0.43              |
| 3:M:183:LEU:O    | 3:M:441:ILE:HG22 | 2.18                     | 0.43              |
| 3:M:251:SER:CB   | 3:M:410:LEU:HD13 | 2.47                     | 0.43              |
| 1:A:44:PHE:HD2   | 1:A:74:PHE:HE2   | 1.66                     | 0.43              |
| 1:A:424:ILE:O    | 1:A:428:VAL:HG13 | 2.19                     | 0.43              |
| 1:A:594:ILE:HA   | 1:A:597:THR:HB   | 2.00                     | 0.43              |
| 2:B:331:PRO:O    | 2:B:335:LYS:HG3  | 2.17                     | 0.43              |
| 2:B:357:GLU:HB3  | 2:B:361:TYR:OH   | 2.18                     | 0.43              |
| 2:B:551:GLU:HG3  | 2:B:554:LEU:HD12 | 1.99                     | 0.43              |
| 3:M:49:ASN:HD21  | 3:M:52:ARG:H     | 1.66                     | 0.43              |
| 3:M:107:LEU:HD21 | 3:M:134:THR:C    | 2.43                     | 0.43              |
| 4:S:34:GLU:O     | 4:S:38:VAL:HG23  | 2.19                     | 0.43              |
| 1:A:192:VAL:O    | 1:A:196:LEU:HG   | 2.19                     | 0.43              |
| 2:B:58:MET:O     | 2:B:60:THR:HG22  | 2.18                     | 0.43              |
| 2:B:399:ILE:HA   | 2:B:407:VAL:HG22 | 1.99                     | 0.43              |
| 2:B:580:ALA:C    | 3:M:52:ARG:HH21  | 2.27                     | 0.43              |
| 3:M:215:GLY:N    | 3:M:414:TYR:O    | 2.33                     | 0.43              |
| 3:M:259:PHE:CE2  | 3:M:265:LEU:HD21 | 2.53                     | 0.43              |
| 3:M:352:LYS:NZ   | 3:M:354:LYS:HD2  | 2.34                     | 0.43              |
| 1:A:445:THR:HA   | 1:A:448:ASN:ND2  | 2.34                     | 0.43              |
| 1:A:605:PHE:CG   | 1:A:606:PRO:HD2  | 2.54                     | 0.43              |
| 2:B:143:VAL:HG12 | 2:B:147:LYS:NZ   | 2.34                     | 0.43              |
| 2:B:162:LEU:O    | 2:B:166:ARG:HB2  | 2.18                     | 0.43              |
| 2:B:308:LEU:HG   | 2:B:575:HIS:HE1  | 1.83                     | 0.43              |
| 2:B:347:SER:O    | 2:B:351:ILE:HG23 | 2.18                     | 0.43              |
| 2:B:423:ASN:ND2  | 2:B:455:TYR:OH   | 2.52                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:499:THR:HG23 | 2:B:502:LEU:HD12 | 2.01                     | 0.43              |
| 3:M:39:ALA:HB3   | 3:M:44:ARG:NH1   | 2.33                     | 0.43              |
| 3:M:107:LEU:HB2  | 3:M:135:GLN:HE22 | 1.83                     | 0.43              |
| 4:S:4:PHE:CD1    | 4:S:6:LEU:HG     | 2.54                     | 0.43              |
| 1:A:50:LEU:O     | 1:A:55:LYS:HG3   | 2.18                     | 0.43              |
| 1:A:300:VAL:HG22 | 1:A:304:ASN:OD1  | 2.18                     | 0.43              |
| 1:A:304:ASN:HD22 | 4:S:82:GLU:CD    | 2.27                     | 0.43              |
| 2:B:105:LEU:HA   | 2:B:108:ARG:HG2  | 2.00                     | 0.43              |
| 2:B:225:CYS:HA   | 2:B:228:ASN:OD1  | 2.19                     | 0.43              |
| 2:B:253:SER:OG   | 3:M:76:ALA:HB1   | 2.18                     | 0.43              |
| 2:B:350:ASN:O    | 2:B:353:GLN:HG3  | 2.19                     | 0.43              |
| 2:B:366:ASP:HB3  | 2:B:369:PHE:CE1  | 2.54                     | 0.43              |
| 2:B:367:VAL:HG23 | 2:B:405:TYR:CD2  | 2.54                     | 0.43              |
| 2:B:527:TRP:O    | 2:B:531:SER:OG   | 2.26                     | 0.43              |
| 3:M:2:ILE:HG23   | 3:M:69:THR:HB    | 2.00                     | 0.43              |
| 3:M:37:ILE:HG23  | 3:M:64:TRP:CZ3   | 2.54                     | 0.43              |
| 3:M:147:GLU:HA   | 3:M:150:GLN:HE21 | 1.83                     | 0.43              |
| 3:M:254:ILE:HG12 | 3:M:257:CYS:HB3  | 2.00                     | 0.43              |
| 4:S:21:MET:HE2   | 4:S:23:PHE:CZ    | 2.53                     | 0.43              |
| 4:S:58:ILE:HD13  | 4:S:80:TYR:CB    | 2.49                     | 0.43              |
| 4:S:91:LEU:HD22  | 4:S:95:PHE:CE2   | 2.52                     | 0.43              |
| 1:A:66:PHE:HA    | 1:A:70:HIS:C     | 2.44                     | 0.43              |
| 1:A:485:GLU:HG3  | 1:A:516:ARG:HH22 | 1.84                     | 0.43              |
| 1:A:543:SER:HB3  | 1:A:579:ARG:NH2  | 2.34                     | 0.43              |
| 2:B:114:ARG:HG2  | 2:B:148:LEU:HA   | 2.00                     | 0.43              |
| 2:B:551:GLU:OE1  | 2:B:551:GLU:N    | 2.51                     | 0.43              |
| 3:M:12:GLY:O     | 3:M:33:ARG:NE    | 2.52                     | 0.43              |
| 3:M:74:ASN:O     | 3:M:77:MET:HG3   | 2.19                     | 0.43              |
| 4:S:87:PHE:O     | 4:S:91:LEU:HG    | 2.19                     | 0.43              |
| 1:A:220:GLU:OE1  | 1:A:220:GLU:N    | 2.52                     | 0.43              |
| 1:A:243:ASP:HA   | 1:A:245:GLN:CD   | 2.44                     | 0.43              |
| 1:A:467:GLN:O    | 1:A:471:ASN:ND2  | 2.52                     | 0.43              |
| 1:A:539:ALA:HB1  | 1:A:579:ARG:HH12 | 1.84                     | 0.43              |
| 1:A:615:LYS:HG2  | 1:A:618:LYS:HE2  | 2.01                     | 0.43              |
| 2:B:114:ARG:NH1  | 2:B:147:LYS:HB3  | 2.33                     | 0.43              |
| 2:B:253:SER:O    | 2:B:257:LEU:HG   | 2.19                     | 0.43              |
| 2:B:399:ILE:O    | 2:B:402:LYS:HE3  | 2.18                     | 0.43              |
| 2:B:473:PHE:CZ   | 2:B:509:LEU:HB3  | 2.54                     | 0.43              |
| 3:M:356:LYS:N    | 3:M:361:ALA:O    | 2.41                     | 0.43              |
| 4:S:110:VAL:O    | 4:S:114:VAL:HG23 | 2.19                     | 0.43              |
| 4:S:117:MET:O    | 4:S:124:ARG:N    | 2.51                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:543:SER:HB3  | 1:A:579:ARG:HH22 | 1.83                     | 0.42              |
| 1:A:615:LYS:HE3  | 1:A:615:LYS:HB3  | 1.75                     | 0.42              |
| 2:B:166:ARG:HH22 | 2:B:197:LEU:CB   | 2.32                     | 0.42              |
| 2:B:322:LYS:HA   | 2:B:325:PHE:CE2  | 2.53                     | 0.42              |
| 3:M:3:GLY:HA2    | 3:M:20:TYR:C     | 2.44                     | 0.42              |
| 3:M:20:TYR:HB3   | 3:M:118:PHE:C    | 2.44                     | 0.42              |
| 3:M:90:ALA:HA    | 3:M:94:GLY:O     | 2.19                     | 0.42              |
| 3:M:250:GLN:N    | 3:M:408:SER:O    | 2.52                     | 0.42              |
| 4:S:43:ASP:OD1   | 4:S:46:HIS:CD2   | 2.72                     | 0.42              |
| 4:S:95:PHE:CB    | 4:S:98:VAL:HB    | 2.48                     | 0.42              |
| 1:A:51:ASP:OD1   | 1:A:52:GLY:N     | 2.49                     | 0.42              |
| 1:A:362:SER:OG   | 1:A:365:ALA:HB3  | 2.19                     | 0.42              |
| 2:B:257:LEU:HB3  | 2:B:568:GLY:HA2  | 2.01                     | 0.42              |
| 3:M:59:LYS:HG2   | 3:M:64:TRP:CD1   | 2.54                     | 0.42              |
| 3:M:102:LYS:HA   | 3:M:105:PHE:CE1  | 2.54                     | 0.42              |
| 3:M:419:GLU:HB2  | 3:M:424:TYR:CZ   | 2.53                     | 0.42              |
| 1:A:16:PHE:O     | 1:A:20:ILE:HG22  | 2.19                     | 0.42              |
| 1:A:197:ASN:ND2  | 1:A:228:LEU:HD13 | 2.34                     | 0.42              |
| 2:B:411:ILE:HG22 | 2:B:447:ALA:CB   | 2.49                     | 0.42              |
| 2:B:450:TRP:CE3  | 2:B:451:ILE:HG12 | 2.53                     | 0.42              |
| 1:A:115:ALA:HA   | 1:A:118:ASN:ND2  | 2.34                     | 0.42              |
| 1:A:424:ILE:HA   | 1:A:427:LYS:HG2  | 2.01                     | 0.42              |
| 1:A:512:ALA:O    | 1:A:517:SER:OG   | 2.37                     | 0.42              |
| 3:M:3:GLY:CA     | 3:M:21:ARG:HB2   | 2.50                     | 0.42              |
| 3:M:41:GLN:CD    | 3:M:42:GLN:H     | 2.27                     | 0.42              |
| 3:M:185:MET:HE3  | 3:M:186:SER:O    | 2.19                     | 0.42              |
| 3:M:299:ARG:HD3  | 3:M:321:ASN:CG   | 2.44                     | 0.42              |
| 3:M:310:THR:C    | 3:M:383:LEU:H    | 2.20                     | 0.42              |
| 4:S:3:ARG:HD3    | 4:S:21:MET:CE    | 2.49                     | 0.42              |
| 1:A:50:LEU:O     | 1:A:54:SER:OG    | 2.38                     | 0.42              |
| 2:B:127:ARG:HH12 | 2:B:160:GLY:C    | 2.26                     | 0.42              |
| 2:B:248:LEU:HB3  | 2:B:249:SER:H    | 1.74                     | 0.42              |
| 2:B:534:PRO:HA   | 2:B:537:ALA:HB3  | 2.00                     | 0.42              |
