



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:35 AM UTC

PDB ID : 8WFZ / pdb\_00008wfz  
EMDB ID : EMD-37500  
Title : AtGORK Full length 2  
Authors : Chen, Y.H.; Li, Q.Y.; Qin, L.; Tang, L.H.; zhang, C.R.  
Deposited on : 2023-09-20  
Resolution : 4.30 Å(reported)

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

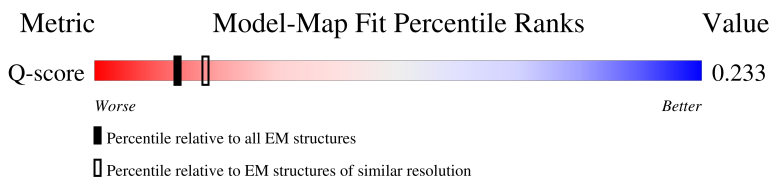
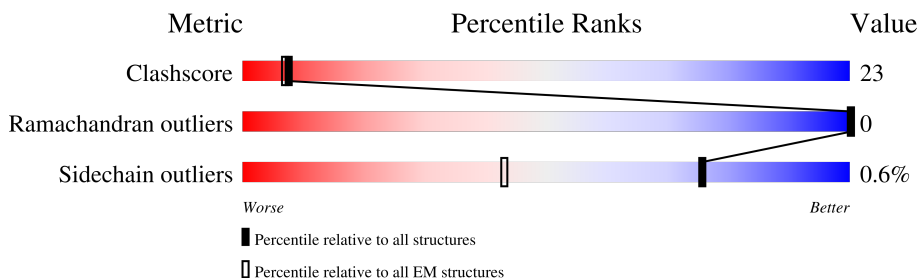
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 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                       | 4585 ( 3.80 - 4.80 )                                     |

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     | 820    | <div> <div>14%</div> <div>45%</div> <div>35%</div> <div>20%</div> </div> |
| 1   | B     | 820    | <div> <div>15%</div> <div>45%</div> <div>35%</div> <div>20%</div> </div> |
| 1   | C     | 820    | <div> <div>16%</div> <div>44%</div> <div>36%</div> <div>20%</div> </div> |
| 1   | D     | 820    | <div> <div>13%</div> <div>48%</div> <div>32%</div> <div>20%</div> </div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21266 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.

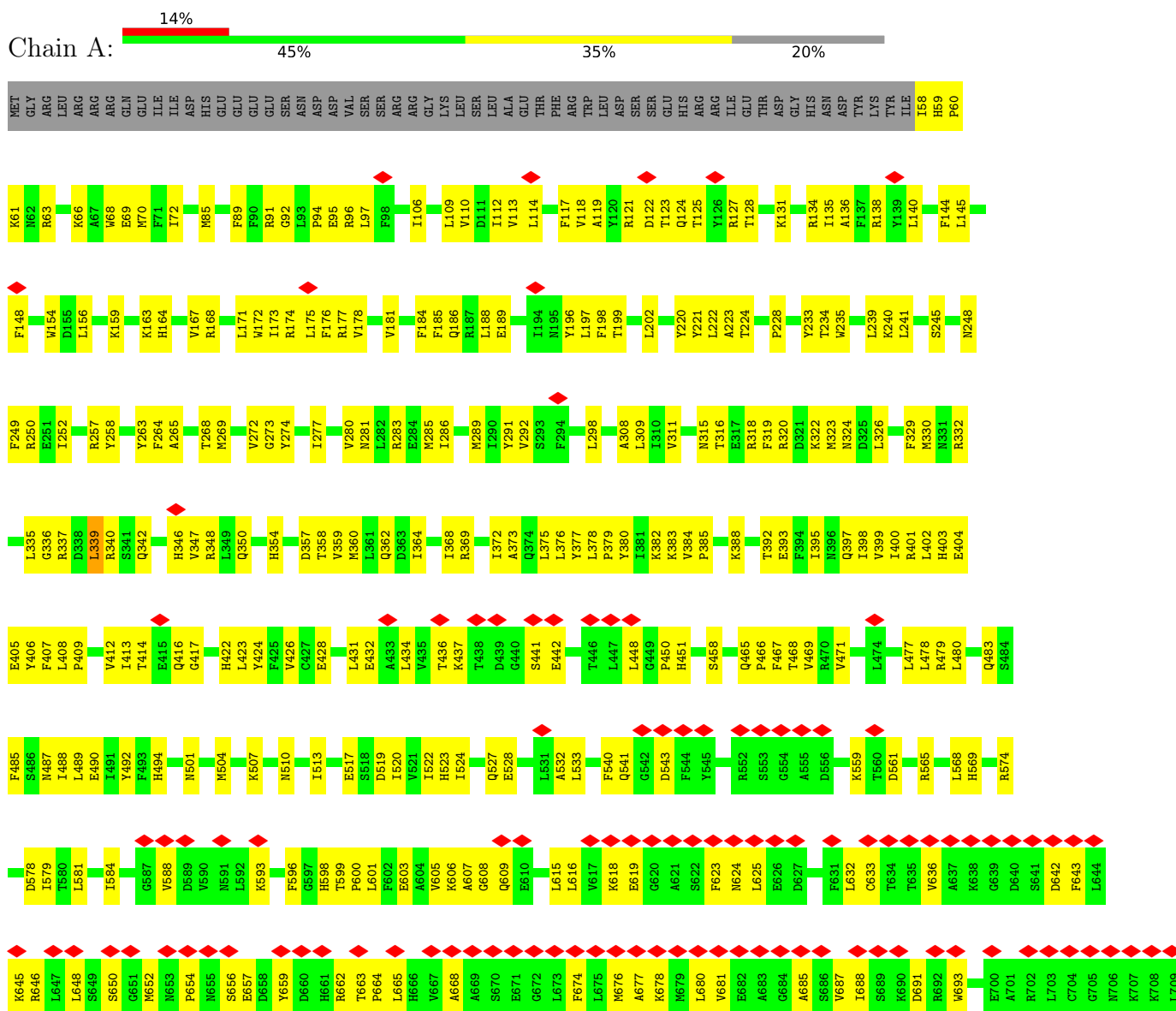
- Molecule 1 is a protein called Potassium channel GORK.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 656      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5315  | 3452 | 885 | 953 | 25 |         |       |
| 1   | B     | 656      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5315  | 3452 | 885 | 953 | 25 |         |       |
| 1   | C     | 656      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5321  | 3455 | 887 | 954 | 25 |         |       |
| 1   | D     | 656      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5315  | 3452 | 885 | 953 | 25 |         |       |

### 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: Potassium channel GORK





Chain C: 16% 44% 36% 20%

Phylogenetic tree showing relationships between various amino acid sequences (e.g., MET, ARG, GLY, LEU, SER, THR, ASP, GLN, VAL, ASN, ASP, VAL, SER, ARG, ARG, GLY, LEU, SER, LEU, ALA, GLU, THR, PHE, ARG, TRP, LEU, LEU, ASP, SER, SER, GLU, HIS, ARG, ARG, ILE, GLU, THR, ASP, GLY, HIS, ASN, ASP, LYS, TYR, ILE, PHE, MET, GLU). The tree is rooted at the top and branches downwards. The sequences are color-coded: red (16%), green (44%), yellow (36%), and grey (20%).

Chain D:

| Color  | Percentage |
|--------|------------|
| Red    | 13%        |
| Green  | 48%        |
| Yellow | 32%        |
| Grey   | 20%        |

AMINO ACID COMPOSITION

| AMINO ACID | PERCENTAGE |
|------------|------------|
| MET        | 0.00       |
| GLY        | 0.00       |
| ARG        | 0.00       |
| LEU        | 0.00       |
| ARG        | 0.00       |
| ARG        | 0.00       |
| ARG        | 0.00       |
| GLN        | 0.00       |
| GLU        | 0.00       |
| ILE        | 0.00       |
| ILE        | 0.00       |
| ASP        | 0.00       |
| HIS        | 0.00       |
| GLU        | 0.00       |
| GLU        | 0.00       |
| GLU        | 0.00       |
| SER        | 0.00       |
| ASN        | 0.00       |
| ASP        | 0.00       |
| ASP        | 0.00       |
| VAL        | 0.00       |
| SER        | 0.00       |
| SER        | 0.00       |
| SER        | 0.00       |
| ARG        | 0.00       |
| ARG        | 0.00       |
| GLY        | 0.00       |
| LYS        | 0.00       |
| LEU        | 0.00       |
| SER        | 0.00       |
| LEU        | 0.00       |
| ALA        | 0.00       |
| GLU        | 0.00       |
| THR        | 0.00       |
| PHE        | 0.00       |
| ARG        | 0.00       |
| TRP        | 0.00       |
| LEU        | 0.00       |
| ASP        | 0.00       |
| SER        | 0.00       |
| SER        | 0.00       |
| GLU        | 0.00       |
| HIS        | 0.00       |
| ARG        | 0.00       |
| ARG        | 0.00       |
| ILE        | 0.00       |
| GLU        | 0.00       |
| THR        | 0.00       |
| ASP        | 0.00       |
| GLY        | 0.00       |
| HIS        | 0.00       |
| ASN        | 0.00       |
| ASP        | 0.00       |
| TYR        | 0.00       |
| LYS        | 0.00       |



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 39551                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 1200                                    | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.363                                   | Depositor |
| Minimum map value                    | -0.173                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.018                                   | Depositor |
| Recommended contour level            | 0.085                                   | Depositor |
| Map size (Å)                         | 305.27997, 305.27997, 305.27997         | wwPDB     |
| Map dimensions                       | 288, 288, 288                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.06, 1.06, 1.06                        | Depositor |



## 5 Model quality

### 5.1 Standard geometry

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         | 0/5438      | 0.52        | 3/7356 (0.0%)   |
| 1   | B     | 0.35         | 0/5438      | 0.62        | 5/7356 (0.1%)   |
| 1   | C     | 0.30         | 0/5445      | 0.56        | 5/7365 (0.1%)   |
| 1   | D     | 0.37         | 0/5438      | 0.63        | 8/7356 (0.1%)   |
| All | All   | 0.33         | 0/21759     | 0.59        | 21/29433 (0.1%) |

There are no bond length outliers.

All (21) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 393 | GLU  | N-CA-C | -9.32 | 101.10      | 111.07   |
| 1   | D     | 186 | GLN  | N-CA-C | -7.88 | 102.69      | 111.28   |
| 1   | B     | 359 | VAL  | N-CA-C | 7.12  | 117.89      | 110.62   |
| 1   | D     | 95  | GLU  | N-CA-C | -7.01 | 103.68      | 111.82   |
| 1   | C     | 326 | LEU  | N-CA-C | -6.92 | 103.73      | 111.28   |
| 1   | C     | 267 | VAL  | N-CA-C | -6.83 | 103.56      | 111.00   |
| 1   | B     | 184 | PHE  | N-CA-C | 6.11  | 118.44      | 111.11   |
| 1   | D     | 436 | THR  | N-CA-C | -5.93 | 101.64      | 110.23   |
| 1   | B     | 512 | ARG  | N-CA-C | -5.92 | 105.71      | 113.12   |
| 1   | A     | 339 | LEU  | N-CA-C | 5.81  | 117.30      | 110.97   |
| 1   | D     | 267 | VAL  | N-CA-C | -5.80 | 104.85      | 110.42   |
| 1   | B     | 516 | LEU  | N-CA-C | -5.79 | 103.92      | 111.74   |
| 1   | C     | 186 | GLN  | N-CA-C | 5.76  | 117.56      | 111.28   |
| 1   | C     | 328 | SER  | N-CA-C | -5.76 | 104.91      | 111.07   |
| 1   | D     | 98  | PHE  | N-CA-C | -5.57 | 105.21      | 111.28   |
| 1   | A     | 154 | TRP  | N-CA-C | -5.52 | 107.55      | 114.56   |
| 1   | B     | 513 | ILE  | N-CA-C | -5.43 | 106.53      | 113.22   |
| 1   | C     | 574 | ARG  | N-CA-C | 5.43  | 118.12      | 111.82   |
| 1   | D     | 250 | ARG  | N-CA-C | 5.20  | 116.63      | 111.07   |
| 1   | D     | 283 | ARG  | N-CA-C | -5.11 | 105.61      | 111.07   |
| 1   | D     | 435 | VAL  | N-CA-C | -5.05 | 107.42      | 111.91   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5315  | 0        | 5344     | 257     | 0            |
| 1   | B     | 5315  | 0        | 5344     | 271     | 0            |
| 1   | C     | 5321  | 0        | 5352     | 268     | 0            |
| 1   | D     | 5315  | 0        | 5344     | 251     | 0            |
| All | All   | 21266 | 0        | 21384    | 977     | 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 23.