| 2:B:544:GLU:C    | 2:B:545:LYS:HD2  | 2.44                     | 0.42              |
| 3:M:395:PRO:HA   | 3:M:396:PRO:HD2  | 1.90                     | 0.42              |
| 3:M:404:PRO:HA   | 3:M:436:ILE:HA   | 2.02                     | 0.42              |
| 4:S:24:ASP:O     | 4:S:28:LYS:N     | 2.36                     | 0.42              |
| 4:S:113:VAL:O    | 4:S:116:GLU:HB3  | 2.19                     | 0.42              |
| 1:A:150:GLU:O    | 1:A:154:ILE:HG12 | 2.18                     | 0.42              |
| 1:A:191:ARG:O    | 1:A:195:LEU:HG   | 2.20                     | 0.42              |
| 1:A:521:ILE:HA   | 1:A:524:ASN:HD21 | 1.84                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:578:PRO:HA   | 2:B:581:PHE:CE2  | 2.55                     | 0.42              |
| 3:M:11:LYS:HE2   | 3:M:13:GLU:OE2   | 2.19                     | 0.42              |
| 3:M:56:PHE:CD2   | 3:M:78:VAL:HG11  | 2.54                     | 0.42              |
| 3:M:221:VAL:O    | 3:M:223:GLU:HG3  | 2.20                     | 0.42              |
| 3:M:271:GLU:HA   | 3:M:272:ARG:NH1  | 2.34                     | 0.42              |
| 1:A:223:LYS:HA   | 1:A:226:VAL:HG23 | 2.01                     | 0.42              |
| 1:A:333:GLN:HB3  | 1:A:337:PHE:CE2  | 2.54                     | 0.42              |
| 1:A:464:ARG:HA   | 1:A:467:GLN:OE1  | 2.20                     | 0.42              |
| 3:M:111:LEU:HD21 | 3:M:133:ILE:HG21 | 2.02                     | 0.42              |
| 3:M:344:VAL:HA   | 3:M:381:ILE:HD13 | 2.01                     | 0.42              |
| 3:M:352:LYS:HZ2  | 3:M:365:LYS:HB3  | 1.84                     | 0.42              |
| 1:A:57:LYS:HE2   | 1:A:57:LYS:HB3   | 1.78                     | 0.42              |
| 1:A:78:GLU:O     | 1:A:81:ASN:HB2   | 2.20                     | 0.42              |
| 1:A:487:LEU:HD12 | 1:A:504:LEU:HD12 | 2.01                     | 0.42              |
| 1:A:505:GLY:HA3  | 1:A:544:THR:HG23 | 2.02                     | 0.42              |
| 1:A:568:GLN:H    | 1:A:568:GLN:CD   | 2.28                     | 0.42              |
| 2:B:440:ASP:OD1  | 2:B:440:ASP:N    | 2.51                     | 0.42              |
| 2:B:501:GLU:HA   | 2:B:504:GLN:CD   | 2.44                     | 0.42              |
| 3:M:14:VAL:HG13  | 3:M:33:ARG:NH2   | 2.34                     | 0.42              |
| 3:M:55:PHE:HB3   | 3:M:57:HIS:CD2   | 2.54                     | 0.42              |
| 3:M:70:LYS:H     | 3:M:71:GLN:NE2   | 2.18                     | 0.42              |
| 3:M:104:ASN:OD1  | 3:M:135:GLN:NE2  | 2.52                     | 0.42              |
| 3:M:268:PHE:HB2  | 3:M:274:ILE:CG2  | 2.50                     | 0.42              |
| 1:A:13:LEU:CD1   | 1:A:61:LYS:HG3   | 2.49                     | 0.42              |
| 1:A:97:PHE:CE2   | 1:A:101:LEU:HD22 | 2.55                     | 0.42              |
| 1:A:231:SER:O    | 1:A:235:ARG:HG2  | 2.19                     | 0.42              |
| 2:B:262:VAL:O    | 2:B:265:LYS:HB3  | 2.19                     | 0.42              |
| 2:B:563:LEU:HD21 | 2:B:578:PRO:HD3  | 2.01                     | 0.42              |
| 4:S:52:PHE:N     | 4:S:55:PHE:O     | 2.37                     | 0.42              |
| 1:A:241:SER:HB3  | 1:A:248:THR:CG2  | 2.50                     | 0.42              |
| 1:A:613:LEU:HD12 | 1:A:614:ALA:N    | 2.35                     | 0.42              |
| 2:B:158:ASP:OD1  | 2:B:159:GLN:N    | 2.53                     | 0.42              |
| 2:B:539:GLU:OE2  | 2:B:539:GLU:N    | 2.48                     | 0.42              |
| 3:M:30:ASP:OD1   | 3:M:31:ALA:N     | 2.52                     | 0.42              |
| 3:M:106:VAL:O    | 3:M:110:GLU:HG3  | 2.20                     | 0.42              |
| 3:M:398:SER:HA   | 3:M:442:TYR:O    | 2.20                     | 0.42              |
| 4:S:67:PHE:HE2   | 4:S:88:VAL:HG22  | 1.85                     | 0.42              |
| 4:S:74:ASN:OD1   | 4:S:74:ASN:N     | 2.53                     | 0.42              |
| 4:S:87:PHE:CE2   | 4:S:91:LEU:HD11  | 2.54                     | 0.42              |
| 1:A:350:LEU:HD23 | 1:A:350:LEU:HA   | 1.83                     | 0.41              |
| 2:B:52:PRO:O     | 2:B:55:VAL:HG12  | 2.19                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:66:LYS:HE3   | 2:B:105:LEU:HD23 | 2.01                     | 0.41              |
| 2:B:118:ILE:HG13 | 2:B:122:LEU:HD23 | 2.01                     | 0.41              |
| 2:B:293:SER:OG   | 3:M:289:ARG:NH2  | 2.53                     | 0.41              |
| 2:B:521:ASP:HA   | 2:B:524:TYR:CG   | 2.55                     | 0.41              |
| 3:M:81:PHE:CZ    | 3:M:116:LEU:HB2  | 2.55                     | 0.41              |
| 3:M:184:LEU:O    | 3:M:192:LEU:N    | 2.53                     | 0.41              |
| 3:M:334:ARG:O    | 3:M:397:ILE:HG23 | 2.19                     | 0.41              |
| 1:A:350:LEU:HB3  | 1:A:388:ARG:HB2  | 2.03                     | 0.41              |
| 1:A:386:ARG:O    | 1:A:390:VAL:HG23 | 2.20                     | 0.41              |
| 1:A:509:ASN:OD1  | 1:A:509:ASN:N    | 2.50                     | 0.41              |
| 2:B:139:LYS:HA   | 2:B:179:ASN:HD21 | 1.85                     | 0.41              |
| 2:B:236:GLU:OE1  | 2:B:236:GLU:N    | 2.47                     | 0.41              |
| 2:B:525:ILE:HA   | 2:B:528:ARG:HE   | 1.85                     | 0.41              |
| 3:M:264:ARG:HA   | 3:M:264:ARG:HD3  | 1.76                     | 0.41              |
| 3:M:340:ASN:O    | 3:M:383:LEU:HD23 | 2.19                     | 0.41              |
| 1:A:161:MET:HE1  | 1:A:163:SER:HB3  | 2.02                     | 0.41              |
| 1:A:185:MET:HA   | 1:A:188:TRP:CH2  | 2.55                     | 0.41              |
| 1:A:409:MET:O    | 1:A:413:LEU:HG   | 2.20                     | 0.41              |
| 1:A:439:TYR:O    | 1:A:443:VAL:HG23 | 2.21                     | 0.41              |
| 1:A:546:ILE:HD12 | 1:A:546:ILE:HA   | 1.95                     | 0.41              |
| 1:A:605:PHE:HE1  | 2:B:520:ARG:HD2  | 1.86                     | 0.41              |
| 2:B:492:PHE:CD1  | 2:B:496:PRO:HA   | 2.55                     | 0.41              |
| 3:M:399:MET:HE2  | 3:M:399:MET:HB3  | 1.80                     | 0.41              |
| 1:A:231:SER:HB3  | 1:A:279:ARG:NH1  | 2.35                     | 0.41              |
| 1:A:357:ALA:CB   | 1:A:392:LEU:HD12 | 2.50                     | 0.41              |
| 1:A:397:CYS:SG   | 1:A:401:ASN:ND2  | 2.93                     | 0.41              |
| 2:B:115:VAL:HG22 | 2:B:116:ASP:OD1  | 2.21                     | 0.41              |
| 2:B:190:SER:O    | 2:B:192:PRO:HD2  | 2.20                     | 0.41              |
| 2:B:316:ILE:C    | 2:B:318:LYS:N    | 2.78                     | 0.41              |
| 2:B:339:LEU:O    | 2:B:342:MET:HB2  | 2.20                     | 0.41              |
| 2:B:566:HIS:CG   | 2:B:571:ALA:HB3  | 2.56                     | 0.41              |
| 3:M:19:VAL:HG13  | 3:M:24:ILE:HG13  | 2.03                     | 0.41              |
| 3:M:37:ILE:HG12  | 3:M:64:TRP:HZ3   | 1.85                     | 0.41              |
| 3:M:180:SER:HB2  | 3:M:438:ARG:HH21 | 1.85                     | 0.41              |
| 3:M:240:LYS:HG2  | 3:M:242:ILE:H    | 1.85                     | 0.41              |
| 3:M:258:THR:O    | 3:M:286:MET:HE2  | 2.20                     | 0.41              |
| 4:S:86:ASN:O     | 4:S:90:VAL:HG23  | 2.20                     | 0.41              |
| 1:A:18:SER:HA    | 1:A:21:ARG:NH1   | 2.35                     | 0.41              |
| 1:A:29:GLU:O     | 1:A:33:ILE:HG13  | 2.20                     | 0.41              |
| 1:A:380:GLU:HB3  | 1:A:386:ARG:CZ   | 2.51                     | 0.41              |
| 1:A:485:GLU:HA   | 1:A:488:GLN:CD   | 2.46                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:143:VAL:HG12 | 2:B:147:LYS:HZ3  | 1.84                     | 0.41              |
| 3:M:296:LEU:HA   | 3:M:297:PRO:HD3  | 1.97                     | 0.41              |
| 3:M:324:PRO:HA   | 3:M:371:GLY:N    | 2.35                     | 0.41              |
| 1:A:401:ASN:O    | 1:A:405:ILE:HG12 | 2.21                     | 0.41              |
| 2:B:127:ARG:HB3  | 2:B:131:LYS:NZ   | 2.36                     | 0.41              |
| 2:B:423:ASN:OD1  | 2:B:458:ARG:NH1  | 2.54                     | 0.41              |
| 2:B:464:GLU:HG2  | 2:B:465:LEU:H    | 1.86                     | 0.41              |
| 3:M:65:LEU:HD11  | 3:M:85:MET:SD    | 2.61                     | 0.41              |
| 3:M:341:THR:HG23 | 3:M:381:ILE:HG23 | 2.03                     | 0.41              |
| 1:A:250:TYR:HB3  | 1:A:302:HIS:CE1  | 2.56                     | 0.41              |
| 1:A:370:ILE:O    | 1:A:374:ILE:HG13 | 2.21                     | 0.41              |
| 1:A:505:GLY:O    | 1:A:551:LEU:HD12 | 2.20                     | 0.41              |
| 2:B:151:ILE:HG23 | 2:B:152:ASN:OD1  | 2.20                     | 0.41              |
| 3:M:83:TYR:O     | 3:M:84:LYS:C     | 2.63                     | 0.41              |
| 3:M:108:ILE:O    | 3:M:112:LEU:HD23 | 2.20                     | 0.41              |
| 4:S:86:ASN:HA    | 4:S:89:GLU:OE2   | 2.20                     | 0.41              |
| 1:A:43:LYS:HG2   | 1:A:58:TYR:CE2   | 2.54                     | 0.41              |
| 1:A:270:PRO:HB3  | 1:A:320:HIS:ND1  | 2.35                     | 0.41              |
| 1:A:462:TRP:HB2  | 1:A:499:VAL:HG21 | 2.02                     | 0.41              |
| 1:A:533:CYS:SG   | 1:A:538:ARG:HG2  | 2.61                     | 0.41              |
| 2:B:94:ASP:HA    | 2:B:97:ASP:OD2   | 2.21                     | 0.41              |
| 2:B:468:SER:O    | 2:B:471:GLU:N    | 2.44                     | 0.41              |
| 3:M:80:GLU:HA    | 3:M:83:TYR:CD2   | 2.55                     | 0.41              |
| 3:M:313:GLU:HG2  | 3:M:380:GLU:HB3  | 2.03                     | 0.41              |
| 3:M:338:PRO:HG2  | 3:M:381:ILE:HB   | 2.02                     | 0.41              |
| 4:S:37:ALA:O     | 4:S:41:VAL:HG22  | 2.20                     | 0.41              |
| 4:S:49:PHE:CE1   | 4:S:77:ASN:HB3   | 2.55                     | 0.41              |
| 1:A:95:TYR:HD1   | 1:A:134:CYS:SG   | 2.43                     | 0.41              |
| 1:A:116:ILE:HG23 | 1:A:131:ALA:HB1  | 2.02                     | 0.41              |
| 1:A:232:ARG:O    | 1:A:236:ILE:HG13 | 2.21                     | 0.41              |
| 1:A:246:ASP:OD2  | 4:S:130:LYS:HG3  | 2.21                     | 0.41              |
| 1:A:404:GLN:CD   | 1:A:404:GLN:H    | 2.29                     | 0.41              |
| 1:A:569:LEU:O    | 1:A:570:LYS:HE2  | 2.21                     | 0.41              |
| 1:A:591:SER:OG   | 1:A:593:ASP:OD1  | 2.21                     | 0.41              |
| 2:B:4:SER:OG     | 3:M:105:PHE:N    | 2.54                     | 0.41              |
| 2:B:10:ASN:O     | 2:B:11:LYS:HB2   | 2.20                     | 0.41              |
| 2:B:282:LYS:HG3  | 2:B:283:LYS:N    | 2.36                     | 0.41              |
| 2:B:286:PRO:HD2  | 2:B:287:PRO:HD2  | 2.03                     | 0.41              |
| 2:B:379:ARG:O    | 2:B:383:LYS:HG3  | 2.20                     | 0.41              |
| 2:B:455:TYR:HA   | 2:B:457:GLU:OE2  | 2.21                     | 0.41              |
| 3:M:20:TYR:HB3   | 3:M:118:PHE:CA   | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:170:ARG:NH1  | 3:M:428:ASP:O    | 2.42                     | 0.41              |
| 3:M:355:TYR:HE2  | 3:M:357:ALA:HB2  | 1.85                     | 0.41              |
| 2:B:205:ASN:O    | 2:B:209:THR:HG23 | 2.21                     | 0.41              |
| 2:B:208:LEU:HD13 | 2:B:243:ARG:HG3  | 2.03                     | 0.41              |
| 2:B:263:LEU:O    | 2:B:266:PHE:N    | 2.51                     | 0.41              |
| 2:B:280:LEU:HA   | 2:B:283:LYS:HG2  | 2.02                     | 0.41              |
| 2:B:306:ILE:HD13 | 2:B:309:ILE:HD12 | 2.03                     | 0.41              |
| 2:B:347:SER:O    | 2:B:350:ASN:N    | 2.54                     | 0.41              |
| 3:M:126:THR:HA   | 3:M:129:LEU:HG   | 2.02                     | 0.41              |
| 3:M:340:ASN:HD22 | 3:M:384:LEU:H    | 1.68                     | 0.41              |
| 1:A:31:LYS:O     | 1:A:35:LYS:HG3   | 2.21                     | 0.40              |
| 1:A:88:TYR:N     | 4:S:142:GLU:OXT  | 2.54                     | 0.40              |
| 1:A:417:ASP:O    | 1:A:421:ARG:HB2  | 2.21                     | 0.40              |
| 2:B:62:ASN:OD1   | 2:B:64:GLU:HG2   | 2.20                     | 0.40              |
| 2:B:304:ARG:CZ   | 2:B:575:HIS:CD2  | 3.04                     | 0.40              |
| 2:B:370:VAL:O    | 2:B:374:VAL:HG23 | 2.21                     | 0.40              |
| 2:B:374:VAL:HG21 | 2:B:406:VAL:HG13 | 2.02                     | 0.40              |
| 3:M:5:LEU:C      | 3:M:6:PHE:HD1    | 2.29                     | 0.40              |
| 3:M:123:ASN:OD1  | 3:M:124:SER:N    | 2.53                     | 0.40              |
| 3:M:171:ASN:HA   | 3:M:205:TYR:O    | 2.21                     | 0.40              |
| 3:M:185:MET:HE1  | 3:M:300:VAL:O    | 2.21                     | 0.40              |
| 3:M:318:ILE:O    | 3:M:374:GLU:HA   | 2.20                     | 0.40              |
| 3:M:345:GLN:O    | 3:M:379:ALA:HA   | 2.20                     | 0.40              |
| 4:S:55:PHE:HD2   | 4:S:71:VAL:O     | 2.04                     | 0.40              |
| 4:S:57:ILE:HA    | 4:S:70:CYS:HA    | 2.03                     | 0.40              |
| 1:A:173:LEU:HD13 | 1:A:210:LEU:HD13 | 2.03                     | 0.40              |
| 1:A:271:PRO:HA   | 1:A:277:ARG:NH1  | 2.37                     | 0.40              |
| 1:A:277:ARG:O    | 1:A:280:LEU:HB3  | 2.22                     | 0.40              |
| 1:A:333:GLN:HA   | 1:A:336:GLN:OE1  | 2.22                     | 0.40              |
| 2:B:11:LYS:CG    | 2:B:12:LYS:HG3   | 2.50                     | 0.40              |
| 2:B:248:LEU:HD13 | 2:B:248:LEU:HA   | 1.93                     | 0.40              |
| 2:B:271:PRO:HA   | 2:B:277:TYR:HB3  | 2.03                     | 0.40              |
| 2:B:378:GLY:HA3  | 2:B:413:VAL:CG1  | 2.52                     | 0.40              |
| 2:B:501:GLU:O    | 2:B:505:GLN:HG3  | 2.22                     | 0.40              |
| 1:A:94:GLY:O     | 1:A:98:ILE:HG12  | 2.20                     | 0.40              |
| 1:A:155:LEU:HD12 | 1:A:165:LYS:HD3  | 2.04                     | 0.40              |
| 1:A:463:TYR:HE1  | 2:B:516:ASN:HA   | 1.87                     | 0.40              |
| 1:A:559:ILE:HA   | 1:A:562:VAL:HG22 | 2.03                     | 0.40              |
| 1:A:600:GLU:CD   | 1:A:602:MET:H    | 2.29                     | 0.40              |
| 2:B:99:ASN:HB3   | 2:B:102:ILE:HB   | 2.02                     | 0.40              |
| 2:B:305:ASN:O    | 2:B:309:ILE:HG13 | 2.21                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:B:405:TYR:O   | 2:B:408:GLN:HB2  | 2.22                     | 0.40              |
| 2:B:437:ASP:OD1 | 2:B:437:ASP:N    | 2.53                     | 0.40              |
| 2:B:575:HIS:C   | 2:B:576:LYS:HD3  | 2.46                     | 0.40              |
| 3:M:6:PHE:CD1   | 3:M:17:SER:HA    | 2.57                     | 0.40              |
| 3:M:409:GLY:O   | 3:M:411:LYS:HE2  | 2.21                     | 0.40              |
| 4:S:8:GLN:HA    | 4:S:14:THR:HA    | 2.03                     | 0.40              |
| 4:S:49:PHE:CD1  | 4:S:77:ASN:HB3   | 2.56                     | 0.40              |
| 3:M:59:LYS:C    | 3:M:61:SER:H     | 2.29                     | 0.40              |
| 3:M:112:LEU:HA  | 3:M:115:ILE:HG22 | 2.03                     | 0.40              |
| 3:M:181:VAL:HB  | 3:M:439:SER:HA   | 2.04                     | 0.40              |
| 3:M:214:PHE:CE1 | 3:M:412:VAL:HG22 | 2.56                     | 0.40              |
| 4:S:1:MET:H2    | 4:S:3:ARG:HH21   | 1.69                     | 0.40              |
| 4:S:15:ARG:CZ   | 4:S:15:ARG:HA    | 2.52                     | 0.40              |
| 1:A:10:MET:CG   | 1:A:57:LYS:HB2   | 2.52                     | 0.40              |
| 1:A:222:PHE:O   | 1:A:268:TYR:OH   | 2.37                     | 0.40              |
| 1:A:347:TYR:O   | 1:A:350:LEU:HB2  | 2.22                     | 0.40              |
| 1:A:467:GLN:HA  | 1:A:470:ILE:HG12 | 2.03                     | 0.40              |
| 1:A:591:SER:O   | 1:A:592:THR:OG1  | 2.33                     | 0.40              |
| 3:M:203:LYS:HD3 | 3:M:282:GLU:HB2  | 2.03                     | 0.40              |
| 3:M:328:ALA:C   | 3:M:331:ILE:HD11 | 2.46                     | 0.40              |
| 4:S:87:PHE:CZ   | 4:S:91:LEU:HD21  | 2.57                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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   | A     | 611/628 (97%) | 546 (89%) | 65 (11%) | 0        | 100         | 100 |
| 2   | B     | 577/944 (61%) | 509 (88%) | 67 (12%) | 1 (0%)   | 43          | 78  |
| 3   | M     | 422/446 (95%) | 357 (85%) | 65 (15%) | 0        | 100         | 100 |
| 4   | S     | 140/142 (99%) | 116 (83%) | 24 (17%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| All | All   | 1750/2160 (81%) | 1528 (87%) | 221 (13%) | 1 (0%)   | 49          | 83 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 316 | ILE  |