All (977) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:339:LEU:CD1  | 1:A:340:ARG:HG2  | 1.52                     | 1.36              |
| 1:C:271:THR:HA   | 1:D:272:VAL:CG2  | 1.63                     | 1.25              |
| 1:C:356:THR:HG22 | 1:C:360:MET:CE   | 1.68                     | 1.23              |
| 1:C:271:THR:CA   | 1:D:272:VAL:HG22 | 1.73                     | 1.18              |
| 1:A:265:ALA:O    | 1:A:268:THR:HG22 | 1.41                     | 1.17              |
| 1:B:568:LEU:CD1  | 1:B:583:LEU:HD21 | 1.76                     | 1.15              |
| 1:A:339:LEU:HD12 | 1:A:340:ARG:HG2  | 1.21                     | 1.15              |
| 1:B:448:LEU:HD11 | 1:B:452:THR:HG21 | 1.30                     | 1.08              |
| 1:B:448:LEU:CD1  | 1:B:452:THR:HG21 | 1.85                     | 1.07              |
| 1:A:339:LEU:HD13 | 1:A:340:ARG:HG2  | 1.33                     | 1.06              |
| 1:C:356:THR:CG2  | 1:C:360:MET:HE1  | 1.90                     | 1.01              |
| 1:A:339:LEU:CD1  | 1:A:340:ARG:CG   | 2.41                     | 0.99              |
| 1:B:568:LEU:HD12 | 1:B:583:LEU:HD21 | 1.41                     | 0.99              |
| 1:C:356:THR:HG22 | 1:C:360:MET:HE1  | 1.01                     | 0.98              |
| 1:D:333:LYS:O    | 1:D:334:LYS:HG2  | 1.62                     | 0.98              |
| 1:A:520:ILE:HD12 | 1:A:523:HIS:HE1  | 1.30                     | 0.96              |
| 1:C:271:THR:HA   | 1:D:272:VAL:HG22 | 0.96                     | 0.95              |
| 1:B:568:LEU:HD13 | 1:B:583:LEU:CD2  | 1.97                     | 0.95              |
| 1:A:339:LEU:HD12 | 1:A:340:ARG:CG   | 1.98                     | 0.93              |
| 1:D:104:GLY:O    | 1:D:108:PHE:CD2  | 2.22                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:240:LYS:HD3  | 1:C:245:SER:HB3  | 1.50                     | 0.91              |
| 1:B:568:LEU:CD1  | 1:B:583:LEU:CD2  | 2.48                     | 0.90              |
| 1:A:339:LEU:HD12 | 1:A:340:ARG:N    | 1.86                     | 0.89              |
| 1:B:357:ASP:O    | 1:B:361:LEU:HG   | 1.73                     | 0.89              |
| 1:D:73:LEU:HB3   | 1:D:180:LYS:HZ2  | 1.37                     | 0.88              |
| 1:A:265:ALA:O    | 1:A:268:THR:CG2  | 2.22                     | 0.87              |
| 1:B:568:LEU:HD13 | 1:B:583:LEU:HD21 | 1.55                     | 0.87              |
| 1:D:266:ILE:HA   | 1:D:269:MET:HG2  | 1.56                     | 0.87              |
| 1:B:448:LEU:CG   | 1:B:452:THR:HG21 | 2.05                     | 0.86              |
| 1:B:568:LEU:HD13 | 1:B:583:LEU:CD1  | 2.06                     | 0.85              |
| 1:C:376:LEU:HD21 | 1:D:333:LYS:HD2  | 1.58                     | 0.85              |
| 1:C:356:THR:HG22 | 1:C:360:MET:SD   | 2.16                     | 0.84              |
| 1:C:289:MET:HE1  | 1:D:262:LEU:HD23 | 1.58                     | 0.84              |
| 1:C:350:GLN:HG3  | 1:C:354:HIS:HB2  | 1.61                     | 0.82              |
| 1:A:274:TYR:O    | 1:D:275:GLY:HA2  | 1.77                     | 0.82              |
| 1:B:373:ALA:HB1  | 1:B:399:VAL:HG22 | 1.59                     | 0.82              |
| 1:B:448:LEU:HD11 | 1:B:452:THR:CG2  | 2.07                     | 0.81              |
| 1:A:407:PHE:HE2  | 1:A:477:LEU:HB2  | 1.46                     | 0.81              |
| 1:B:364:ILE:HG21 | 1:B:369:ARG:HB2  | 1.62                     | 0.81              |
| 1:D:430:LEU:HD11 | 1:D:447:LEU:HD13 | 1.62                     | 0.81              |
| 1:B:188:LEU:HD12 | 1:B:188:LEU:O    | 1.81                     | 0.81              |
| 1:B:514:LYS:NZ   | 1:B:520:ILE:HG21 | 1.95                     | 0.81              |
| 1:D:281:ASN:HB3  | 1:D:284:GLU:HG2  | 1.63                     | 0.79              |
| 1:D:333:LYS:O    | 1:D:334:LYS:CG   | 2.31                     | 0.79              |
| 1:D:104:GLY:O    | 1:D:108:PHE:HD2  | 1.62                     | 0.79              |
| 1:A:69:GLU:HA    | 1:A:72:ILE:HG12  | 1.65                     | 0.78              |
| 1:B:289:MET:CE   | 1:C:266:ILE:HD11 | 2.13                     | 0.78              |
| 1:A:417:GLY:H    | 1:A:466:PRO:HA   | 1.49                     | 0.78              |
| 1:A:605:VAL:HG11 | 1:A:650:SER:HB3  | 1.67                     | 0.77              |
| 1:D:266:ILE:O    | 1:D:269:MET:HG2  | 1.85                     | 0.77              |
| 1:B:568:LEU:HD13 | 1:B:583:LEU:HD11 | 1.67                     | 0.77              |
| 1:D:272:VAL:O    | 1:D:274:TYR:CD2  | 2.37                     | 0.77              |
| 1:D:593:LYS:HB3  | 1:D:597:GLY:HA2  | 1.67                     | 0.76              |
| 1:B:301:TYR:HD1  | 1:C:306:ILE:HD11 | 1.48                     | 0.76              |
| 1:B:289:MET:HE3  | 1:C:266:ILE:HD11 | 1.68                     | 0.76              |
| 1:C:289:MET:HE1  | 1:D:262:LEU:CD2  | 2.14                     | 0.76              |
| 1:A:402:LEU:HD11 | 1:A:478:LEU:HB3  | 1.67                     | 0.76              |
| 1:A:268:THR:CG2  | 1:A:291:TYR:HE2  | 1.99                     | 0.75              |
| 1:A:323:MET:HG2  | 1:A:348:ARG:HD3  | 1.68                     | 0.75              |
| 1:A:369:ARG:NH1  | 1:A:400:ILE:O    | 2.20                     | 0.75              |
| 1:A:264:PHE:HB2  | 1:A:277:ILE:HD13 | 1.69                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:330:MET:HG3  | 1:A:335:LEU:HD12 | 1.69                     | 0.74              |
| 1:C:304:GLY:HA2  | 1:D:307:THR:HG22 | 1.69                     | 0.74              |
| 1:D:266:ILE:HG13 | 1:D:269:MET:SD   | 2.28                     | 0.74              |
| 1:A:520:ILE:HD12 | 1:A:523:HIS:CE1  | 2.21                     | 0.73              |
| 1:B:448:LEU:HD21 | 1:B:452:THR:HG22 | 1.68                     | 0.73              |
| 1:B:416:GLN:NE2  | 1:B:466:PRO:O    | 2.22                     | 0.73              |
| 1:D:435:VAL:HG12 | 1:D:435:VAL:O    | 1.86                     | 0.73              |
| 1:A:528:GLU:OE1  | 1:A:559:LYS:NZ   | 2.21                     | 0.73              |
| 1:D:330:MET:HG2  | 1:D:340:ARG:HG2  | 1.71                     | 0.73              |
| 1:D:543:ASP:HB3  | 1:D:546:GLN:HB2  | 1.70                     | 0.73              |
| 1:D:264:PHE:CE2  | 1:D:277:ILE:HG22 | 2.24                     | 0.72              |
| 1:A:145:LEU:HA   | 1:A:148:PHE:CE1  | 2.23                     | 0.72              |
| 1:B:558:ASN:OD1  | 1:B:558:ASN:O    | 2.06                     | 0.72              |
| 1:B:92:GLY:H     | 1:B:168:ARG:HH12 | 1.35                     | 0.72              |
| 1:C:470:ARG:NH1  | 1:C:471:VAL:O    | 2.22                     | 0.72              |
| 1:A:95:GLU:HG2   | 1:A:96:ARG:HD3   | 1.72                     | 0.72              |
| 1:C:518:SER:CB   | 1:C:523:HIS:HE1  | 2.02                     | 0.72              |
| 1:C:356:THR:CG2  | 1:C:360:MET:SD   | 2.76                     | 0.72              |
| 1:A:186:GLN:O    | 1:A:189:GLU:HG2  | 1.89                     | 0.72              |
| 1:C:518:SER:HB2  | 1:C:523:HIS:HE1  | 1.54                     | 0.72              |
| 1:C:519:ASP:HB2  | 1:C:522:ILE:HG12 | 1.72                     | 0.72              |
| 1:D:131:LYS:HE3  | 1:D:134:ARG:HH12 | 1.56                     | 0.71              |
| 1:B:430:LEU:HB3  | 1:B:447:LEU:HD12 | 1.71                     | 0.71              |
| 1:C:699:ASP:OD1  | 1:C:702:ARG:NH2  | 2.23                     | 0.71              |
| 1:D:143:HIS:NE2  | 1:D:179:ARG:HD3  | 2.04                     | 0.71              |
| 1:B:424:TYR:HB3  | 1:B:477:LEU:HD12 | 1.71                     | 0.71              |
| 1:D:402:LEU:HD22 | 1:D:478:LEU:HD12 | 1.73                     | 0.71              |
| 1:A:131:LYS:HG3  | 1:A:134:ARG:HG2  | 1.73                     | 0.70              |
| 1:D:208:GLU:OE2  | 1:D:269:MET:HE3  | 1.90                     | 0.70              |
| 1:A:678:LYS:HB2  | 1:A:712:LEU:HD13 | 1.73                     | 0.70              |
| 1:A:426:VAL:O    | 1:A:451:HIS:N    | 2.24                     | 0.70              |
| 1:D:266:ILE:CA   | 1:D:269:MET:HG2  | 2.21                     | 0.70              |
| 1:D:378:LEU:HG   | 1:D:382:LYS:HE2  | 1.72                     | 0.70              |
| 1:C:404:GLU:HG2  | 1:C:476:HIS:HE1  | 1.57                     | 0.70              |
| 1:A:265:ALA:C    | 1:A:268:THR:HG22 | 2.17                     | 0.69              |
| 1:A:263:TYR:CD1  | 1:D:285:MET:SD   | 2.85                     | 0.69              |
| 1:D:115:GLN:HG2  | 1:D:139:TYR:CE2  | 2.26                     | 0.69              |
| 1:A:385:PRO:O    | 1:A:388:LYS:NZ   | 2.25                     | 0.69              |
| 1:C:383:LYS:HD2  | 1:C:451:HIS:CD2  | 2.26                     | 0.69              |
| 1:A:431:LEU:HB2  | 1:A:448:LEU:HB2  | 1.76                     | 0.68              |
| 1:C:271:THR:C    | 1:D:272:VAL:HG22 | 2.19                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:333:LYS:C    | 1:D:334:LYS:HG2  | 2.19                     | 0.68              |
| 1:A:402:LEU:HG   | 1:A:478:LEU:HD12 | 1.76                     | 0.67              |
| 1:C:374:GLN:HA   | 1:C:399:VAL:HG11 | 1.76                     | 0.67              |
| 1:A:414:THR:HG22 | 1:A:469:VAL:HG22 | 1.77                     | 0.67              |
| 1:C:518:SER:HB2  | 1:C:523:HIS:CE1  | 2.30                     | 0.67              |
| 1:A:663:THR:HG22 | 1:A:665:LEU:H    | 1.59                     | 0.67              |
| 1:C:569:HIS:O    | 1:C:573:CYS:SG   | 2.53                     | 0.67              |
| 1:C:289:MET:HE1  | 1:D:262:LEU:CG   | 2.25                     | 0.67              |
| 1:A:268:THR:HG21 | 1:A:291:TYR:CE2  | 2.30                     | 0.67              |
| 1:C:91:ARG:HD2   | 1:C:168:ARG:HH11 | 1.59                     | 0.66              |
| 1:B:312:LYS:NZ   | 1:C:311:VAL:HG23 | 2.11                     | 0.66              |
| 1:D:239:LEU:HD11 | 1:D:246:TYR:CD2  | 2.30                     | 0.66              |
| 1:D:266:ILE:HA   | 1:D:269:MET:CG   | 2.25                     | 0.66              |
| 1:B:329:PHE:HA   | 1:B:332:ARG:HE   | 1.60                     | 0.66              |
| 1:D:281:ASN:HB3  | 1:D:284:GLU:CG   | 2.25                     | 0.66              |
| 1:A:109:LEU:O    | 1:A:112:ILE:HG22 | 1.95                     | 0.66              |
| 1:A:510:ASN:HB3  | 1:A:513:ILE:HG22 | 1.76                     | 0.66              |
| 1:A:642:ASP:HA   | 1:A:645:LYS:HE3  | 1.78                     | 0.66              |
| 1:C:93:LEU:HD12  | 1:C:94:PRO:HD2   | 1.78                     | 0.66              |
| 1:D:336:GLY:HA2  | 1:D:340:ARG:HE   | 1.61                     | 0.66              |
| 1:A:645:LYS:HA   | 1:A:648:LEU:HD12 | 1.79                     | 0.65              |
| 1:C:404:GLU:HG2  | 1:C:476:HIS:CE1  | 2.30                     | 0.65              |
| 1:D:220:TYR:CE1  | 1:D:236:ILE:HD13 | 2.31                     | 0.65              |
| 1:B:593:LYS:HG3  | 1:B:599:THR:HG22 | 1.77                     | 0.65              |
| 1:B:208:GLU:O    | 1:B:212:THR:HG23 | 1.96                     | 0.65              |
| 1:B:140:LEU:HA   | 1:B:144:PHE:HB3  | 1.79                     | 0.65              |
| 1:D:364:ILE:O    | 1:D:369:ARG:NH2  | 2.29                     | 0.65              |
| 1:A:319:PHE:O    | 1:A:323:MET:HG3  | 1.96                     | 0.65              |
| 1:A:681:VAL:HA   | 1:A:685:ALA:HB3  | 1.77                     | 0.65              |
| 1:C:601:LEU:HD13 | 1:C:616:LEU:HD22 | 1.77                     | 0.65              |
| 1:D:630:ASN:HD22 | 1:D:659:TYR:HB3  | 1.61                     | 0.65              |
| 1:A:119:ALA:O    | 1:A:138:ARG:NH2  | 2.30                     | 0.65              |
| 1:C:356:THR:HG21 | 1:D:329:PHE:CD1  | 2.32                     | 0.65              |
| 1:B:448:LEU:HG   | 1:B:452:THR:HG21 | 1.78                     | 0.64              |
| 1:B:663:THR:HB   | 1:B:666:HIS:CG   | 2.32                     | 0.64              |
| 1:D:220:TYR:HE1  | 1:D:236:ILE:HD13 | 1.59                     | 0.64              |
| 1:D:330:MET:HE1  | 1:D:339:LEU:HD23 | 1.79                     | 0.64              |
| 1:B:172:TRP:HZ2  | 1:B:218:ILE:HD11 | 1.61                     | 0.64              |
| 1:B:312:LYS:HZ2  | 1:C:311:VAL:HG23 | 1.62                     | 0.64              |
| 1:B:345:GLY:HA2  | 1:B:348:ARG:HE   | 1.62                     | 0.64              |
| 1:B:511:ASP:HA   | 1:B:514:LYS:HB3  | 1.79                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:61:LYS:O     | 1:C:66:LYS:NZ    | 2.31                     | 0.64              |
| 1:C:568:LEU:HD21 | 1:C:590:VAL:HG22 | 1.79                     | 0.64              |
| 1:C:356:THR:CG2  | 1:C:360:MET:CE   | 2.61                     | 0.64              |
| 1:A:173:ILE:HD12 | 1:A:176:PHE:HD2  | 1.62                     | 0.64              |
| 1:A:268:THR:CG2  | 1:A:291:TYR:CE2  | 2.79                     | 0.64              |
| 1:C:573:CYS:SG   | 1:C:603:GLU:OE1  | 2.55                     | 0.64              |
| 1:D:347:VAL:O    | 1:D:350:GLN:HG3  | 1.97                     | 0.64              |
| 1:C:408:LEU:HA   | 1:C:474:LEU:HG   | 1.80                     | 0.64              |
| 1:D:431:LEU:HD22 | 1:D:448:LEU:HD12 | 1.80                     | 0.64              |
| 1:C:678:LYS:HB2  | 1:C:712:LEU:HD13 | 1.80                     | 0.64              |
| 1:A:268:THR:HG21 | 1:A:291:TYR:HE2  | 1.61                     | 0.64              |
| 1:A:156:LEU:HD12 | 1:A:159:LYS:HE2  | 1.80                     | 0.63              |
| 1:D:208:GLU:OE2  | 1:D:269:MET:CE   | 2.46                     | 0.63              |
| 1:D:337:ARG:HD2  | 1:D:339:LEU:H    | 1.62                     | 0.63              |
| 1:B:197:LEU:HB2  | 1:B:309:LEU:HD13 | 1.80                     | 0.63              |
| 1:D:565:ARG:HD3  | 1:D:569:HIS:HB3  | 1.78                     | 0.63              |
| 1:B:336:GLY:O    | 1:B:337:ARG:HG2  | 1.98                     | 0.63              |
| 1:B:507:LYS:HE3  | 1:B:514:LYS:HE2  | 1.80                     | 0.63              |
| 1:C:599:THR:HB   | 1:C:624:ASN:HB2  | 1.80                     | 0.63              |
| 1:D:424:TYR:HB3  | 1:D:477:LEU:HD11 | 1.79                     | 0.63              |
| 1:A:517:GLU:O    | 1:A:520:ILE:HG22 | 1.99                     | 0.63              |
| 1:B:94:PRO:HG2   | 1:B:97:LEU:HD13  | 1.81                     | 0.63              |
| 1:C:266:ILE:HA   | 1:C:269:MET:HB2  | 1.80                     | 0.63              |
| 1:C:535:VAL:HG22 | 1:C:550:LEU:HD21 | 1.81                     | 0.63              |
| 1:B:568:LEU:HD12 | 1:B:583:LEU:CD2  | 2.19                     | 0.62              |
| 1:B:329:PHE:O    | 1:B:332:ARG:HG2  | 1.99                     | 0.62              |
| 1:D:690:LYS:HD2  | 1:D:694:GLY:HA2  | 1.81                     | 0.62              |
| 1:C:428:GLU:O    | 1:C:475:CYS:HA   | 1.99                     | 0.62              |
| 1:C:573:CYS:SG   | 1:C:603:GLU:HB3  | 2.39                     | 0.62              |
| 1:A:140:LEU:HA   | 1:A:144:PHE:HB3  | 1.81                     | 0.62              |
| 1:B:122:ASP:O    | 1:B:126:TYR:N    | 2.28                     | 0.62              |
| 1:B:337:ARG:HG3  | 1:B:338:ASP:H    | 1.64                     | 0.62              |
| 1:C:497:ARG:HA   | 1:C:500:LEU:HD12 | 1.82                     | 0.62              |
| 1:A:324:ASN:ND2  | 1:D:192:THR:O    | 2.33                     | 0.62              |
| 1:C:428:GLU:HG3  | 1:C:476:HIS:HB3  | 1.82                     | 0.62              |
| 1:D:108:PHE:CE1  | 1:D:177:ARG:HD3  | 2.35                     | 0.61              |
| 1:D:561:ASP:OD1  | 1:D:565:ARG:N    | 2.32                     | 0.61              |
| 1:A:578:ASP:OD1  | 1:A:579:ILE:HD12 | 1.99                     | 0.61              |
| 1:B:285:MET:O    | 1:B:289:MET:HG2  | 2.00                     | 0.61              |
| 1:B:574:ARG:NH2  | 1:B:576:TYR:OH   | 2.34                     | 0.61              |
| 1:B:632:LEU:HD13 | 1:B:654:PRO:HA   | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:500:LEU:HD22 | 1:B:524:ILE:HD13 | 1.81                     | 0.61              |
| 1:C:289:MET:HE1  | 1:D:262:LEU:HG   | 1.83                     | 0.61              |
| 1:A:163:LYS:HG3  | 1:A:164:HIS:H    | 1.65                     | 0.61              |
| 1:D:401:ARG:HH21 | 1:D:488:ILE:HD11 | 1.66                     | 0.61              |
| 1:B:693:TRP:HE1  | 1:C:662:ARG:HH22 | 1.49                     | 0.61              |
| 1:C:268:THR:HG23 | 1:D:274:TYR:OH   | 2.01                     | 0.61              |
| 1:A:434:LEU:HD22 | 1:A:442:GLU:HB2  | 1.82                     | 0.60              |
| 1:B:105:GLN:OE1  | 1:B:174:ARG:NH2  | 2.34                     | 0.60              |
| 1:B:544:PHE:HA   | 1:B:547:LEU:HD12 | 1.83                     | 0.60              |
| 1:B:252:ILE:O    | 1:B:257:ARG:NH2  | 2.34                     | 0.60              |
| 1:C:266:ILE:HB   | 1:C:269:MET:HE3  | 1.81                     | 0.60              |
| 1:D:266:ILE:C    | 1:D:269:MET:HG2  | 2.25                     | 0.60              |
| 1:D:458:SER:HA   | 1:D:463:ILE:HG23 | 1.83                     | 0.60              |