### 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   | A     | 537/548 (98%)   | 535 (100%)  | 2 (0%)   | 84          | 84  |
| 2   | B     | 522/840 (62%)   | 522 (100%)  | 0        | 100         | 100 |
| 3   | M     | 384/398 (96%)   | 381 (99%)   | 3 (1%)   | 73          | 80  |
| 4   | S     | 131/131 (100%)  | 131 (100%)  | 0        | 100         | 100 |
| All | All   | 1574/1917 (82%) | 1569 (100%) | 5 (0%)   | 84          | 86  |

All (5) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 563 | LEU  |
| 1   | A     | 599 | LEU  |
| 3   | M     | 115 | ILE  |
| 3   | M     | 252 | ILE  |
| 3   | M     | 322 | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 22  | ASN  |
| 1   | A     | 34  | ASN  |
| 1   | A     | 70  | HIS  |
| 1   | A     | 105 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 118 | ASN  |
| 1   | A     | 124 | ASN  |
| 1   | A     | 194 | HIS  |
| 1   | A     | 197 | ASN  |
| 1   | A     | 200 | HIS  |
| 1   | A     | 266 | GLN  |
| 1   | A     | 302 | HIS  |
| 1   | A     | 333 | GLN  |
| 1   | A     | 363 | HIS  |
| 1   | A     | 448 | ASN  |
| 1   | A     | 495 | ASN  |
| 1   | A     | 522 | GLN  |
| 1   | A     | 531 | HIS  |
| 2   | B     | 89  | ASN  |
| 2   | B     | 191 | HIS  |
| 2   | B     | 195 | ASN  |
| 2   | B     | 238 | GLN  |
| 2   | B     | 305 | ASN  |
| 2   | B     | 353 | GLN  |
| 2   | B     | 423 | ASN  |
| 2   | B     | 474 | HIS  |
| 2   | B     | 504 | GLN  |
| 3   | M     | 38  | HIS  |
| 3   | M     | 72  | ASN  |
| 3   | M     | 135 | GLN  |
| 3   | M     | 150 | GLN  |
| 3   | M     | 154 | GLN  |
| 3   | M     | 182 | ASN  |
| 3   | M     | 250 | GLN  |
| 3   | M     | 376 | GLN  |
| 3   | M     | 427 | HIS  |
| 4   | S     | 92  | 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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-10751. These allow visual inspection of the internal detail of the map and identification of artifacts.

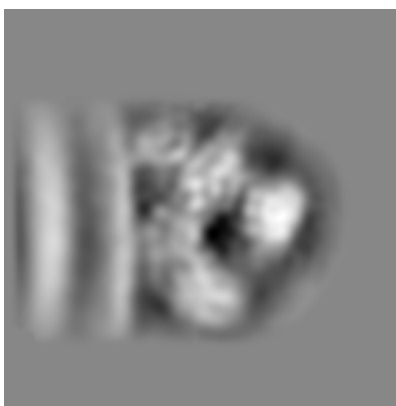
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



X

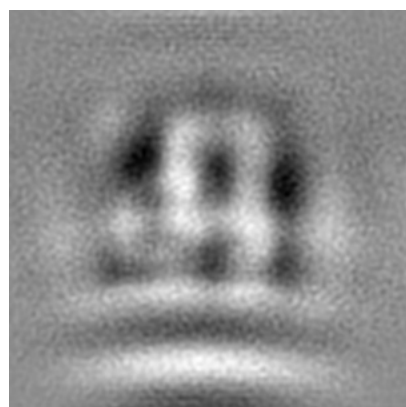


Y

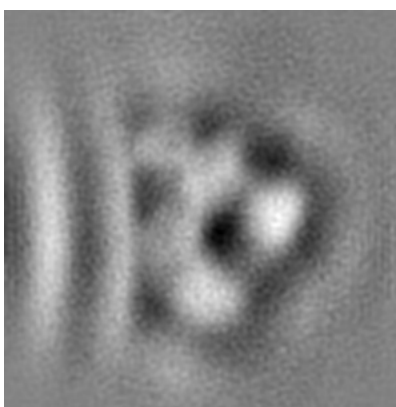


Z

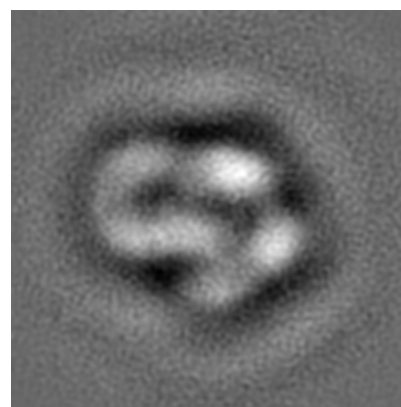
#### 6.1.2 Raw map



X



Y



Z

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

## 6.2 Central slices [i](#)

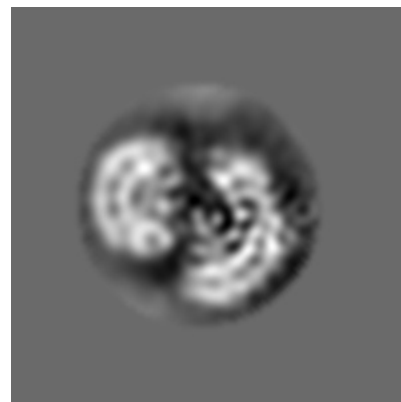
### 6.2.1 Primary map



X Index: 60

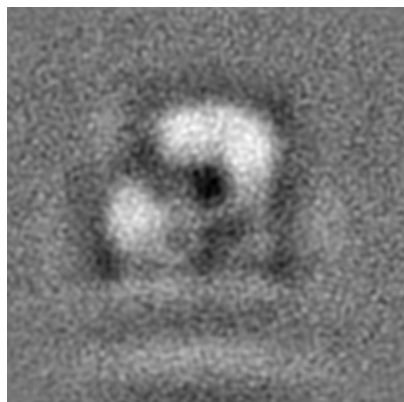


Y Index: 60

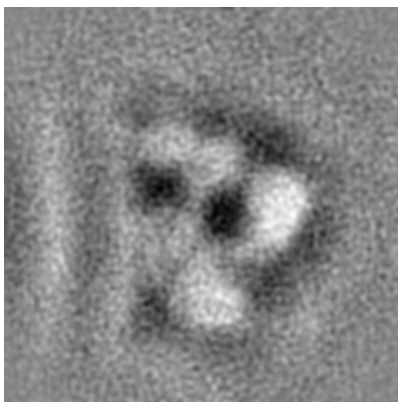


Z Index: 60

### 6.2.2 Raw map



X Index: 60



Y Index: 60

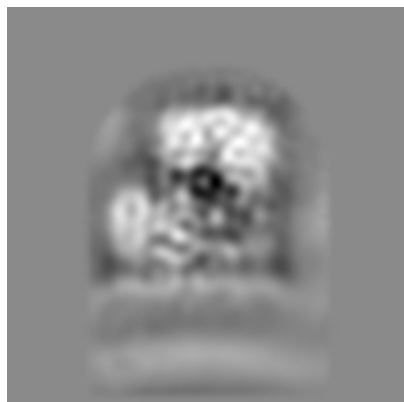


Z Index: 60

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

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

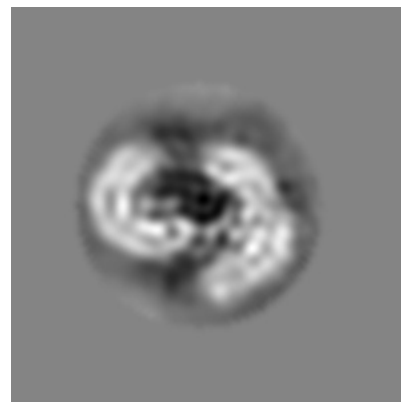
### 6.3.1 Primary map



X Index: 58



Y Index: 69

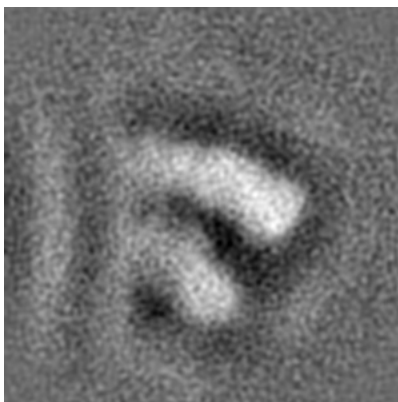


Z Index: 65

### 6.3.2 Raw map



X Index: 59



Y Index: 69



Z Index: 65

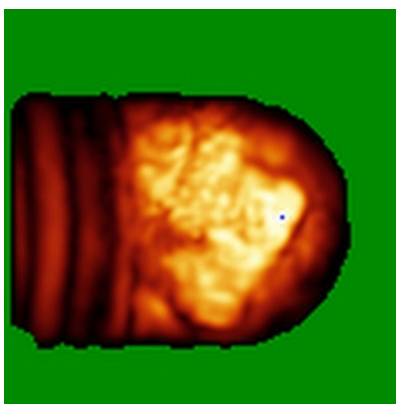
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

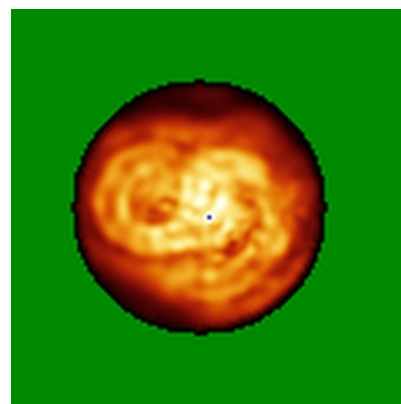
### 6.4.1 Primary map



X



Y

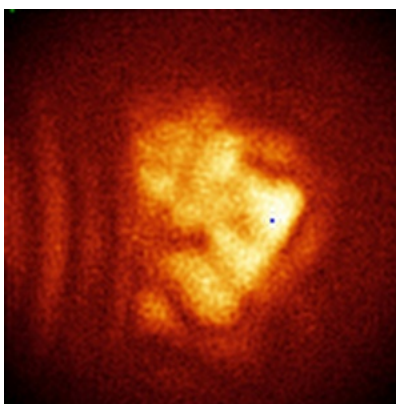


Z

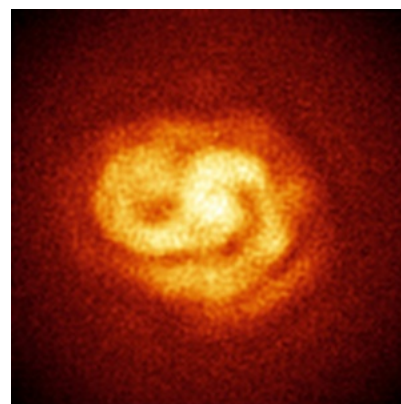
### 6.4.2 Raw map



X



Y

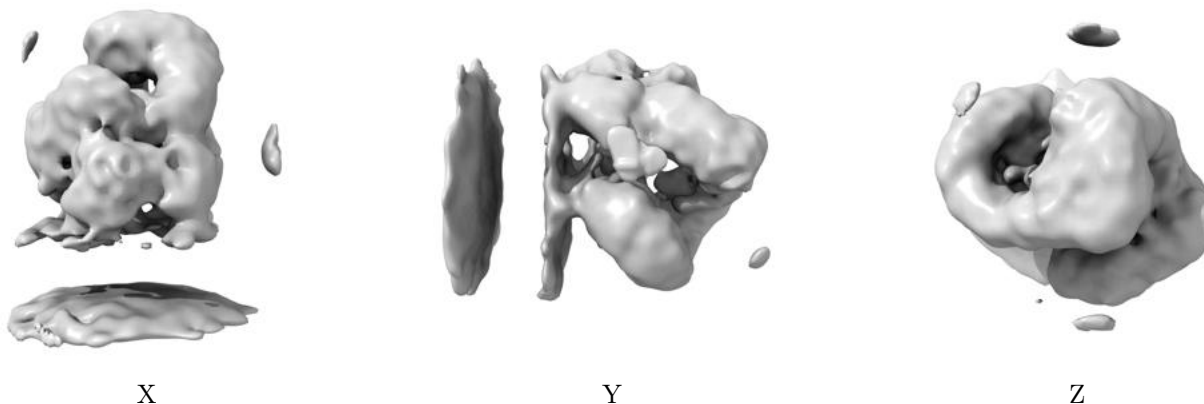


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

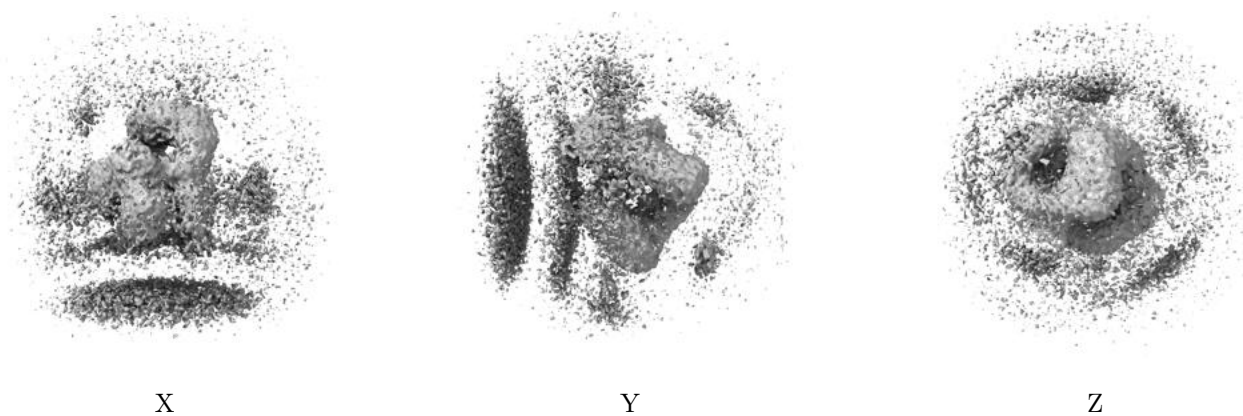
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