| 1:A:364:ILE:HD11 | 1:A:368:ILE:HB   | 1.83                     | 0.60              |
| 1:D:185:PHE:CD1  | 1:D:188:LEU:HD12 | 2.37                     | 0.60              |
| 1:A:286:ILE:O    | 1:A:289:MET:HB2  | 2.00                     | 0.60              |
| 1:A:593:LYS:NZ   | 1:A:624:ASN:HB2  | 2.16                     | 0.60              |
| 1:C:269:MET:HG2  | 1:C:295:ASP:OD2  | 2.01                     | 0.59              |
| 1:D:272:VAL:HB   | 1:D:274:TYR:CE2  | 2.37                     | 0.59              |
| 1:B:360:MET:SD   | 1:B:403:HIS:HD2  | 2.25                     | 0.59              |
| 1:A:280:VAL:HG12 | 1:B:241:LEU:HG   | 1.85                     | 0.59              |
| 1:D:115:GLN:HG2  | 1:D:139:TYR:HE2  | 1.66                     | 0.59              |
| 1:A:196:TYR:O    | 1:A:199:THR:OG1  | 2.20                     | 0.59              |
| 1:B:514:LYS:CE   | 1:B:520:ILE:HG21 | 2.32                     | 0.59              |
| 1:D:660:ASP:HB3  | 1:D:662:ARG:HG3  | 1.84                     | 0.59              |
| 1:C:356:THR:HG21 | 1:D:329:PHE:CE1  | 2.37                     | 0.59              |
| 1:A:561:ASP:OD1  | 1:A:565:ARG:N    | 2.35                     | 0.59              |
| 1:B:593:LYS:HB3  | 1:B:599:THR:HA   | 1.83                     | 0.59              |
| 1:B:417:GLY:N    | 1:B:465:GLN:O    | 2.36                     | 0.59              |
| 1:D:272:VAL:O    | 1:D:274:TYR:HD2  | 1.86                     | 0.59              |
| 1:A:323:MET:HE3  | 1:A:348:ARG:HH11 | 1.67                     | 0.59              |
| 1:B:431:LEU:HB2  | 1:B:448:LEU:HB3  | 1.84                     | 0.59              |
| 1:D:121:ARG:HD3  | 1:D:126:TYR:HA   | 1.85                     | 0.59              |
| 1:A:178:VAL:O    | 1:A:181:VAL:HG12 | 2.03                     | 0.59              |
| 1:D:264:PHE:HE2  | 1:D:277:ILE:HG22 | 1.67                     | 0.58              |
| 1:A:431:LEU:O    | 1:A:448:LEU:N    | 2.36                     | 0.58              |
| 1:A:360:MET:HE1  | 1:B:329:PHE:CE2  | 2.38                     | 0.58              |
| 1:C:394:PHE:HD1  | 1:C:492:TYR:HD2  | 1.50                     | 0.58              |
| 1:A:66:LYS:O     | 1:A:70:MET:HG2   | 2.04                     | 0.58              |
| 1:A:369:ARG:HA   | 1:A:372:ILE:HG12 | 1.84                     | 0.58              |
| 1:D:240:LYS:HG2  | 1:D:240:LYS:O    | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:285:MET:SD   | 1:B:263:TYR:CD1  | 2.97                     | 0.58              |
| 1:A:339:LEU:HD12 | 1:A:340:ARG:CB   | 2.32                     | 0.58              |
| 1:A:504:MET:O    | 1:A:507:LYS:HG2  | 2.03                     | 0.58              |
| 1:B:223:ALA:HB2  | 1:B:235:TRP:HE1  | 1.68                     | 0.58              |
| 1:B:190:LYS:HD3  | 1:C:344:THR:HG21 | 1.85                     | 0.58              |
| 1:B:151:CYS:HA   | 1:B:174:ARG:HH22 | 1.69                     | 0.58              |
| 1:C:266:ILE:HA   | 1:C:269:MET:CB   | 2.33                     | 0.58              |
| 1:C:385:PRO:HA   | 1:C:388:LYS:HG3  | 1.86                     | 0.57              |
| 1:A:533:LEU:HD21 | 1:D:533:LEU:HB3  | 1.85                     | 0.57              |
| 1:B:448:LEU:HD21 | 1:B:452:THR:CG2  | 2.34                     | 0.57              |
| 1:C:518:SER:CB   | 1:C:523:HIS:CE1  | 2.86                     | 0.57              |
| 1:D:548:LYS:O    | 1:D:552:ARG:HG2  | 2.04                     | 0.57              |
| 1:A:409:PRO:HD3  | 1:D:127:ARG:CZ   | 2.34                     | 0.57              |
| 1:B:448:LEU:CG   | 1:B:452:THR:CG2  | 2.81                     | 0.57              |
| 1:C:180:LYS:O    | 1:C:183:GLU:HG3  | 2.03                     | 0.57              |
| 1:C:409:PRO:HD3  | 1:C:474:LEU:HG   | 1.87                     | 0.57              |
| 1:C:601:LEU:HD23 | 1:C:623:PHE:HB3  | 1.86                     | 0.57              |
| 1:C:642:ASP:O    | 1:C:646:ARG:HG2  | 2.04                     | 0.57              |
| 1:D:669:ALA:HA   | 1:D:709:LEU:HD21 | 1.86                     | 0.57              |
| 1:B:189:GLU:HG2  | 1:B:192:THR:HG23 | 1.86                     | 0.57              |
| 1:B:356:THR:HG22 | 1:C:329:PHE:CE1  | 2.39                     | 0.57              |
| 1:B:301:TYR:O    | 1:B:305:ASN:OD1  | 2.23                     | 0.57              |
| 1:D:366:ALA:HA   | 1:D:369:ARG:HG2  | 1.85                     | 0.57              |
| 1:A:339:LEU:HD13 | 1:A:340:ARG:CG   | 2.19                     | 0.57              |
| 1:A:347:VAL:O    | 1:A:350:GLN:HG2  | 2.04                     | 0.57              |
| 1:B:248:ASN:HB3  | 1:B:251:GLU:CD   | 2.30                     | 0.57              |
| 1:A:600:PRO:HB2  | 1:A:616:LEU:HD21 | 1.87                     | 0.57              |
| 1:B:240:LYS:O    | 1:B:240:LYS:HD3  | 2.05                     | 0.57              |
| 1:C:381:ILE:HG21 | 1:C:395:ILE:HG23 | 1.87                     | 0.57              |
| 1:C:493:PHE:HB2  | 1:C:497:ARG:HH12 | 1.70                     | 0.57              |
| 1:A:431:LEU:HD13 | 1:A:471:VAL:HA   | 1.84                     | 0.57              |
| 1:A:532:ALA:HB2  | 1:A:559:LYS:HE3  | 1.87                     | 0.56              |
| 1:B:580:THR:O    | 1:B:583:LEU:HG   | 2.05                     | 0.56              |
| 1:D:264:PHE:CD2  | 1:D:277:ILE:HG22 | 2.40                     | 0.56              |
| 1:C:518:SER:OG   | 1:C:523:HIS:CE1  | 2.59                     | 0.56              |
| 1:C:599:THR:HG23 | 1:C:602:PHE:H    | 1.69                     | 0.56              |
| 1:B:233:TYR:CE2  | 1:B:281:ASN:HA   | 2.40                     | 0.56              |
| 1:C:662:ARG:NH1  | 1:C:691:ASP:OD2  | 2.38                     | 0.56              |
| 1:A:134:ARG:HH12 | 1:A:138:ARG:HE   | 1.52                     | 0.56              |
| 1:C:493:PHE:HB2  | 1:C:497:ARG:NH1  | 2.20                     | 0.56              |
| 1:D:425:PHE:CD1  | 1:D:453:SER:HB2  | 2.40                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:417:GLY:N    | 1:A:466:PRO:HA   | 2.19                     | 0.56              |
| 1:B:153:PRO:HB2  | 1:B:156:LEU:HD13 | 1.87                     | 0.56              |
| 1:C:374:GLN:O    | 1:C:378:LEU:HG   | 2.05                     | 0.56              |
| 1:A:329:PHE:CZ   | 1:D:356:THR:HG22 | 2.40                     | 0.56              |
| 1:A:398:ILE:HD11 | 1:A:488:ILE:HG21 | 1.86                     | 0.56              |
| 1:A:606:LYS:HG2  | 1:A:643:PHE:HE1  | 1.70                     | 0.56              |
| 1:C:330:MET:HE2  | 1:C:343:ILE:HD11 | 1.88                     | 0.56              |
| 1:D:155:ASP:OD1  | 1:D:159:LYS:NZ   | 2.37                     | 0.56              |
| 1:D:459:ILE:HG12 | 1:D:482:LYS:HZ2  | 1.71                     | 0.56              |
| 1:B:644:LEU:HD23 | 1:B:648:LEU:HD23 | 1.87                     | 0.56              |
| 1:B:122:ASP:HB3  | 1:B:124:GLN:CD   | 2.31                     | 0.56              |
| 1:B:170:LEU:O    | 1:B:173:ILE:HG12 | 2.06                     | 0.56              |
| 1:C:72:ILE:HD12  | 1:C:180:LYS:NZ   | 2.21                     | 0.56              |
| 1:D:397:GLN:HB3  | 1:D:401:ARG:HH22 | 1.71                     | 0.56              |
| 1:A:106:ILE:O    | 1:A:110:VAL:HG23 | 2.06                     | 0.55              |
| 1:C:466:PRO:HB3  | 1:C:517:GLU:HG2  | 1.89                     | 0.55              |
| 1:C:507:LYS:HA   | 1:C:514:LYS:HD2  | 1.88                     | 0.55              |
| 1:A:263:TYR:CG   | 1:D:285:MET:SD   | 2.99                     | 0.55              |
| 1:D:500:LEU:HA   | 1:D:503:ILE:HD12 | 1.88                     | 0.55              |
| 1:D:591:ASN:HD21 | 1:D:624:ASN:HB2  | 1.71                     | 0.55              |
| 1:A:234:THR:HG22 | 1:A:235:TRP:N    | 2.21                     | 0.55              |
| 1:A:593:LYS:HZ1  | 1:A:624:ASN:HB2  | 1.71                     | 0.55              |
| 1:B:364:ILE:HG22 | 1:B:366:ALA:H    | 1.72                     | 0.55              |
| 1:B:692:ARG:HH22 | 1:C:666:HIS:HB3  | 1.71                     | 0.55              |
| 1:A:407:PHE:CE2  | 1:A:477:LEU:HB2  | 2.34                     | 0.55              |
| 1:B:337:ARG:HG3  | 1:B:338:ASP:N    | 2.21                     | 0.55              |
| 1:C:296:MET:HE1  | 1:D:269:MET:HE2  | 1.87                     | 0.55              |
| 1:D:407:PHE:O    | 1:D:474:LEU:HA   | 2.06                     | 0.55              |
| 1:B:409:PRO:HD3  | 1:B:474:LEU:HB3  | 1.87                     | 0.55              |
| 1:B:673:LEU:HD23 | 1:B:676:MET:HG3  | 1.87                     | 0.55              |
| 1:A:377:TYR:HB2  | 1:A:399:VAL:HG13 | 1.89                     | 0.55              |
| 1:B:368:ILE:O    | 1:B:372:ILE:HG12 | 2.07                     | 0.55              |
| 1:A:228:PRO:HG3  | 1:A:250:ARG:HH12 | 1.71                     | 0.55              |
| 1:A:618:LYS:NZ   | 1:A:619:GLU:OE2  | 2.40                     | 0.55              |
| 1:D:431:LEU:HD21 | 1:D:469:VAL:HG23 | 1.89                     | 0.55              |
| 1:A:519:ASP:HA   | 1:A:522:ILE:HG12 | 1.89                     | 0.55              |
| 1:C:281:ASN:HB3  | 1:C:284:GLU:OE2  | 2.07                     | 0.55              |
| 1:C:567:PRO:HA   | 1:C:570:LEU:HD13 | 1.89                     | 0.55              |
| 1:D:330:MET:HE3  | 1:D:336:GLY:H    | 1.73                     | 0.55              |
| 1:D:572:ALA:HA   | 1:D:612:VAL:HG11 | 1.87                     | 0.55              |
| 1:A:329:PHE:O    | 1:A:332:ARG:HG2  | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:560:THR:HG22 | 1:B:566:SER:HA   | 1.89                     | 0.54              |
| 1:C:416:GLN:HG3  | 1:C:436:THR:HB   | 1.87                     | 0.54              |
| 1:C:514:LYS:HB2  | 1:C:520:ILE:HD11 | 1.89                     | 0.54              |
| 1:A:319:PHE:CZ   | 1:A:348:ARG:HG2  | 2.42                     | 0.54              |
| 1:B:188:LEU:HD12 | 1:B:188:LEU:C    | 2.31                     | 0.54              |
| 1:B:380:TYR:CZ   | 1:B:427:CYS:HA   | 2.43                     | 0.54              |
| 1:B:507:LYS:HB2  | 1:B:514:LYS:HG2  | 1.89                     | 0.54              |
| 1:C:413:ILE:HB   | 1:C:469:VAL:HB   | 1.88                     | 0.54              |
| 1:D:446:THR:HG23 | 1:D:511:ASP:HB2  | 1.90                     | 0.54              |
| 1:A:487:ASN:O    | 1:A:490:GLU:HG3  | 2.07                     | 0.54              |
| 1:A:523:HIS:O    | 1:A:527:GLN:N    | 2.23                     | 0.54              |
| 1:B:220:TYR:CZ   | 1:B:257:ARG:HD3  | 2.43                     | 0.54              |
| 1:B:435:VAL:O    | 1:B:443:GLU:HG3  | 2.07                     | 0.54              |
| 1:B:109:LEU:O    | 1:B:112:ILE:HG22 | 2.06                     | 0.54              |
| 1:C:519:ASP:CB   | 1:C:522:ILE:HG12 | 2.38                     | 0.54              |
| 1:C:355:TYR:O    | 1:C:358:THR:OG1  | 2.26                     | 0.54              |
| 1:B:79:SER:O     | 1:B:83:THR:HG23  | 2.08                     | 0.54              |
| 1:C:286:ILE:O    | 1:C:289:MET:HB2  | 2.08                     | 0.54              |
| 1:D:630:ASN:ND2  | 1:D:659:TYR:HB3  | 2.22                     | 0.54              |
| 1:B:514:LYS:HZ2  | 1:B:520:ILE:HG21 | 1.71                     | 0.54              |
| 1:C:657:GLU:HA   | 1:C:664:PRO:HD3  | 1.90                     | 0.54              |
| 1:D:445:VAL:HG12 | 1:D:446:THR:N    | 2.23                     | 0.54              |
| 1:A:330:MET:HG2  | 1:A:337:ARG:HH22 | 1.73                     | 0.54              |
| 1:B:329:PHE:CE2  | 1:B:333:LYS:HG3  | 2.43                     | 0.54              |
| 1:D:337:ARG:HD2  | 1:D:338:ASP:N    | 2.23                     | 0.54              |
| 1:B:335:LEU:HD12 | 1:B:339:LEU:HD22 | 1.89                     | 0.53              |
| 1:C:178:VAL:O    | 1:C:181:VAL:HG22 | 2.09                     | 0.53              |
| 1:C:394:PHE:CE1  | 1:C:488:ILE:HG12 | 2.43                     | 0.53              |
| 1:D:691:ASP:OD1  | 1:D:692:ARG:N    | 2.38                     | 0.53              |
| 1:B:421:ASP:OD1  | 1:B:482:LYS:HB3  | 2.08                     | 0.53              |
| 1:C:574:ARG:NH2  | 1:C:576:TYR:OH   | 2.41                     | 0.53              |
| 1:D:86:GLU:HG3   | 1:D:171:LEU:HD21 | 1.89                     | 0.53              |
| 1:C:409:PRO:HG3  | 1:C:473:GLU:HA   | 1.90                     | 0.53              |
| 1:C:410:GLY:H    | 1:C:470:ARG:NH1  | 2.05                     | 0.53              |
| 1:C:669:ALA:HA   | 1:C:709:LEU:HD21 | 1.91                     | 0.53              |
| 1:B:603:GLU:HA   | 1:B:606:LYS:HG2  | 1.91                     | 0.53              |
| 1:A:272:VAL:O    | 1:D:273:GLY:HA3  | 2.08                     | 0.53              |
| 1:A:520:ILE:O    | 1:A:524:ILE:HG12 | 2.09                     | 0.53              |
| 1:A:593:LYS:NZ   | 1:A:599:THR:HB   | 2.24                     | 0.53              |
| 1:B:565:ARG:HG3  | 1:B:594:ASP:OD1  | 2.08                     | 0.53              |
| 1:C:275:GLY:O    | 1:C:278:HIS:NE2  | 2.42                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:623:PHE:HB2  | 1:B:652:MET:SD   | 2.48                     | 0.53              |
| 1:D:179:ARG:HA   | 1:D:182:VAL:HG12 | 1.91                     | 0.53              |
| 1:B:180:LYS:HA   | 1:B:183:GLU:OE1  | 2.08                     | 0.53              |
| 1:A:357:ASP:HA   | 1:A:360:MET:HE3  | 1.90                     | 0.53              |
| 1:C:413:ILE:HD13 | 1:C:469:VAL:HG12 | 1.91                     | 0.53              |
| 1:D:69:GLU:O     | 1:D:180:LYS:NZ   | 2.41                     | 0.53              |
| 1:C:284:GLU:OE2  | 1:C:284:GLU:N    | 2.34                     | 0.53              |
| 1:D:347:VAL:HG22 | 1:D:351:TYR:CE2  | 2.44                     | 0.53              |
| 1:C:706:ASN:HB3  | 1:C:709:LEU:HB3  | 1.90                     | 0.52              |
| 1:D:435:VAL:O    | 1:D:435:VAL:CG1  | 2.56                     | 0.52              |
| 1:D:615:LEU:HA   | 1:D:618:LYS:HG2  | 1.91                     | 0.52              |
| 1:B:308:ALA:HA   | 1:B:312:LYS:HZ3  | 1.74                     | 0.52              |
| 1:A:606:LYS:HE2  | 1:D:596:PHE:HE1  | 1.74                     | 0.52              |
| 1:B:500:LEU:HA   | 1:B:503:ILE:HG12 | 1.90                     | 0.52              |
| 1:C:91:ARG:HD2   | 1:C:168:ARG:NH1  | 2.24                     | 0.52              |
| 1:C:363:ASP:OD1  | 1:C:364:ILE:N    | 2.43                     | 0.52              |
| 1:D:92:GLY:H     | 1:D:168:ARG:HH12 | 1.55                     | 0.52              |
| 1:A:607:ALA:HB1  | 1:A:609:GLN:HE22 | 1.74                     | 0.52              |
| 1:B:249:PHE:O    | 1:B:257:ARG:NH2  | 2.23                     | 0.52              |
| 1:C:59:HIS:CG    | 1:C:60:PRO:HD2   | 2.45                     | 0.52              |
| 1:A:189:GLU:HA   | 1:A:199:THR:HG21 | 1.91                     | 0.52              |
| 1:B:666:HIS:CE1  | 1:B:691:ASP:HB2  | 2.43                     | 0.52              |
| 1:A:168:ARG:O    | 1:A:171:LEU:HD23 | 2.09                     | 0.52              |
| 1:A:272:VAL:O    | 1:D:273:GLY:CA   | 2.57                     | 0.52              |
| 1:A:492:TYR:HD1  | 1:A:494:HIS:CE1  | 2.28                     | 0.52              |
| 1:A:603:GLU:HA   | 1:A:606:LYS:HB2  | 1.92                     | 0.52              |
| 1:B:311:VAL:HG12 | 1:B:312:LYS:HD3  | 1.92                     | 0.52              |
| 1:B:328:SER:HA   | 1:B:331:ASN:HD21 | 1.75                     | 0.52              |
| 1:B:329:PHE:HA   | 1:B:332:ARG:NE   | 2.25                     | 0.52              |
| 1:C:369:ARG:NH1  | 1:C:372:ILE:HD11 | 2.24                     | 0.52              |
| 1:C:393:GLU:HA   | 1:C:396:ASN:HD21 | 1.73                     | 0.52              |
| 1:C:518:SER:OG   | 1:C:523:HIS:HE1  | 1.92                     | 0.52              |
| 1:C:543:ASP:OD1  | 1:C:543:ASP:N    | 2.43                     | 0.52              |
| 1:C:605:VAL:HG11 | 1:C:652:MET:HE1  | 1.91                     | 0.52              |
| 1:A:128:THR:HB   | 1:A:135:ILE:HD11 | 1.91                     | 0.52              |
| 1:C:349:LEU:HD21 | 1:C:406:TYR:HB3  | 1.92                     | 0.52              |
| 1:C:410:GLY:H    | 1:C:470:ARG:CZ   | 2.22                     | 0.52              |
| 1:D:272:VAL:O    | 1:D:274:TYR:CE2  | 2.61                     | 0.52              |
| 1:D:336:GLY:HA2  | 1:D:340:ARG:NE   | 2.23                     | 0.52              |
| 1:A:69:GLU:HG3   | 1:A:70:MET:HE3   | 1.92                     | 0.52              |
| 1:A:402:LEU:HD21 | 1:A:478:LEU:HG   | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:699:ASP:HA   | 1:B:702:ARG:NH1  | 2.26                     | 0.51              |
| 1:C:121:ARG:HB2  | 1:C:128:THR:HG22 | 1.92                     | 0.51              |
| 1:D:329:PHE:CE1  | 1:D:333:LYS:HE2  | 2.45                     | 0.51              |
| 1:D:445:VAL:HG12 | 1:D:446:THR:H    | 1.75                     | 0.51              |
| 1:D:540:PHE:HA   | 1:D:570:LEU:HD21 | 1.92                     | 0.51              |