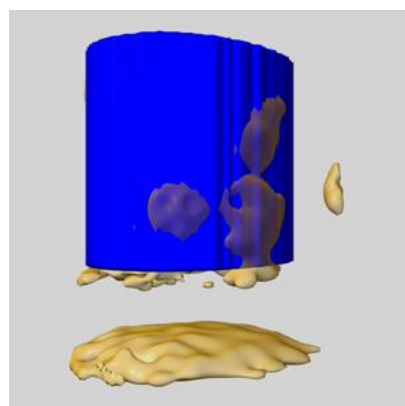
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

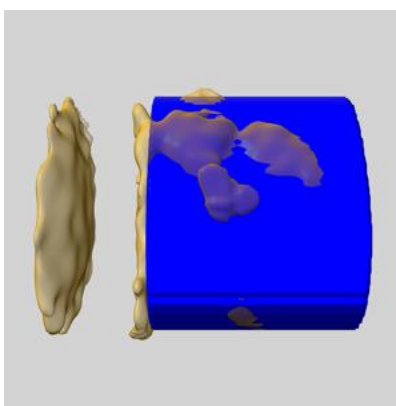
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

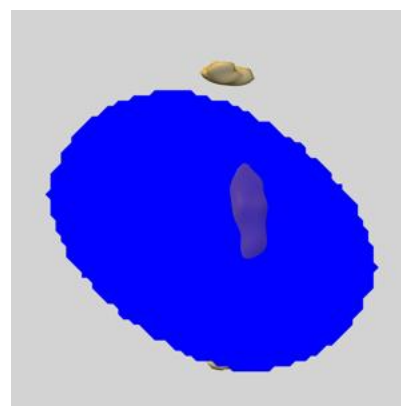
### 6.6.1 emd\_10751\_msk\_1.map [i](#)



X



Y



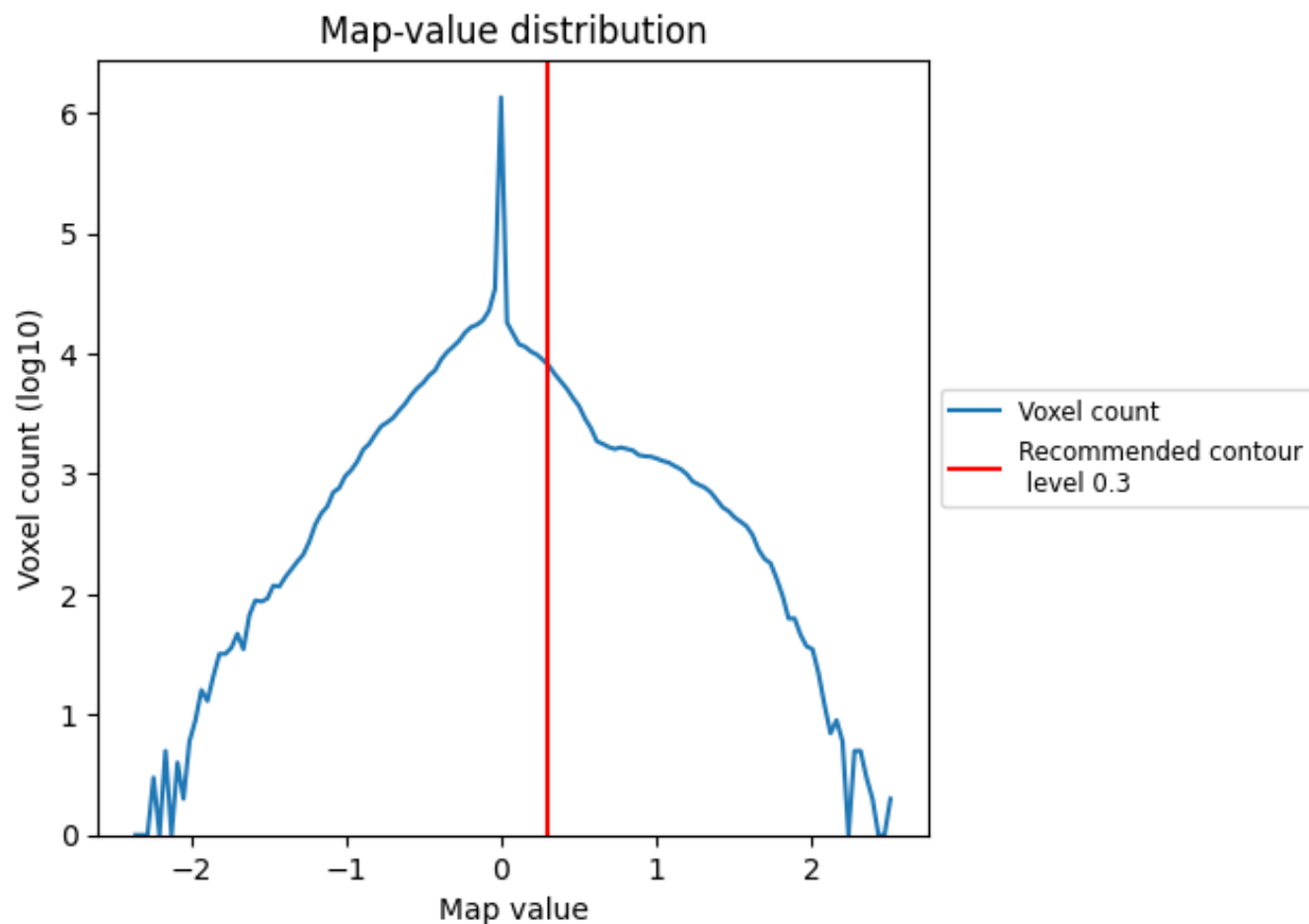
Z



## 7 Map analysis [i](#)

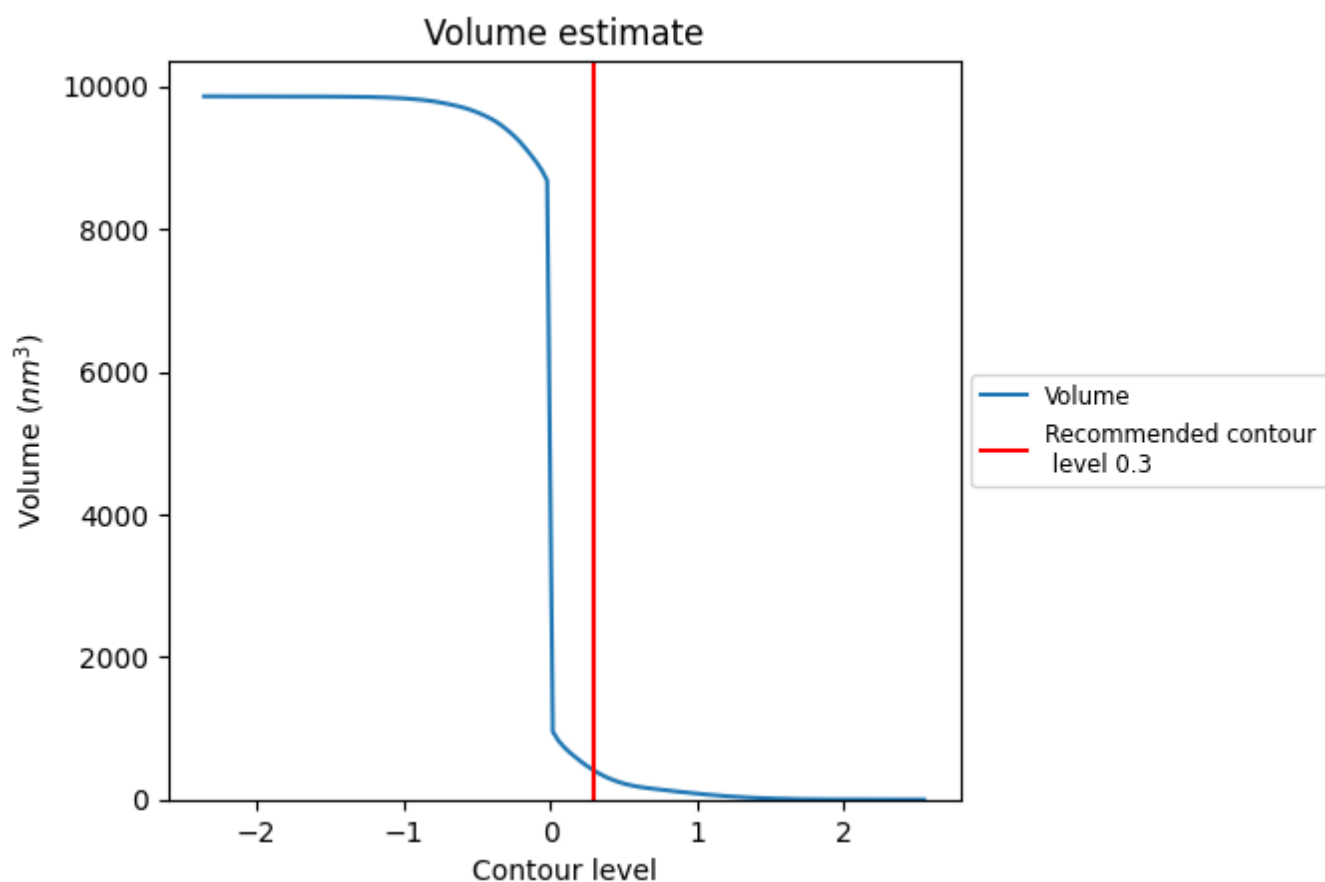
This section contains the results of statistical analysis of the map.