| 1:B:565:ARG:HG3  | 1:B:594:ASP:CG   | 2.35                     | 0.51              |
| 1:C:540:PHE:HA   | 1:C:574:ARG:HG3  | 1.92                     | 0.51              |
| 1:B:205:LEU:O    | 1:B:208:GLU:HB2  | 2.10                     | 0.51              |
| 1:C:152:PHE:O    | 1:C:174:ARG:NH2  | 2.43                     | 0.51              |
| 1:C:547:LEU:O    | 1:C:551:ILE:HG12 | 2.10                     | 0.51              |
| 1:C:319:PHE:CD2  | 1:C:351:TYR:CD1  | 2.98                     | 0.51              |
| 1:C:415:GLU:HG2  | 1:C:416:GLN:H    | 1.76                     | 0.51              |
| 1:D:530:GLU:O    | 1:D:534:LYS:HG2  | 2.11                     | 0.51              |
| 1:A:131:LYS:HZ2  | 1:A:134:ARG:HB3  | 1.75                     | 0.51              |
| 1:A:174:ARG:HB3  | 1:A:177:ARG:NH2  | 2.26                     | 0.51              |
| 1:D:70:MET:O     | 1:D:73:LEU:HG    | 2.10                     | 0.51              |
| 1:A:533:LEU:HD11 | 1:D:533:LEU:HB3  | 1.93                     | 0.51              |
| 1:D:266:ILE:HA   | 1:D:269:MET:SD   | 2.51                     | 0.51              |
| 1:C:432:GLU:HG2  | 1:C:470:ARG:HB3  | 1.92                     | 0.51              |
| 1:B:521:VAL:O    | 1:B:524:ILE:HG22 | 2.11                     | 0.51              |
| 1:D:109:LEU:O    | 1:D:112:ILE:HG22 | 2.11                     | 0.51              |
| 1:B:190:LYS:NZ   | 1:C:337:ARG:HH22 | 2.08                     | 0.51              |
| 1:C:394:PHE:HD1  | 1:C:492:TYR:CD2  | 2.29                     | 0.51              |
| 1:C:110:VAL:HA   | 1:C:113:VAL:HG12 | 1.93                     | 0.51              |
| 1:C:281:ASN:OD1  | 1:C:282:LEU:N    | 2.44                     | 0.51              |
| 1:D:65:TYR:HE1   | 1:D:114:LEU:HD21 | 1.76                     | 0.51              |
| 1:B:358:THR:HA   | 1:B:361:LEU:HD12 | 1.92                     | 0.50              |
| 1:C:282:LEU:HD11 | 1:D:259:THR:HG21 | 1.92                     | 0.50              |
| 1:C:459:ILE:HG12 | 1:C:482:LYS:HE2  | 1.92                     | 0.50              |
| 1:D:231:GLU:O    | 1:D:234:THR:OG1  | 2.27                     | 0.50              |
| 1:B:221:TYR:O    | 1:B:224:THR:OG1  | 2.20                     | 0.50              |
| 1:B:120:TYR:HB3  | 1:B:135:ILE:HG12 | 1.93                     | 0.50              |
| 1:B:507:LYS:HE3  | 1:B:514:LYS:CE   | 2.41                     | 0.50              |
| 1:C:531:LEU:O    | 1:C:535:VAL:HG23 | 2.11                     | 0.50              |
| 1:A:350:GLN:NE2  | 1:A:405:GLU:OE2  | 2.44                     | 0.50              |
| 1:A:378:LEU:O    | 1:A:382:LYS:HG2  | 2.12                     | 0.50              |
| 1:D:236:ILE:HA   | 1:D:239:LEU:HD23 | 1.92                     | 0.50              |
| 1:A:543:ASP:OD1  | 1:A:543:ASP:N    | 2.45                     | 0.50              |
| 1:B:417:GLY:H    | 1:B:466:PRO:HA   | 1.77                     | 0.50              |
| 1:D:337:ARG:HH11 | 1:D:338:ASP:HB3  | 1.77                     | 0.50              |
| 1:A:615:LEU:O    | 1:A:618:LYS:HG2  | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:701:ALA:HB2  | 1:C:713:LEU:HD23 | 1.94                     | 0.50              |
| 1:A:112:ILE:HG13 | 1:A:144:PHE:CE1  | 2.47                     | 0.50              |
| 1:A:197:LEU:HB3  | 1:A:309:LEU:HD12 | 1.94                     | 0.50              |
| 1:A:625:LEU:HD21 | 1:A:652:MET:SD   | 2.52                     | 0.50              |
| 1:B:190:LYS:HZ1  | 1:C:337:ARG:HH22 | 1.58                     | 0.50              |
| 1:C:212:THR:HG21 | 1:C:269:MET:HE2  | 1.93                     | 0.50              |
| 1:C:346:HIS:HD2  | 1:C:349:LEU:HD23 | 1.77                     | 0.50              |
| 1:D:329:PHE:HE1  | 1:D:333:LYS:HE2  | 1.77                     | 0.50              |
| 1:A:85:MET:O     | 1:A:89:PHE:N     | 2.40                     | 0.49              |
| 1:A:329:PHE:CD1  | 1:A:332:ARG:HD3  | 2.47                     | 0.49              |
| 1:A:354:HIS:O    | 1:A:358:THR:HG23 | 2.12                     | 0.49              |
| 1:B:548:LYS:HZ3  | 1:B:582:PHE:HD2  | 1.60                     | 0.49              |
| 1:C:87:PHE:HA    | 1:C:168:ARG:NH2  | 2.27                     | 0.49              |
| 1:A:385:PRO:O    | 1:A:388:LYS:HG3  | 2.11                     | 0.49              |
| 1:B:138:ARG:O    | 1:B:141:LYS:HG2  | 2.12                     | 0.49              |
| 1:B:401:ARG:CZ   | 1:B:481:ASP:HB2  | 2.42                     | 0.49              |
| 1:D:394:PHE:CE2  | 1:D:488:ILE:HG22 | 2.47                     | 0.49              |
| 1:D:592:LEU:O    | 1:D:599:THR:HA   | 2.12                     | 0.49              |
| 1:A:319:PHE:CE1  | 1:A:348:ARG:HG2  | 2.47                     | 0.49              |
| 1:A:404:GLU:O    | 1:A:479:ARG:NE   | 2.44                     | 0.49              |
| 1:C:289:MET:CE   | 1:D:262:LEU:HG   | 2.42                     | 0.49              |
| 1:C:575:GLY:HA2  | 1:C:612:VAL:HG11 | 1.94                     | 0.49              |
| 1:A:424:TYR:HB3  | 1:A:477:LEU:HD12 | 1.93                     | 0.49              |
| 1:B:422:HIS:HA   | 1:B:480:LEU:O    | 2.12                     | 0.49              |
| 1:C:272:VAL:HG23 | 1:C:273:GLY:H    | 1.76                     | 0.49              |
| 1:C:610:GLU:OE2  | 1:C:646:ARG:NH1  | 2.46                     | 0.49              |
| 1:C:209:VAL:O    | 1:C:212:THR:OG1  | 2.24                     | 0.49              |
| 1:A:185:PHE:HA   | 1:A:188:LEU:HD12 | 1.95                     | 0.49              |
| 1:A:601:LEU:HD23 | 1:A:623:PHE:HD2  | 1.78                     | 0.49              |
| 1:D:154:TRP:CZ3  | 1:D:170:LEU:HB3  | 2.48                     | 0.49              |
| 1:D:226:LEU:HD21 | 1:D:281:ASN:HD21 | 1.78                     | 0.49              |
| 1:A:268:THR:HG23 | 1:A:269:MET:N    | 2.27                     | 0.49              |
| 1:A:569:HIS:HD2  | 1:A:600:PRO:HG3  | 1.77                     | 0.49              |
| 1:B:522:ILE:O    | 1:B:526:LYS:HG3  | 2.12                     | 0.49              |
| 1:B:568:LEU:HD13 | 1:B:583:LEU:CG   | 2.42                     | 0.49              |
| 1:A:66:LYS:O     | 1:A:69:GLU:HG2   | 2.13                     | 0.49              |
| 1:A:400:ILE:HG13 | 1:A:401:ARG:HD3  | 1.95                     | 0.49              |
| 1:A:596:PHE:HB2  | 1:A:598:HIS:CD2  | 2.48                     | 0.49              |
| 1:B:353:SER:O    | 1:B:356:THR:OG1  | 2.25                     | 0.49              |
| 1:B:386:LEU:HD22 | 1:B:453:SER:HB2  | 1.94                     | 0.49              |
| 1:C:375:LEU:HD11 | 1:D:335:LEU:HD12 | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:643:PHE:HD1  | 1:A:646:ARG:HH21 | 1.60                     | 0.49              |
| 1:B:401:ARG:NH2  | 1:B:481:ASP:HB2  | 2.28                     | 0.49              |
| 1:B:551:ILE:HA   | 1:B:555:ALA:HB3  | 1.93                     | 0.49              |
| 1:D:387:PHE:HE1  | 1:D:394:PHE:HE1  | 1.61                     | 0.49              |
| 1:D:154:TRP:HZ3  | 1:D:170:LEU:HB3  | 1.78                     | 0.49              |
| 1:A:240:LYS:HD2  | 1:A:245:SER:HB2  | 1.94                     | 0.48              |
| 1:B:504:MET:O    | 1:B:507:LYS:HG2  | 2.12                     | 0.48              |
| 1:C:356:THR:CG2  | 1:D:329:PHE:CD1  | 2.96                     | 0.48              |
| 1:B:189:GLU:CG   | 1:B:192:THR:HG23 | 2.43                     | 0.48              |
| 1:C:247:GLU:OE1  | 1:C:247:GLU:N    | 2.40                     | 0.48              |
| 1:A:426:VAL:HG22 | 1:A:477:LEU:HD11 | 1.94                     | 0.48              |
| 1:B:328:SER:HA   | 1:B:331:ASN:ND2  | 2.27                     | 0.48              |
| 1:C:414:THR:HG21 | 1:C:465:GLN:HG2  | 1.95                     | 0.48              |
| 1:A:346:HIS:HB3  | 1:A:408:LEU:HG   | 1.95                     | 0.48              |
| 1:A:380:TYR:O    | 1:A:384:VAL:HG23 | 2.14                     | 0.48              |
| 1:B:565:ARG:HD3  | 1:C:596:PHE:HZ   | 1.77                     | 0.48              |
| 1:B:612:VAL:O    | 1:B:615:LEU:HG   | 2.13                     | 0.48              |
| 1:A:136:ALA:O    | 1:A:140:LEU:HB2  | 2.13                     | 0.48              |
| 1:A:541:GLN:NE2  | 1:D:562:TYR:OH   | 2.42                     | 0.48              |
| 1:B:368:ILE:HD13 | 1:C:343:ILE:HG22 | 1.96                     | 0.48              |
| 1:B:448:LEU:HG   | 1:B:452:THR:CG2  | 2.43                     | 0.48              |
| 1:B:500:LEU:HD23 | 1:B:503:ILE:HD11 | 1.95                     | 0.48              |
| 1:C:59:HIS:CD2   | 1:C:60:PRO:HD2   | 2.49                     | 0.48              |
| 1:C:252:ILE:O    | 1:C:257:ARG:NH1  | 2.46                     | 0.48              |
| 1:C:375:LEU:CD1  | 1:D:335:LEU:HD12 | 2.44                     | 0.48              |
| 1:A:360:MET:HE1  | 1:B:329:PHE:CZ   | 2.49                     | 0.48              |
| 1:C:240:LYS:HG3  | 1:C:240:LYS:O    | 2.14                     | 0.48              |
| 1:C:409:PRO:HA   | 1:C:471:VAL:HG23 | 1.96                     | 0.48              |
| 1:C:535:VAL:HG22 | 1:C:550:LEU:HD11 | 1.96                     | 0.48              |
| 1:C:665:LEU:HD22 | 1:C:713:LEU:HD13 | 1.95                     | 0.48              |
| 1:A:483:GLN:OE1  | 1:A:487:ASN:ND2  | 2.46                     | 0.48              |
| 1:A:517:GLU:HA   | 1:A:520:ILE:HG22 | 1.96                     | 0.48              |
| 1:B:63:ARG:HD2   | 1:B:66:LYS:HZ1   | 1.78                     | 0.48              |
| 1:B:158:TYR:CE2  | 1:B:163:LYS:HG3  | 2.49                     | 0.48              |
| 1:B:484:SER:O    | 1:B:488:ILE:HG12 | 2.14                     | 0.48              |
| 1:C:132:PRO:HA   | 1:C:135:ILE:HD12 | 1.95                     | 0.48              |
| 1:D:86:GLU:O     | 1:D:168:ARG:NH2  | 2.47                     | 0.48              |
| 1:D:358:THR:HB   | 1:D:362:GLN:HE22 | 1.78                     | 0.48              |
| 1:A:408:LEU:O    | 1:A:471:VAL:HG21 | 2.13                     | 0.48              |
| 1:B:323:MET:O    | 1:B:327:ILE:HG12 | 2.14                     | 0.48              |
| 1:B:565:ARG:NH2  | 1:C:563:ASP:OD2  | 2.37                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:364:ILE:HD13 | 1:A:369:ARG:HB3  | 1.96                     | 0.48              |
| 1:A:416:GLN:CD   | 1:A:436:THR:HB   | 2.38                     | 0.48              |
| 1:D:143:HIS:CD2  | 1:D:179:ARG:HD3  | 2.49                     | 0.48              |
| 1:D:331:ASN:OD1  | 1:D:340:ARG:NH2  | 2.44                     | 0.48              |
| 1:A:268:THR:HG23 | 1:A:291:TYR:CE2  | 2.48                     | 0.48              |
| 1:A:401:ARG:HH22 | 1:A:488:ILE:HD13 | 1.79                     | 0.48              |
| 1:A:507:LYS:HA   | 1:A:513:ILE:HG12 | 1.96                     | 0.48              |
| 1:A:674:PHE:HB2  | 1:A:712:LEU:HD12 | 1.95                     | 0.48              |
| 1:C:83:THR:OG1   | 1:C:84:PRO:HD3   | 2.14                     | 0.48              |
| 1:C:385:PRO:HA   | 1:C:388:LYS:HE2  | 1.96                     | 0.48              |
| 1:C:460:ILE:HD11 | 1:C:500:LEU:HD23 | 1.96                     | 0.48              |
| 1:A:581:LEU:HA   | 1:A:584:ILE:HD12 | 1.95                     | 0.47              |
| 1:B:501:ASN:HA   | 1:B:504:MET:HE3  | 1.96                     | 0.47              |
| 1:C:103:VAL:O    | 1:C:106:ILE:HG22 | 2.13                     | 0.47              |
| 1:A:59:HIS:CD2   | 1:A:61:LYS:H     | 2.32                     | 0.47              |
| 1:A:501:ASN:O    | 1:A:504:MET:HG3  | 2.14                     | 0.47              |
| 1:A:520:ILE:HA   | 1:A:523:HIS:CE1  | 2.49                     | 0.47              |
| 1:A:615:LEU:O    | 1:A:618:LYS:N    | 2.47                     | 0.47              |
| 1:B:113:VAL:HA   | 1:B:116:PHE:HD2  | 1.78                     | 0.47              |
| 1:C:145:LEU:O    | 1:C:149:ILE:HG13 | 2.14                     | 0.47              |
| 1:C:352:ASP:OD1  | 1:C:353:SER:N    | 2.47                     | 0.47              |
| 1:D:411:GLU:O    | 1:D:471:VAL:HG12 | 2.13                     | 0.47              |
| 1:A:323:MET:HG2  | 1:A:348:ARG:CD   | 2.42                     | 0.47              |
| 1:B:239:LEU:HD23 | 1:B:246:TYR:CE2  | 2.49                     | 0.47              |
| 1:B:558:ASN:OD1  | 1:B:558:ASN:C    | 2.58                     | 0.47              |
| 1:B:637:ALA:HB1  | 1:C:659:TYR:CG   | 2.49                     | 0.47              |
| 1:D:89:PHE:CZ    | 1:D:258:TYR:HA   | 2.50                     | 0.47              |
| 1:C:356:THR:O    | 1:C:359:VAL:HG22 | 2.15                     | 0.47              |
| 1:D:108:PHE:CE1  | 1:D:177:ARG:CD   | 2.97                     | 0.47              |
| 1:A:198:PHE:O    | 1:A:202:LEU:HD23 | 2.14                     | 0.47              |
| 1:B:150:GLY:O    | 1:B:174:ARG:NH2  | 2.47                     | 0.47              |
| 1:B:239:LEU:HD23 | 1:B:246:TYR:HE2  | 1.80                     | 0.47              |
| 1:B:364:ILE:CG2  | 1:B:369:ARG:HB2  | 2.38                     | 0.47              |
| 1:B:504:MET:HG2  | 1:B:507:LYS:HZ3  | 1.79                     | 0.47              |
| 1:D:565:ARG:NH2  | 1:D:594:ASP:OD2  | 2.47                     | 0.47              |
| 1:A:376:LEU:O    | 1:A:379:PRO:HD2  | 2.14                     | 0.47              |
| 1:A:569:HIS:CD2  | 1:A:600:PRO:HG3  | 2.50                     | 0.47              |
| 1:D:323:MET:O    | 1:D:327:ILE:HG12 | 2.14                     | 0.47              |
| 1:D:335:LEU:HD22 | 1:D:339:LEU:CB   | 2.45                     | 0.47              |
| 1:A:339:LEU:HD12 | 1:A:340:ARG:H    | 1.71                     | 0.47              |
| 1:A:662:ARG:HH12 | 1:A:693:TRP:HB2  | 1.79                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:264:PHE:HB2  | 1:B:277:ILE:HD12 | 1.96                     | 0.47              |
| 1:B:425:PHE:HD1  | 1:B:453:SER:HG   | 1.62                     | 0.47              |
| 1:B:655:ASN:HB3  | 1:B:685:ALA:HA   | 1.97                     | 0.47              |
| 1:B:662:ARG:HG3  | 1:B:663:THR:N    | 2.30                     | 0.47              |
| 1:B:690:LYS:HD2  | 1:B:690:LYS:HA   | 1.41                     | 0.47              |
| 1:C:431:LEU:HB2  | 1:C:448:LEU:HB2  | 1.96                     | 0.47              |
| 1:C:550:LEU:HG   | 1:C:555:ALA:HB3  | 1.97                     | 0.47              |
| 1:D:86:GLU:HG2   | 1:D:87:PHE:N     | 2.28                     | 0.47              |
| 1:D:319:PHE:O    | 1:D:323:MET:HG2  | 2.14                     | 0.47              |
| 1:D:640:ASP:OD1  | 1:D:640:ASP:N    | 2.48                     | 0.47              |
| 1:A:59:HIS:CD2   | 1:A:61:LYS:HB2   | 2.50                     | 0.47              |
| 1:A:68:TRP:O     | 1:A:72:ILE:HG23  | 2.15                     | 0.47              |
| 1:B:255:TRP:O    | 1:B:259:THR:HG23 | 2.15                     | 0.47              |
| 1:B:407:PHE:CD2  | 1:B:471:VAL:HG21 | 2.49                     | 0.47              |
| 1:B:693:TRP:HE1  | 1:C:662:ARG:NH2  | 2.13                     | 0.47              |
| 1:C:599:THR:HG21 | 1:C:624:ASN:H    | 1.80                     | 0.47              |
| 1:D:323:MET:HE1  | 1:D:347:VAL:HG11 | 1.95                     | 0.47              |
| 1:B:194:ILE:HD12 | 1:B:199:THR:HG22 | 1.96                     | 0.47              |
| 1:B:416:GLN:NE2  | 1:B:435:VAL:HG23 | 2.30                     | 0.47              |
| 1:D:235:TRP:CZ3  | 1:D:277:ILE:HG21 | 2.50                     | 0.47              |
| 1:D:335:LEU:HD22 | 1:D:339:LEU:HB3  | 1.97                     | 0.47              |
| 1:D:404:GLU:OE1  | 1:D:476:HIS:NE2  | 2.48                     | 0.47              |
| 1:D:428:GLU:HB3  | 1:D:476:HIS:HB3  | 1.97                     | 0.47              |
| 1:C:434:LEU:HB3  | 1:C:442:GLU:OE1  | 2.15                     | 0.47              |
| 1:A:315:ASN:OD1  | 1:A:316:THR:N    | 2.48                     | 0.46              |
| 1:B:418:ASN:O    | 1:B:465:GLN:HG2  | 2.15                     | 0.46              |
| 1:D:263:TYR:O    | 1:D:266:ILE:HG22 | 2.15                     | 0.46              |
| 1:D:264:PHE:CD2  | 1:D:277:ILE:CG2  | 2.97                     | 0.46              |
| 1:D:357:ASP:O    | 1:D:361:LEU:HG   | 2.15                     | 0.46              |
| 1:D:461:CYS:HB3  | 1:D:519:ASP:CG   | 2.40                     | 0.46              |
| 1:D:503:ILE:HA   | 1:D:506:GLU:OE2  | 2.16                     | 0.46              |
| 1:A:636:VAL:HG21 | 1:A:664:PRO:HB3  | 1.97                     | 0.46              |
| 1:B:349:LEU:HD23 | 1:B:408:LEU:HG   | 1.97                     | 0.46              |
| 1:B:431:LEU:HD13 | 1:B:471:VAL:HG22 | 1.97                     | 0.46              |
| 1:C:112:ILE:HG21 | 1:C:148:PHE:CE2  | 2.50                     | 0.46              |
| 1:D:181:VAL:HG12 | 1:D:185:PHE:HE2  | 1.80                     | 0.46              |
| 1:D:556:ASP:O    | 1:D:559:LYS:HG2  | 2.16                     | 0.46              |
| 1:A:368:ILE:O    | 1:A:372:ILE:HG23 | 2.15                     | 0.46              |
| 1:A:465:GLN:HE21 | 1:A:467:PHE:HB2  | 1.81                     | 0.46              |