### 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.

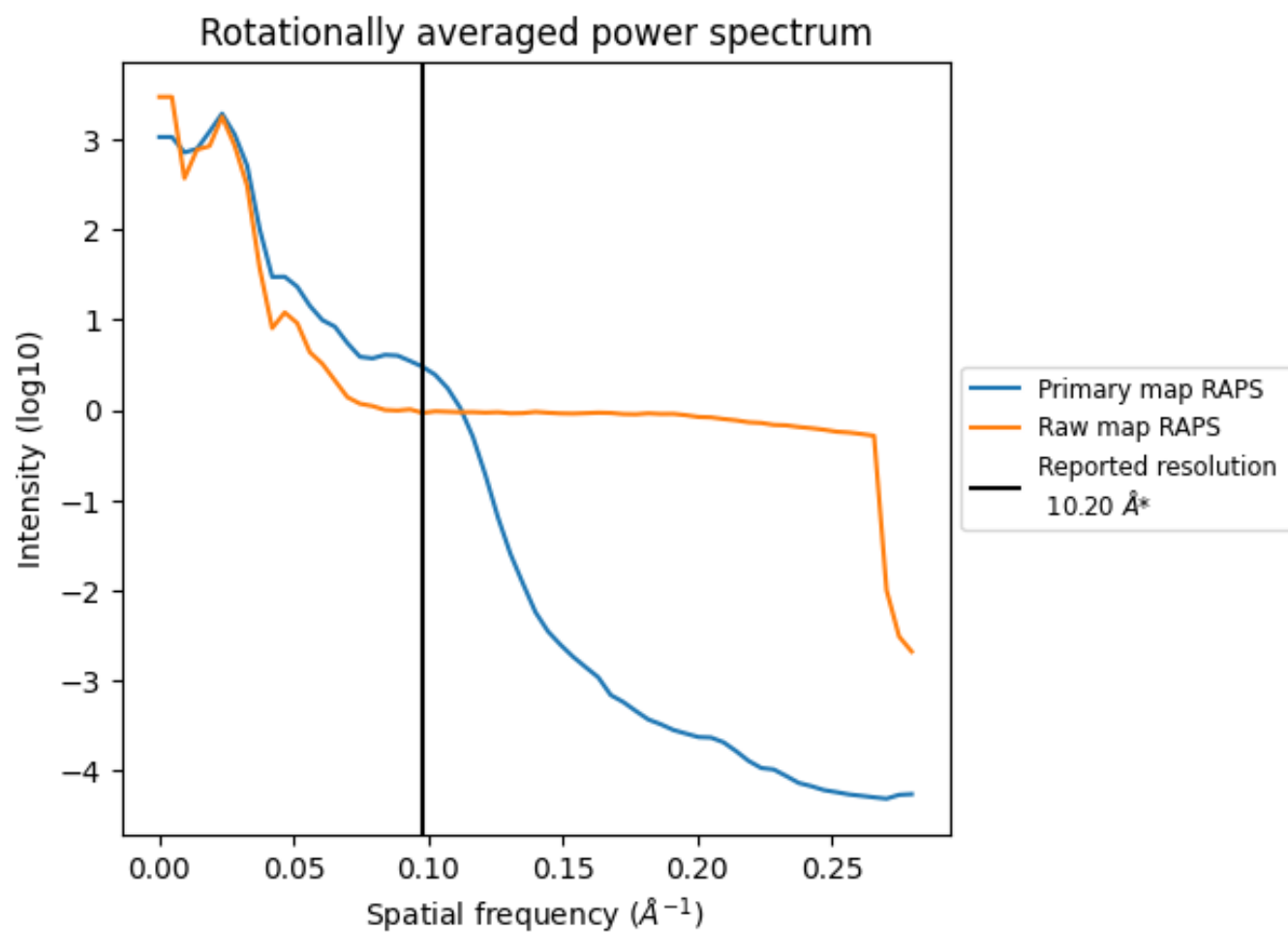
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 408 nm<sup>3</sup>; this corresponds to an approximate mass of 368 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 ⓘ

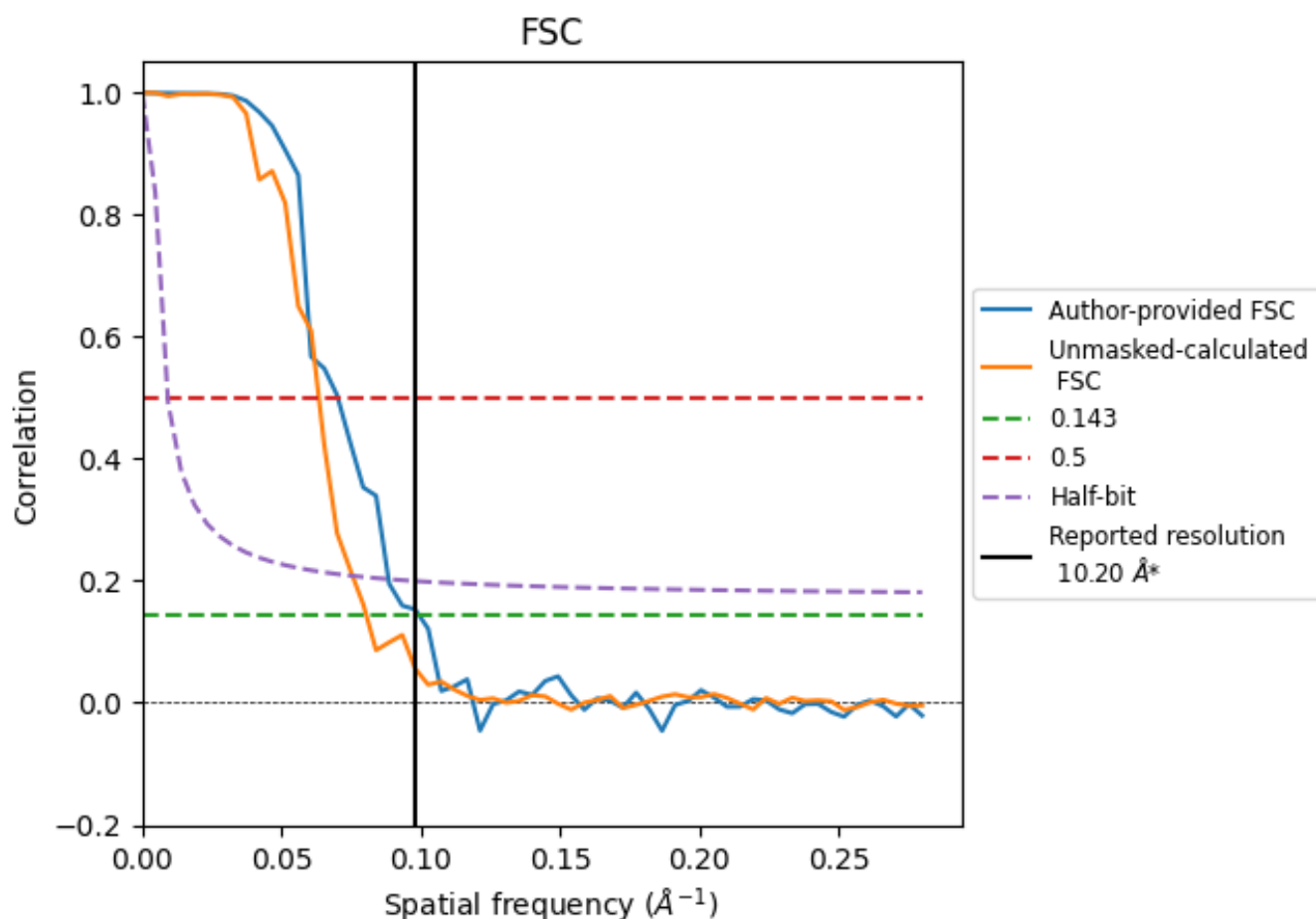


\*Reported resolution corresponds to spatial frequency of 0.098 Å⁻¹

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.098  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