| 1:B:167:VAL:HA   | 1:B:170:LEU:HD12 | 1.98                     | 0.46              |
| 1:B:220:TYR:O    | 1:B:224:THR:HG23 | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:527:GLN:O    | 1:B:530:GLU:HG3  | 2.15                     | 0.46              |
| 1:C:71:PHE:O     | 1:C:75:TRP:HD1   | 1.98                     | 0.46              |
| 1:D:158:TYR:HE2  | 1:D:163:LYS:HZ2  | 1.63                     | 0.46              |
| 1:B:102:ILE:O    | 1:B:106:ILE:HG12 | 2.15                     | 0.46              |
| 1:C:272:VAL:HG23 | 1:C:273:GLY:N    | 2.31                     | 0.46              |
| 1:C:397:GLN:O    | 1:C:400:ILE:HG12 | 2.15                     | 0.46              |
| 1:A:606:LYS:HG2  | 1:A:643:PHE:CE1  | 2.49                     | 0.46              |
| 1:B:642:ASP:O    | 1:B:645:LYS:HG2  | 2.15                     | 0.46              |
| 1:C:149:ILE:HG23 | 1:C:154:TRP:HZ2  | 1.80                     | 0.46              |
| 1:C:315:ASN:HA   | 1:C:318:ARG:CZ   | 2.45                     | 0.46              |
| 1:C:522:ILE:HG13 | 1:C:523:HIS:CD2  | 2.51                     | 0.46              |
| 1:A:326:LEU:HD11 | 1:A:348:ARG:NH2  | 2.30                     | 0.46              |
| 1:B:330:MET:HE1  | 1:B:340:ARG:N    | 2.30                     | 0.46              |
| 1:B:540:PHE:HA   | 1:B:570:LEU:HD21 | 1.97                     | 0.46              |
| 1:C:189:GLU:HB2  | 1:C:199:THR:HG21 | 1.96                     | 0.46              |
| 1:C:402:LEU:HD22 | 1:C:478:LEU:HB3  | 1.98                     | 0.46              |
| 1:C:481:ASP:OD2  | 1:C:483:GLN:HB3  | 2.16                     | 0.46              |
| 1:C:506:GLU:HA   | 1:C:509:SER:OG   | 2.16                     | 0.46              |
| 1:A:249:PHE:HA   | 1:A:252:ILE:HD13 | 1.97                     | 0.46              |
| 1:B:90:PHE:O     | 1:B:168:ARG:NH2  | 2.47                     | 0.46              |
| 1:B:281:ASN:OD1  | 1:B:283:ARG:N    | 2.39                     | 0.46              |
| 1:B:336:GLY:C    | 1:B:337:ARG:HG2  | 2.41                     | 0.46              |
| 1:B:402:LEU:HB3  | 1:B:478:LEU:HD12 | 1.98                     | 0.46              |
| 1:C:393:GLU:HA   | 1:C:396:ASN:ND2  | 2.31                     | 0.46              |
| 1:D:420:VAL:O    | 1:D:482:LYS:HD2  | 2.15                     | 0.46              |
| 1:D:434:LEU:O    | 1:D:467:PHE:HB2  | 2.15                     | 0.46              |
| 1:D:625:LEU:HD23 | 1:D:625:LEU:HA   | 1.77                     | 0.46              |
| 1:B:666:HIS:HE1  | 1:B:691:ASP:HB2  | 1.81                     | 0.46              |
| 1:C:426:VAL:O    | 1:C:451:HIS:N    | 2.48                     | 0.46              |
| 1:C:636:VAL:HG11 | 1:C:667:VAL:HG23 | 1.98                     | 0.46              |
| 1:D:73:LEU:HB3   | 1:D:180:LYS:NZ   | 2.21                     | 0.46              |
| 1:D:83:THR:HA    | 1:D:86:GLU:CD    | 2.41                     | 0.46              |
| 1:D:671:GLU:HG3  | 1:D:673:LEU:HG   | 1.97                     | 0.46              |
| 1:A:357:ASP:HA   | 1:A:360:MET:CE   | 2.46                     | 0.46              |
| 1:B:82:PHE:O     | 1:B:85:MET:HG2   | 2.15                     | 0.46              |
| 1:C:398:ILE:HG13 | 1:C:399:VAL:N    | 2.30                     | 0.46              |
| 1:D:129:VAL:HG13 | 1:D:135:ILE:HD11 | 1.97                     | 0.46              |
| 1:A:668:ALA:HB1  | 1:A:677:ALA:HB2  | 1.97                     | 0.46              |
| 1:B:523:HIS:HA   | 1:B:526:LYS:HE2  | 1.97                     | 0.46              |
| 1:C:380:TYR:CE1  | 1:C:427:CYS:HB3  | 2.51                     | 0.46              |
| 1:C:394:PHE:HA   | 1:C:488:ILE:HD11 | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:561:ASP:OD2  | 1:C:565:ARG:NH2  | 2.46                     | 0.46              |
| 1:A:164:HIS:O    | 1:A:167:VAL:HG12 | 2.15                     | 0.45              |
| 1:A:403:HIS:HB2  | 1:A:479:ARG:HG3  | 1.97                     | 0.45              |
| 1:A:422:HIS:HA   | 1:A:480:LEU:O    | 2.17                     | 0.45              |
| 1:B:565:ARG:NH2  | 1:C:565:ARG:NH1  | 2.64                     | 0.45              |
| 1:C:344:THR:O    | 1:C:348:ARG:HG2  | 2.17                     | 0.45              |
| 1:A:423:LEU:HB2  | 1:A:480:LEU:HB3  | 1.97                     | 0.45              |
| 1:B:319:PHE:HA   | 1:B:322:LYS:HE2  | 1.98                     | 0.45              |
| 1:C:271:THR:HA   | 1:D:272:VAL:HG21 | 1.81                     | 0.45              |
| 1:C:663:THR:HG22 | 1:C:665:LEU:H    | 1.82                     | 0.45              |
| 1:D:504:MET:O    | 1:D:507:LYS:HB2  | 2.16                     | 0.45              |
| 1:A:398:ILE:O    | 1:A:402:LEU:HB2  | 2.16                     | 0.45              |
| 1:B:307:THR:O    | 1:B:311:VAL:HG23 | 2.15                     | 0.45              |
| 1:B:514:LYS:O    | 1:B:514:LYS:HG3  | 2.17                     | 0.45              |
| 1:B:603:GLU:HA   | 1:B:606:LYS:HE3  | 1.98                     | 0.45              |
| 1:C:384:VAL:HG12 | 1:C:387:PHE:H    | 1.81                     | 0.45              |
| 1:C:465:GLN:CD   | 1:C:465:GLN:H    | 2.24                     | 0.45              |
| 1:C:525:GLY:O    | 1:C:528:GLU:HG2  | 2.16                     | 0.45              |
| 1:D:431:LEU:HD21 | 1:D:469:VAL:CG2  | 2.46                     | 0.45              |
| 1:A:135:ILE:HG12 | 1:A:138:ARG:NH2  | 2.31                     | 0.45              |
| 1:C:512:ARG:HA   | 1:C:516:LEU:HD12 | 1.98                     | 0.45              |
| 1:D:565:ARG:HH12 | 1:D:603:GLU:CD   | 2.24                     | 0.45              |
| 1:A:128:THR:HG21 | 1:A:134:ARG:HD3  | 1.98                     | 0.45              |
| 1:B:301:TYR:CD1  | 1:C:306:ILE:HD11 | 2.39                     | 0.45              |
| 1:C:174:ARG:HG3  | 1:C:177:ARG:NH2  | 2.30                     | 0.45              |
| 1:C:237:GLY:HA2  | 1:C:247:GLU:HA   | 1.97                     | 0.45              |
| 1:D:628:SER:HB2  | 1:D:652:MET:SD   | 2.56                     | 0.45              |
| 1:A:397:GLN:HB3  | 1:A:401:ARG:HH12 | 1.82                     | 0.45              |
| 1:A:485:PHE:CE2  | 1:A:489:LEU:HD11 | 2.52                     | 0.45              |
| 1:B:226:LEU:HD21 | 1:B:283:ARG:CZ   | 2.46                     | 0.45              |
| 1:C:115:GLN:O    | 1:C:118:VAL:HG12 | 2.17                     | 0.45              |
| 1:C:130:TYR:CG   | 1:C:130:TYR:O    | 2.68                     | 0.45              |
| 1:D:445:VAL:CG1  | 1:D:446:THR:H    | 2.30                     | 0.45              |
| 1:A:60:PRO:HD3   | 1:A:118:VAL:HG13 | 1.98                     | 0.45              |
| 1:A:330:MET:HE3  | 1:A:337:ARG:HH22 | 1.82                     | 0.45              |
| 1:B:514:LYS:HE3  | 1:B:520:ILE:HG21 | 1.98                     | 0.45              |
| 1:D:623:PHE:CD2  | 1:D:625:LEU:HB2  | 2.52                     | 0.45              |
| 1:A:94:PRO:HD2   | 1:A:97:LEU:HD12  | 1.97                     | 0.45              |
| 1:A:184:PHE:O    | 1:A:188:LEU:HG   | 2.17                     | 0.45              |
| 1:A:380:TYR:HA   | 1:A:383:LYS:HD2  | 1.99                     | 0.45              |
| 1:B:415:GLU:O    | 1:B:465:GLN:HG3  | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:393:GLU:HG2  | 1:D:394:PHE:N    | 2.31                     | 0.45              |
| 1:A:163:LYS:HG3  | 1:A:164:HIS:N    | 2.32                     | 0.45              |
| 1:B:120:TYR:CE2  | 1:B:138:ARG:HG3  | 2.51                     | 0.45              |
| 1:B:402:LEU:HD23 | 1:B:402:LEU:HA   | 1.82                     | 0.45              |
| 1:B:428:GLU:O    | 1:B:475:CYS:HB2  | 2.16                     | 0.45              |
| 1:B:433:ALA:HB1  | 1:B:467:PHE:CE2  | 2.51                     | 0.45              |
| 1:B:662:ARG:NH2  | 1:C:692:ARG:HH21 | 2.14                     | 0.45              |
| 1:C:223:ALA:HB2  | 1:C:235:TRP:NE1  | 2.32                     | 0.45              |
| 1:D:394:PHE:O    | 1:D:398:ILE:HG12 | 2.16                     | 0.45              |
| 1:D:409:PRO:HB3  | 1:D:473:GLU:HA   | 1.99                     | 0.45              |
| 1:A:298:LEU:HD23 | 1:A:298:LEU:HA   | 1.85                     | 0.45              |
| 1:A:616:LEU:HD12 | 1:A:616:LEU:HA   | 1.85                     | 0.45              |
| 1:B:372:ILE:O    | 1:B:375:LEU:HG   | 2.17                     | 0.45              |
| 1:B:514:LYS:HZ1  | 1:B:520:ILE:HG21 | 1.80                     | 0.45              |
| 1:C:173:ILE:HD12 | 1:C:173:ILE:H    | 1.82                     | 0.45              |
| 1:D:174:ARG:HG2  | 1:D:177:ARG:HH12 | 1.82                     | 0.45              |
| 1:A:221:TYR:O    | 1:A:224:THR:OG1  | 2.26                     | 0.44              |
| 1:C:239:LEU:HD12 | 1:C:246:TYR:OH   | 2.16                     | 0.44              |
| 1:D:303:ILE:O    | 1:D:307:THR:HG23 | 2.17                     | 0.44              |
| 1:C:540:PHE:CD1  | 1:C:574:ARG:HD3  | 2.51                     | 0.44              |
| 1:D:81:LEU:O     | 1:D:84:PRO:HD2   | 2.17                     | 0.44              |
| 1:A:222:LEU:HD22 | 1:A:283:ARG:HB3  | 1.99                     | 0.44              |
| 1:A:372:ILE:HG13 | 1:A:373:ALA:N    | 2.32                     | 0.44              |
| 1:A:636:VAL:HG13 | 1:A:676:MET:HE1  | 1.98                     | 0.44              |
| 1:A:654:PRO:HB3  | 1:A:680:LEU:HD23 | 2.00                     | 0.44              |
| 1:B:539:ALA:HA   | 1:B:547:LEU:HD11 | 1.99                     | 0.44              |
| 1:C:285:MET:O    | 1:C:288:VAL:HG12 | 2.18                     | 0.44              |
| 1:D:93:LEU:H     | 1:D:159:LYS:NZ   | 2.15                     | 0.44              |
| 1:D:547:LEU:HD22 | 1:D:579:ILE:HD12 | 1.99                     | 0.44              |
| 1:D:547:LEU:O    | 1:D:551:ILE:HG12 | 2.16                     | 0.44              |
| 1:D:678:LYS:HA   | 1:D:681:VAL:HG22 | 2.00                     | 0.44              |
| 1:A:110:VAL:O    | 1:A:114:LEU:HD23 | 2.18                     | 0.44              |
| 1:C:304:GLY:C    | 1:D:310:ILE:HD11 | 2.43                     | 0.44              |
| 1:D:374:GLN:HA   | 1:D:399:VAL:HG11 | 1.99                     | 0.44              |
| 1:A:124:GLN:HG2  | 1:A:125:THR:N    | 2.32                     | 0.44              |
| 1:B:188:LEU:O    | 1:B:188:LEU:CD1  | 2.60                     | 0.44              |
| 1:B:265:ALA:O    | 1:B:268:THR:OG1  | 2.31                     | 0.44              |
| 1:B:378:LEU:HB3  | 1:B:379:PRO:HD3  | 2.00                     | 0.44              |
| 1:C:418:ASN:C    | 1:C:465:GLN:HE22 | 2.25                     | 0.44              |
| 1:C:538:ALA:HA   | 1:C:541:GLN:HG2  | 2.00                     | 0.44              |
| 1:C:569:HIS:NE2  | 1:C:600:PRO:HD3  | 2.32                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:149:ILE:H    | 1:D:149:ILE:HD12 | 1.83                     | 0.44              |
| 1:D:235:TRP:HZ3  | 1:D:277:ILE:HG21 | 1.81                     | 0.44              |
| 1:A:140:LEU:HG   | 1:A:144:PHE:CD2  | 2.53                     | 0.44              |
| 1:A:308:ALA:HA   | 1:A:311:VAL:HG12 | 2.00                     | 0.44              |
| 1:A:326:LEU:HD11 | 1:A:348:ARG:HH21 | 1.82                     | 0.44              |
| 1:B:356:THR:HG22 | 1:C:329:PHE:HE1  | 1.83                     | 0.44              |
| 1:B:568:LEU:CD1  | 1:B:583:LEU:HD11 | 2.42                     | 0.44              |
| 1:C:121:ARG:HA   | 1:C:128:THR:HA   | 2.00                     | 0.44              |
| 1:C:418:ASN:O    | 1:C:465:GLN:NE2  | 2.50                     | 0.44              |
| 1:C:647:LEU:HG   | 1:C:652:MET:HB2  | 1.99                     | 0.44              |
| 1:D:339:LEU:O    | 1:D:343:ILE:HD12 | 2.17                     | 0.44              |
| 1:A:122:ASP:OD2  | 1:A:124:GLN:NE2  | 2.39                     | 0.44              |
| 1:A:659:TYR:CG   | 1:D:637:ALA:HB1  | 2.52                     | 0.44              |
| 1:B:407:PHE:HD2  | 1:B:471:VAL:HG21 | 1.82                     | 0.44              |
| 1:B:596:PHE:HB2  | 1:B:598:HIS:ND1  | 2.33                     | 0.44              |
| 1:C:86:GLU:HG3   | 1:C:90:PHE:CE1   | 2.53                     | 0.44              |
| 1:C:487:ASN:O    | 1:C:490:GLU:HG3  | 2.18                     | 0.44              |
| 1:D:251:GLU:C    | 1:D:251:GLU:CD   | 2.85                     | 0.44              |
| 1:A:239:LEU:CD2  | 1:A:241:LEU:HB2  | 2.48                     | 0.44              |
| 1:A:432:GLU:OE2  | 1:A:434:LEU:HB3  | 2.18                     | 0.44              |
| 1:A:593:LYS:HZ3  | 1:A:599:THR:HB   | 1.82                     | 0.44              |
| 1:A:687:VAL:HG23 | 1:A:688:ILE:HG23 | 1.99                     | 0.44              |
| 1:B:355:TYR:O    | 1:B:359:VAL:HG13 | 2.18                     | 0.44              |
| 1:B:564:GLY:N    | 1:B:595:LYS:HB3  | 2.32                     | 0.44              |
| 1:C:358:THR:O    | 1:C:362:GLN:OE1  | 2.35                     | 0.44              |
| 1:C:488:ILE:HA   | 1:C:491:ILE:HG22 | 1.99                     | 0.44              |
| 1:D:115:GLN:HE22 | 1:D:140:LEU:HA   | 1.81                     | 0.44              |
| 1:A:479:ARG:H    | 1:A:479:ARG:HG2  | 1.66                     | 0.44              |
| 1:A:608:GLY:HA2  | 1:A:646:ARG:HD2  | 2.00                     | 0.44              |
| 1:B:437:LYS:HB3  | 1:B:441:SER:HB3  | 2.00                     | 0.44              |
| 1:B:659:TYR:HB2  | 1:C:637:ALA:HB2  | 2.00                     | 0.44              |
| 1:C:149:ILE:HG23 | 1:C:154:TRP:CZ2  | 2.53                     | 0.44              |
| 1:A:124:GLN:HG2  | 1:A:125:THR:HG23 | 2.00                     | 0.43              |
| 1:A:281:ASN:O    | 1:A:285:MET:N    | 2.51                     | 0.43              |
| 1:A:330:MET:HE3  | 1:A:337:ARG:NH2  | 2.32                     | 0.43              |
| 1:B:196:TYR:HB2  | 1:C:320:ARG:HE   | 1.83                     | 0.43              |
| 1:B:525:GLY:O    | 1:B:528:GLU:HG3  | 2.17                     | 0.43              |
| 1:B:642:ASP:OD1  | 1:B:642:ASP:N    | 2.50                     | 0.43              |
| 1:D:137:PHE:O    | 1:D:141:LYS:HG3  | 2.17                     | 0.43              |
| 1:D:514:LYS:HB3  | 1:D:514:LYS:HE2  | 1.71                     | 0.43              |
| 1:D:575:GLY:HA2  | 1:D:612:VAL:HG21 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:375:LEU:HD21 | 1:B:337:ARG:HH22 | 1.83                     | 0.43              |
| 1:A:382:LYS:HZ3  | 1:A:392:THR:HA   | 1.83                     | 0.43              |
| 1:C:343:ILE:HG13 | 1:C:344:THR:N    | 2.33                     | 0.43              |
| 1:C:383:LYS:HD2  | 1:C:451:HIS:CG   | 2.53                     | 0.43              |
| 1:D:131:LYS:CE   | 1:D:134:ARG:HH12 | 2.27                     | 0.43              |
| 1:A:172:TRP:O    | 1:A:175:LEU:HB3  | 2.19                     | 0.43              |
| 1:A:485:PHE:O    | 1:A:488:ILE:HG22 | 2.18                     | 0.43              |
| 1:C:308:ALA:HA   | 1:C:311:VAL:HG12 | 2.01                     | 0.43              |
| 1:C:583:LEU:O    | 1:C:586:GLU:HB2  | 2.19                     | 0.43              |
| 1:D:394:PHE:HB2  | 1:D:495:ASP:OD2  | 2.19                     | 0.43              |
| 1:D:527:GLN:O    | 1:D:530:GLU:HG3  | 2.18                     | 0.43              |
| 1:A:59:HIS:ND1   | 1:A:60:PRO:HD2   | 2.33                     | 0.43              |
| 1:A:91:ARG:HA    | 1:A:168:ARG:NH1  | 2.33                     | 0.43              |
| 1:A:289:MET:O    | 1:A:292:VAL:HG22 | 2.18                     | 0.43              |
| 1:D:68:TRP:CZ2   | 1:D:72:ILE:HD11  | 2.53                     | 0.43              |
| 1:D:393:GLU:O    | 1:D:397:GLN:HG2  | 2.18                     | 0.43              |
| 1:D:487:ASN:O    | 1:D:490:GLU:HG3  | 2.18                     | 0.43              |
| 1:D:497:ARG:NH1  | 1:D:553:SER:O    | 2.51                     | 0.43              |
| 1:A:60:PRO:HG3   | 1:A:117:PHE:HE2  | 1.83                     | 0.43              |
| 1:A:397:GLN:O    | 1:A:400:ILE:HG12 | 2.19                     | 0.43              |
| 1:A:485:PHE:CZ   | 1:A:489:LEU:HD11 | 2.54                     | 0.43              |
| 1:B:527:GLN:O    | 1:B:531:LEU:HG   | 2.18                     | 0.43              |
| 1:D:106:ILE:HD12 | 1:D:109:LEU:HD12 | 1.99                     | 0.43              |
| 1:D:507:LYS:C    | 1:D:509:SER:H    | 2.26                     | 0.43              |
| 1:D:535:VAL:HG12 | 1:D:550:LEU:HD22 | 2.00                     | 0.43              |
| 1:D:601:LEU:HD11 | 1:D:621:ALA:HB3  | 2.01                     | 0.43              |
| 1:B:194:ILE:CD1  | 1:B:199:THR:HG22 | 2.49                     | 0.43              |
| 1:D:269:MET:HA   | 1:D:295:ASP:OD2  | 2.18                     | 0.43              |
| 1:D:425:PHE:HD1  | 1:D:453:SER:HB2  | 1.82                     | 0.43              |
| 1:D:547:LEU:O    | 1:D:550:LEU:HG   | 2.19                     | 0.43              |
| 1:B:384:VAL:HA   | 1:B:451:HIS:HB3  | 2.00                     | 0.43              |
| 1:B:433:ALA:HB3  | 1:B:446:THR:OG1  | 2.19                     | 0.43              |