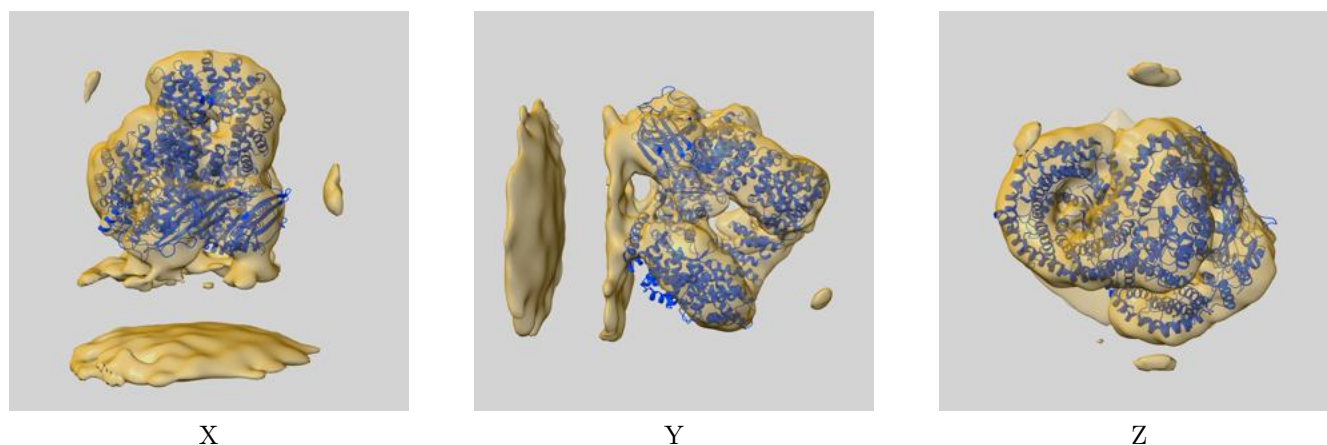
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 10.20                              | -     | -        |
| Author-provided FSC curve | 10.06                              | 14.25 | 11.31    |
| Unmasked-calculated*      | 12.44                              | 15.77 | 13.25    |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 12.44 differs from the reported value 10.2 by more than 10 %

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

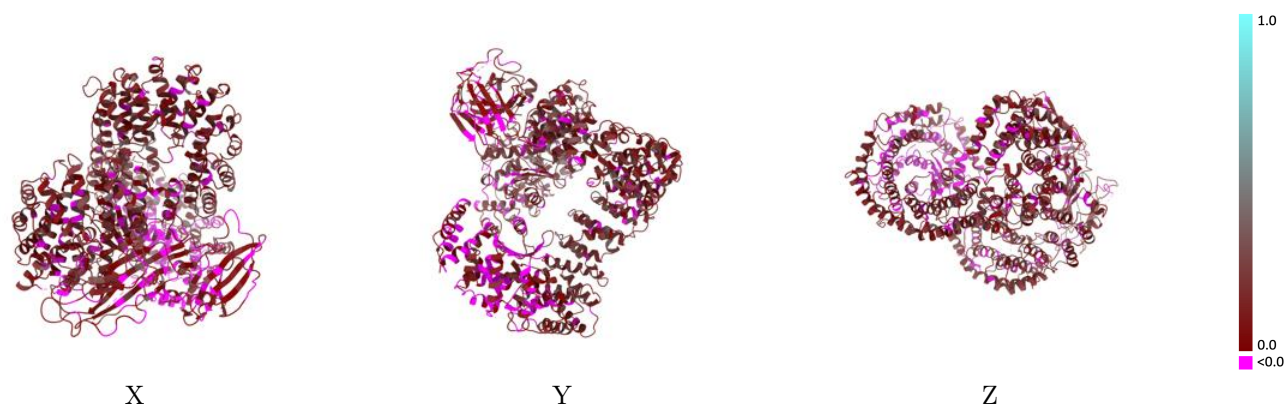
This section contains information regarding the fit between EMDB map EMD-10751 and PDB model 6YAH. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



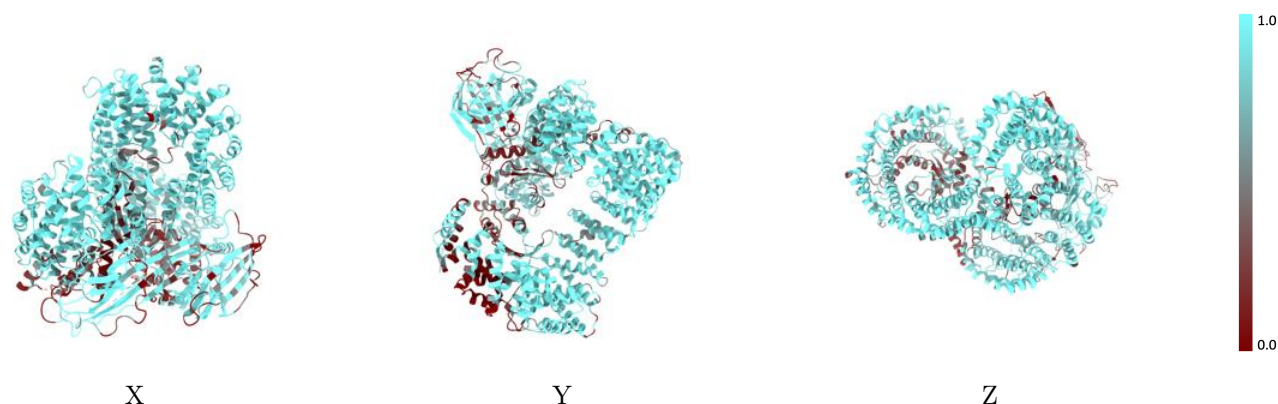
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

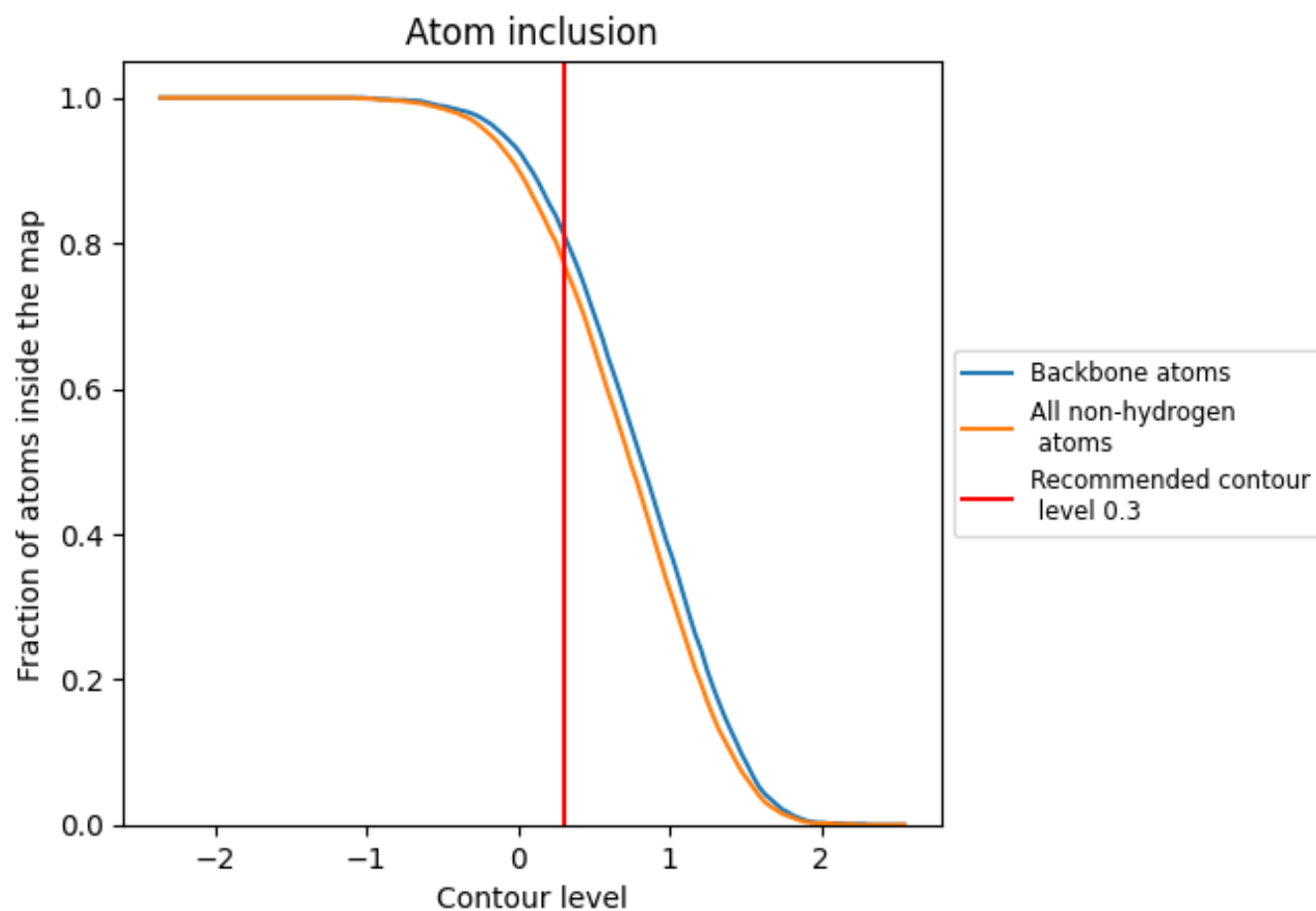
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.3).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.3) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score             |
|-------|--------------------|---------------------|
| All   | <div></div> 0.7740 | <div></div> 0.1050  |
| A     | <div></div> 0.8510 | <div></div> 0.1080  |
| B     | <div></div> 0.8590 | <div></div> 0.1330  |
| M     | <div></div> 0.6700 | <div></div> 0.0980  |
| S     | <div></div> 0.4310 | <div></div> -0.0020 |