| 1:C:511:ASP:HB2  | 1:C:515:LYS:HB3  | 2.01                     | 0.43              |
| 1:A:273:GLY:HA3  | 1:B:272:VAL:O    | 2.19                     | 0.43              |
| 1:B:378:LEU:HA   | 1:B:381:ILE:HG22 | 2.00                     | 0.43              |
| 1:C:383:LYS:O    | 1:C:383:LYS:HG2  | 2.18                     | 0.43              |
| 1:C:435:VAL:HG22 | 1:C:467:PHE:CD1  | 2.54                     | 0.43              |
| 1:C:576:TYR:O    | 1:C:580:THR:HG23 | 2.18                     | 0.43              |
| 1:A:326:LEU:HD12 | 1:A:326:LEU:C    | 2.44                     | 0.43              |
| 1:B:507:LYS:CB   | 1:B:514:LYS:HG2  | 2.49                     | 0.43              |
| 1:C:402:LEU:HD23 | 1:C:402:LEU:HA   | 1.83                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:239:LEU:HD11 | 1:D:246:TYR:CE2  | 2.54                     | 0.43              |
| 1:D:589:ASP:OD1  | 1:D:589:ASP:N    | 2.51                     | 0.43              |
| 1:A:223:ALA:HB2  | 1:A:235:TRP:HE1  | 1.83                     | 0.43              |
| 1:B:424:TYR:HA   | 1:B:478:LEU:O    | 2.18                     | 0.43              |
| 1:B:594:ASP:OD1  | 1:B:595:LYS:N    | 2.49                     | 0.43              |
| 1:C:408:LEU:HD23 | 1:C:409:PRO:O    | 2.19                     | 0.43              |
| 1:A:412:VAL:HG23 | 1:A:468:THR:HG23 | 2.00                     | 0.42              |
| 1:A:507:LYS:HA   | 1:A:513:ILE:HG23 | 2.01                     | 0.42              |
| 1:B:129:VAL:HB   | 1:B:135:ILE:HD11 | 2.01                     | 0.42              |
| 1:B:345:GLY:HA2  | 1:B:348:ARG:HG2  | 2.00                     | 0.42              |
| 1:B:410:GLY:N    | 1:B:471:VAL:O    | 2.50                     | 0.42              |
| 1:C:399:VAL:O    | 1:C:402:LEU:HB2  | 2.19                     | 0.42              |
| 1:C:582:PHE:HA   | 1:C:585:GLN:NE2  | 2.33                     | 0.42              |
| 1:C:593:LYS:HD3  | 1:C:624:ASN:HB3  | 1.99                     | 0.42              |
| 1:D:131:LYS:HE3  | 1:D:134:ARG:NH1  | 2.30                     | 0.42              |
| 1:D:333:LYS:C    | 1:D:334:LYS:CG   | 2.87                     | 0.42              |
| 1:A:223:ALA:HB2  | 1:A:235:TRP:NE1  | 2.34                     | 0.42              |
| 1:B:74:VAL:HA    | 1:B:77:ILE:HG12  | 2.01                     | 0.42              |
| 1:B:448:LEU:CD2  | 1:B:452:THR:CG2  | 2.97                     | 0.42              |
| 1:D:561:ASP:OD2  | 1:D:565:ARG:HB3  | 2.18                     | 0.42              |
| 1:D:645:LYS:HG2  | 1:D:679:MET:HG2  | 2.00                     | 0.42              |
| 1:A:89:PHE:CZ    | 1:A:258:TYR:HA   | 2.54                     | 0.42              |
| 1:B:168:ARG:HA   | 1:B:171:LEU:HD13 | 2.01                     | 0.42              |
| 1:C:549:SER:HA   | 1:C:552:ARG:HG2  | 2.01                     | 0.42              |
| 1:D:251:GLU:CD   | 1:D:251:GLU:O    | 2.63                     | 0.42              |
| 1:D:308:ALA:O    | 1:D:311:VAL:HG12 | 2.18                     | 0.42              |
| 1:D:497:ARG:NH2  | 1:D:553:SER:HB2  | 2.34                     | 0.42              |
| 1:A:63:ARG:HA    | 1:A:66:LYS:HG2   | 2.02                     | 0.42              |
| 1:B:280:VAL:HG11 | 1:C:242:GLY:HA3  | 2.02                     | 0.42              |
| 1:B:336:GLY:O    | 1:B:337:ARG:CG   | 2.66                     | 0.42              |
| 1:B:374:GLN:HA   | 1:B:378:LEU:HB2  | 2.02                     | 0.42              |
| 1:B:615:LEU:HA   | 1:B:618:LYS:HG2  | 2.00                     | 0.42              |
| 1:C:190:LYS:HD3  | 1:C:190:LYS:HA   | 1.64                     | 0.42              |
| 1:C:349:LEU:HD22 | 1:C:474:LEU:HD23 | 1.99                     | 0.42              |
| 1:C:396:ASN:O    | 1:C:400:ILE:HG23 | 2.19                     | 0.42              |
| 1:D:445:VAL:CG1  | 1:D:446:THR:N    | 2.83                     | 0.42              |
| 1:A:220:TYR:OH   | 1:A:257:ARG:HD2  | 2.20                     | 0.42              |
| 1:B:72:ILE:HG12  | 1:B:111:ASP:OD1  | 2.19                     | 0.42              |
| 1:B:83:THR:O     | 1:B:86:GLU:HG3   | 2.19                     | 0.42              |
| 1:B:115:GLN:HB3  | 1:B:139:TYR:CZ   | 2.55                     | 0.42              |
| 1:B:194:ILE:O    | 1:C:320:ARG:NH2  | 2.53                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:222:LEU:HD22 | 1:B:284:GLU:OE1  | 2.20                     | 0.42              |
| 1:C:270:ALA:O    | 1:C:272:VAL:HG13 | 2.19                     | 0.42              |
| 1:D:424:TYR:HA   | 1:D:478:LEU:O    | 2.19                     | 0.42              |
| 1:A:413:ILE:HB   | 1:A:469:VAL:HG23 | 2.01                     | 0.42              |
| 1:A:691:ASP:OD1  | 1:A:691:ASP:N    | 2.52                     | 0.42              |
| 1:B:72:ILE:HD12  | 1:B:72:ILE:HA    | 1.92                     | 0.42              |
| 1:B:393:GLU:H    | 1:B:393:GLU:CD   | 2.25                     | 0.42              |
| 1:C:339:LEU:HA   | 1:C:339:LEU:HD23 | 1.76                     | 0.42              |
| 1:C:456:ASP:OD2  | 1:C:457:ILE:N    | 2.52                     | 0.42              |
| 1:D:185:PHE:HA   | 1:D:188:LEU:HD12 | 2.02                     | 0.42              |
| 1:D:322:LYS:O    | 1:D:326:LEU:HB2  | 2.20                     | 0.42              |
| 1:A:122:ASP:O    | 1:A:123:THR:OG1  | 2.28                     | 0.42              |
| 1:C:579:ILE:HD12 | 1:C:579:ILE:H    | 1.85                     | 0.42              |
| 1:D:226:LEU:CD2  | 1:D:281:ASN:HD21 | 2.32                     | 0.42              |
| 1:D:666:HIS:CD2  | 1:D:700:GLU:HB2  | 2.54                     | 0.42              |
| 1:A:359:VAL:O    | 1:A:362:GLN:HG2  | 2.20                     | 0.42              |
| 1:B:65:TYR:O     | 1:B:69:GLU:HG3   | 2.19                     | 0.42              |
| 1:B:172:TRP:O    | 1:B:175:LEU:HG   | 2.20                     | 0.42              |
| 1:B:700:GLU:H    | 1:B:700:GLU:HG2  | 1.63                     | 0.42              |
| 1:C:89:PHE:HA    | 1:C:220:TYR:CD1  | 2.55                     | 0.42              |
| 1:C:507:LYS:HE2  | 1:C:515:LYS:HD3  | 2.02                     | 0.42              |
| 1:C:533:LEU:HD11 | 1:C:562:TYR:CE1  | 2.55                     | 0.42              |
| 1:C:673:LEU:HD21 | 1:C:676:MET:HE3  | 2.02                     | 0.42              |
| 1:D:181:VAL:CG1  | 1:D:185:PHE:HE2  | 2.33                     | 0.42              |
| 1:A:234:THR:CG2  | 1:A:235:TRP:N    | 2.83                     | 0.42              |
| 1:B:154:TRP:HE1  | 1:B:173:ILE:HD11 | 1.85                     | 0.42              |
| 1:B:281:ASN:HD21 | 1:B:283:ARG:NH2  | 2.17                     | 0.42              |
| 1:B:396:ASN:O    | 1:B:400:ILE:HG23 | 2.19                     | 0.42              |
| 1:B:433:ALA:HB1  | 1:B:467:PHE:HE2  | 1.85                     | 0.42              |
| 1:B:504:MET:O    | 1:B:508:GLU:OE1  | 2.37                     | 0.42              |
| 1:C:584:ILE:HD13 | 1:C:619:GLU:OE2  | 2.19                     | 0.42              |
| 1:A:248:ASN:O    | 1:A:252:ILE:HD12 | 2.20                     | 0.42              |
| 1:B:208:GLU:OE1  | 1:B:298:LEU:HG   | 2.19                     | 0.42              |
| 1:B:310:ILE:HD13 | 1:B:310:ILE:HA   | 1.83                     | 0.42              |
| 1:B:330:MET:HE2  | 1:B:336:GLY:HA2  | 2.02                     | 0.42              |
| 1:C:519:ASP:HB2  | 1:C:522:ILE:CG1  | 2.45                     | 0.42              |
| 1:C:136:ALA:O    | 1:C:140:LEU:HD23 | 2.20                     | 0.41              |
| 1:A:437:LYS:HD2  | 1:A:441:SER:OG   | 2.20                     | 0.41              |
| 1:B:90:PHE:CZ    | 1:B:254:LEU:HD13 | 2.55                     | 0.41              |
| 1:B:239:LEU:CD1  | 1:B:277:ILE:HG22 | 2.50                     | 0.41              |
| 1:B:418:ASN:O    | 1:B:465:GLN:N    | 2.32                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:89:PHE:CZ    | 1:C:258:TYR:HA   | 2.55                     | 0.41              |
| 1:C:540:PHE:HD1  | 1:C:574:ARG:CG   | 2.33                     | 0.41              |
| 1:C:543:ASP:HB2  | 1:C:545:TYR:CE2  | 2.55                     | 0.41              |
| 1:D:158:TYR:HD1  | 1:D:167:VAL:HB   | 1.85                     | 0.41              |
| 1:D:183:GLU:O    | 1:D:187:ARG:NE   | 2.50                     | 0.41              |
| 1:A:233:TYR:HB3  | 1:B:243:ASP:HB2  | 2.01                     | 0.41              |
| 1:B:219:PHE:HD1  | 1:B:284:GLU:OE2  | 2.04                     | 0.41              |
| 1:C:231:GLU:OE2  | 1:C:248:ASN:HA   | 2.21                     | 0.41              |
| 1:C:360:MET:HG3  | 1:C:369:ARG:NH2  | 2.35                     | 0.41              |
| 1:D:62:ASN:OD1   | 1:D:63:ARG:N     | 2.54                     | 0.41              |
| 1:D:264:PHE:HD2  | 1:D:277:ILE:CG2  | 2.33                     | 0.41              |
| 1:D:548:LYS:HG3  | 1:D:552:ARG:HH21 | 1.86                     | 0.41              |
| 1:A:632:LEU:HD23 | 1:A:656:SER:O    | 2.20                     | 0.41              |
| 1:B:352:ASP:O    | 1:B:356:THR:HG23 | 2.20                     | 0.41              |
| 1:B:642:ASP:O    | 1:B:646:ARG:HG2  | 2.20                     | 0.41              |
| 1:C:101:ASP:O    | 1:C:105:GLN:HG2  | 2.20                     | 0.41              |
| 1:C:456:ASP:O    | 1:C:460:ILE:HG22 | 2.21                     | 0.41              |
| 1:C:493:PHE:HD2  | 1:C:497:ARG:HH22 | 1.67                     | 0.41              |
| 1:C:578:ASP:OD1  | 1:C:578:ASP:N    | 2.48                     | 0.41              |
| 1:D:109:LEU:O    | 1:D:113:VAL:HG23 | 2.21                     | 0.41              |
| 1:D:426:VAL:HG13 | 1:D:426:VAL:O    | 2.21                     | 0.41              |
| 1:A:95:GLU:HG2   | 1:A:96:ARG:N     | 2.35                     | 0.41              |
| 1:A:58:ILE:O     | 1:A:118:VAL:HG12 | 2.19                     | 0.41              |
| 1:C:423:LEU:HD12 | 1:C:454:PHE:O    | 2.21                     | 0.41              |
| 1:D:281:ASN:O    | 1:D:284:GLU:HB2  | 2.20                     | 0.41              |
| 1:D:347:VAL:HG22 | 1:D:351:TYR:HE2  | 1.83                     | 0.41              |
| 1:D:397:GLN:HB3  | 1:D:401:ARG:NH2  | 2.33                     | 0.41              |
| 1:D:425:PHE:O    | 1:D:477:LEU:HD12 | 2.20                     | 0.41              |
| 1:A:174:ARG:HG2  | 1:A:177:ARG:HH12 | 1.85                     | 0.41              |
| 1:A:329:PHE:HZ   | 1:D:356:THR:HG22 | 1.82                     | 0.41              |
| 1:B:393:GLU:OE2  | 1:B:393:GLU:N    | 2.40                     | 0.41              |
| 1:C:255:TRP:O    | 1:C:259:THR:HG23 | 2.21                     | 0.41              |
| 1:A:428:GLU:HA   | 1:A:450:PRO:HB3  | 2.02                     | 0.41              |
| 1:A:501:ASN:HA   | 1:A:504:MET:HG3  | 2.02                     | 0.41              |
| 1:B:220:TYR:CE1  | 1:B:257:ARG:HD3  | 2.55                     | 0.41              |
| 1:C:616:LEU:O    | 1:C:620:GLY:N    | 2.52                     | 0.41              |
| 1:D:77:ILE:HG13  | 1:D:78:TYR:N     | 2.36                     | 0.41              |
| 1:D:485:PHE:CE2  | 1:D:489:LEU:HD11 | 2.56                     | 0.41              |
| 1:A:121:ARG:NH1  | 1:A:127:ARG:HB2  | 2.36                     | 0.41              |
| 1:A:134:ARG:HG3  | 1:A:135:ILE:N    | 2.35                     | 0.41              |
| 1:A:336:GLY:O    | 1:A:339:LEU:HG   | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:350:GLN:HB2  | 1:A:406:TYR:HB2  | 2.02                     | 0.41              |
| 1:A:375:LEU:HD22 | 1:B:335:LEU:HD11 | 2.01                     | 0.41              |
| 1:A:540:PHE:CE2  | 1:D:562:TYR:HB3  | 2.55                     | 0.41              |
| 1:B:375:LEU:HD12 | 1:B:376:LEU:HB2  | 2.02                     | 0.41              |
| 1:B:599:THR:HG21 | 1:B:623:PHE:O    | 2.20                     | 0.41              |
| 1:B:666:HIS:CG   | 1:B:700:GLU:HG3  | 2.55                     | 0.41              |
| 1:C:270:ALA:HB3  | 1:C:272:VAL:HG22 | 2.02                     | 0.41              |
| 1:C:273:GLY:N    | 1:D:272:VAL:HG13 | 2.35                     | 0.41              |
| 1:C:397:GLN:HB3  | 1:C:488:ILE:HD12 | 2.03                     | 0.41              |
| 1:C:420:VAL:O    | 1:C:482:LYS:NZ   | 2.51                     | 0.41              |
| 1:C:486:SER:O    | 1:C:489:LEU:HG   | 2.21                     | 0.41              |
| 1:D:58:ILE:HD11  | 1:D:62:ASN:HD22  | 1.86                     | 0.41              |
| 1:D:239:LEU:C    | 1:D:239:LEU:HD12 | 2.45                     | 0.41              |
| 1:D:257:ARG:H    | 1:D:257:ARG:HG3  | 1.73                     | 0.41              |
| 1:D:267:VAL:HG22 | 1:D:274:TYR:CD2  | 2.56                     | 0.41              |
| 1:A:320:ARG:O    | 1:A:323:MET:HB2  | 2.20                     | 0.41              |
| 1:A:458:SER:OG   | 1:A:465:GLN:HB2  | 2.22                     | 0.41              |
| 1:B:496:GLY:O    | 1:B:499:ILE:HG22 | 2.20                     | 0.41              |
| 1:B:524:ILE:HD12 | 1:B:524:ILE:HA   | 1.92                     | 0.41              |
| 1:D:66:LYS:HB3   | 1:D:66:LYS:HE3   | 1.85                     | 0.41              |
| 1:D:91:ARG:NH2   | 1:D:168:ARG:HD2  | 2.36                     | 0.41              |
| 1:B:504:MET:HG2  | 1:B:507:LYS:NZ   | 2.35                     | 0.40              |
| 1:C:200:ARG:O    | 1:C:204:LEU:HD23 | 2.21                     | 0.40              |
| 1:D:335:LEU:HD22 | 1:D:339:LEU:CD2  | 2.51                     | 0.40              |
| 1:D:590:VAL:HB   | 1:D:619:GLU:HG2  | 2.03                     | 0.40              |
| 1:A:568:LEU:HD22 | 1:A:588:VAL:HG13 | 2.03                     | 0.40              |
| 1:A:633:CYS:HB3  | 1:A:657:GLU:O    | 2.22                     | 0.40              |
| 1:B:347:VAL:O    | 1:B:350:GLN:HG2  | 2.21                     | 0.40              |
| 1:C:361:LEU:HD23 | 1:C:369:ARG:HD2  | 2.03                     | 0.40              |
| 1:C:582:PHE:HA   | 1:C:585:GLN:CD   | 2.46                     | 0.40              |
| 1:A:92:GLY:H     | 1:A:168:ARG:HH12 | 1.69                     | 0.40              |
| 1:A:110:VAL:O    | 1:A:113:VAL:HG22 | 2.22                     | 0.40              |
| 1:B:89:PHE:HA    | 1:B:220:TYR:CE2  | 2.56                     | 0.40              |
| 1:B:190:LYS:NZ   | 1:C:337:ARG:NH2  | 2.69                     | 0.40              |
| 1:B:544:PHE:O    | 1:B:548:LYS:HD3  | 2.21                     | 0.40              |
| 1:C:205:LEU:HA   | 1:C:205:LEU:HD12 | 1.80                     | 0.40              |
| 1:C:266:ILE:CG2  | 1:C:269:MET:HE3  | 2.52                     | 0.40              |
| 1:C:377:TYR:HB2  | 1:C:399:VAL:HG13 | 2.04                     | 0.40              |
| 1:D:266:ILE:O    | 1:D:269:MET:CG   | 2.62                     | 0.40              |
| 1:A:318:ARG:C    | 1:A:322:LYS:HZ2  | 2.30                     | 0.40              |
| 1:A:574:ARG:HA   | 1:A:574:ARG:HD2  | 1.89                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:152:PHE:HA   | 1:B:153:PRO:HD3  | 1.97                     | 0.40              |
| 1:B:181:VAL:CG1  | 1:B:185:PHE:HE2  | 2.33                     | 0.40              |
| 1:B:661:HIS:O    | 1:B:661:HIS:CG   | 2.75                     | 0.40              |
| 1:D:349:LEU:HD21 | 1:D:406:TYR:HB2  | 2.04                     | 0.40              |
| 1:D:563:ASP:HA   | 1:D:595:LYS:HG3  | 2.02                     | 0.40              |
| 1:B:84:PRO:HB2   | 1:B:217:CYS:SG   | 2.61                     | 0.40              |
| 1:B:98:PHE:CE2   | 1:B:102:ILE:HD11 | 2.56                     | 0.40              |
| 1:B:172:TRP:CZ2  | 1:B:218:ILE:HD11 | 2.49                     | 0.40              |
| 1:C:220:TYR:O    | 1:C:224:THR:HG23 | 2.22                     | 0.40              |
| 1:C:356:THR:HG23 | 1:C:360:MET:SD   | 2.59                     | 0.40              |
| 1:C:572:ALA:HB1  | 1:C:604:ALA:HB2  | 2.04                     | 0.40              |
| 1:D:190:LYS:HD3  | 1:D:190:LYS:HA   | 1.90                     | 0.40              |
| 1:D:591:ASN:ND2  | 1:D:624:ASN:OD1  | 2.55                     | 0.40              |
| 1:D:676:MET:SD   | 1:D:677:ALA:N    | 2.95                     | 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     | 654/820 (80%)   | 634 (97%)  | 20 (3%) | 0        | 100         | 100 |
| 1   | B     | 654/820 (80%)   | 637 (97%)  | 17 (3%) | 0        | 100         | 100 |
| 1   | C     | 654/820 (80%)   | 640 (98%)  | 14 (2%) | 0        | 100         | 100 |
| 1   | D     | 654/820 (80%)   | 642 (98%)  | 12 (2%) | 0        | 100         | 100 |
| All | All   | 2616/3280 (80%) | 2553 (98%) | 63 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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     | 577/729 (79%)   | 575 (100%) | 2 (0%)   | 86          | 84 |
| 1   | B     | 577/729 (79%)   | 572 (99%)  | 5 (1%)   | 70          | 76 |
| 1   | C     | 579/729 (79%)   | 576 (100%) | 3 (0%)   | 81          | 81 |
| 1   | D     | 577/729 (79%)   | 574 (100%) | 3 (0%)   | 81          | 81 |
| All | All   | 2310/2916 (79%) | 2297 (99%) | 13 (1%)  | 76          | 80 |

All (13) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 342 | GLN  |
| 1   | A     | 395 | ILE  |
| 1   | B     | 359 | VAL  |
| 1   | B     | 513 | ILE  |
| 1   | B     | 566 | SER  |
| 1   | B     | 688 | ILE  |
| 1   | B     | 690 | LYS  |
| 1   | C     | 267 | VAL  |
| 1   | C     | 326 | LEU  |
| 1   | C     | 327 | ILE  |
| 1   | D     | 247 | GLU  |
| 1   | D     | 253 | ASP  |
| 1   | D     | 267 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 465 | GLN  |
| 1   | A     | 487 | ASN  |
| 1   | A     | 501 | ASN  |
| 1   | A     | 527 | GLN  |
| 1   | A     | 666 | HIS  |
| 1   | B     | 248 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 346 | HIS  |
| 1   | B     | 350 | GLN  |
| 1   | B     | 403 | HIS  |
| 1   | B     | 465 | GLN  |
| 1   | B     | 558 | ASN  |
| 1   | B     | 591 | ASN  |
| 1   | B     | 666 | HIS  |
| 1   | C     | 186 | GLN  |
| 1   | C     | 350 | GLN  |
| 1   | C     | 397 | GLN  |
| 1   | C     | 487 | ASN  |
| 1   | C     | 523 | HIS  |
| 1   | C     | 630 | ASN  |
| 1   | C     | 653 | ASN  |
| 1   | D     | 59  | HIS  |
| 1   | D     | 124 | GLN  |
| 1   | D     | 502 | ASN  |
| 1   | D     | 558 | ASN  |
| 1   | D     | 655 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

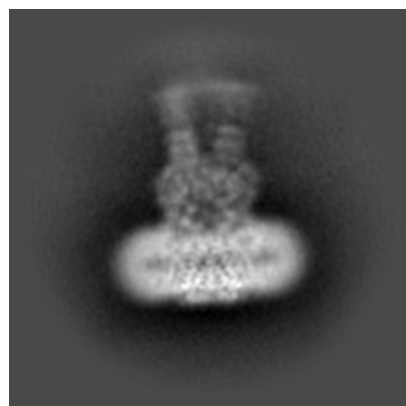
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37500. These allow visual inspection of the internal detail of the map and identification of artifacts.

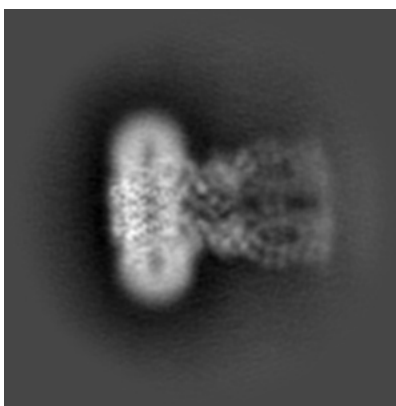
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

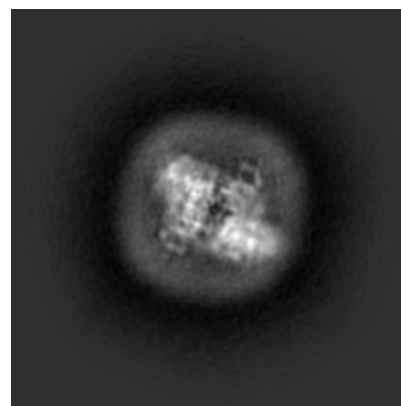
#### 6.1.1 Primary map



X

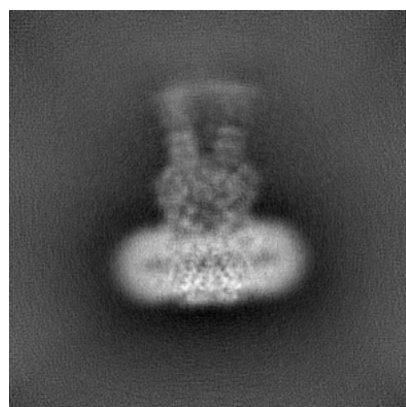


Y

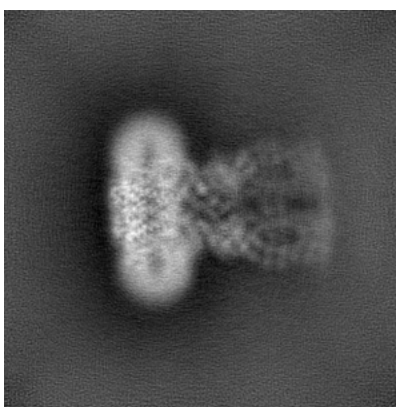


Z

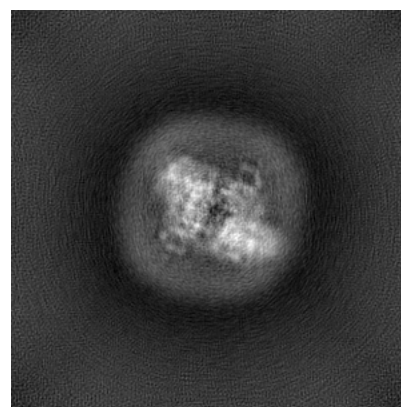
#### 6.1.2 Raw map



X



Y



Z

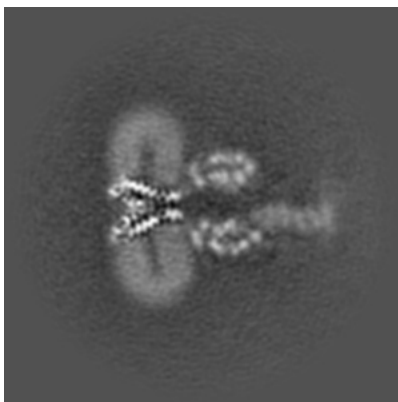
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

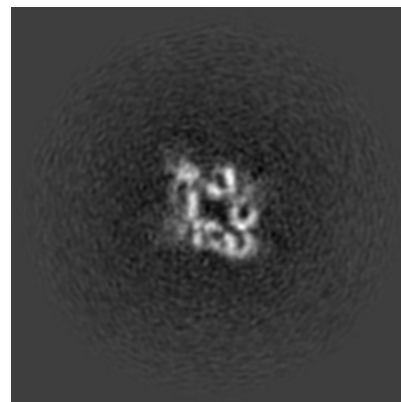
### 6.2.1 Primary map



X Index: 144

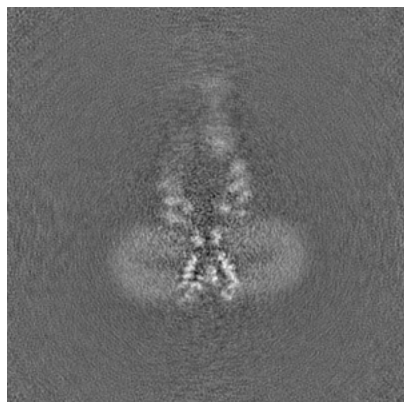


Y Index: 144

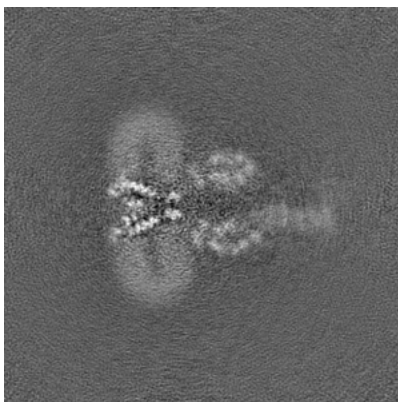


Z Index: 144

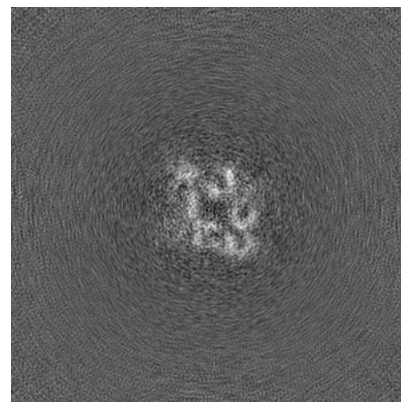
### 6.2.2 Raw map



X Index: 144



Y Index: 144



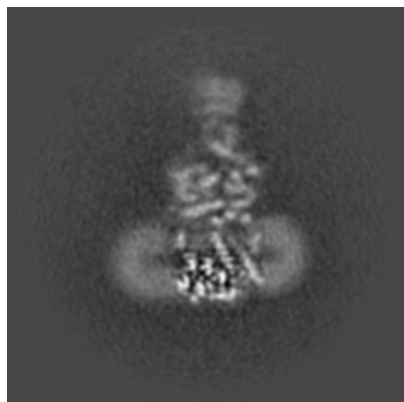
Z Index: 144

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

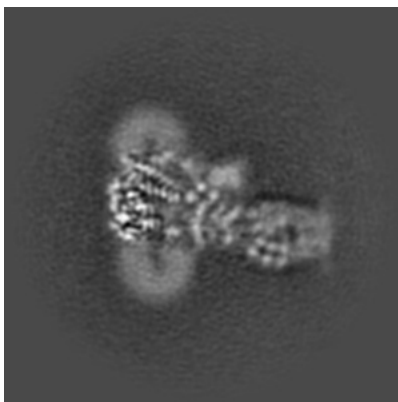


## 6.3 Largest variance slices [i](#)

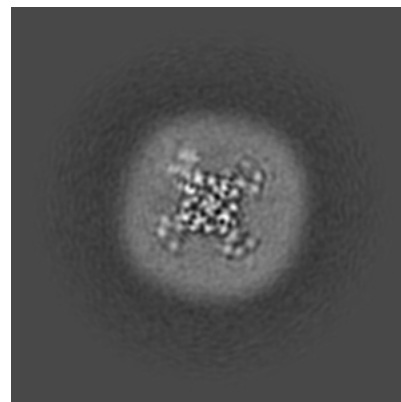
### 6.3.1 Primary map



X Index: 130

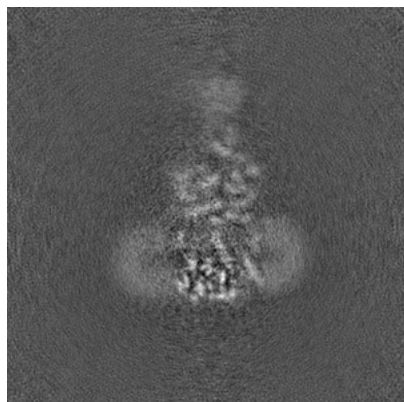


Y Index: 159

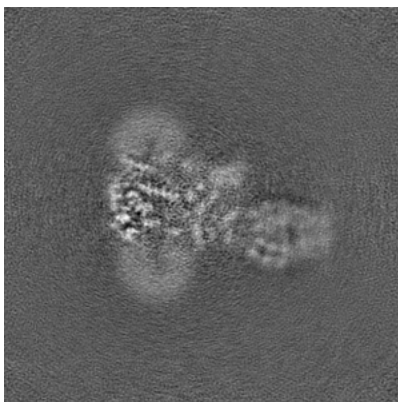


Z Index: 92

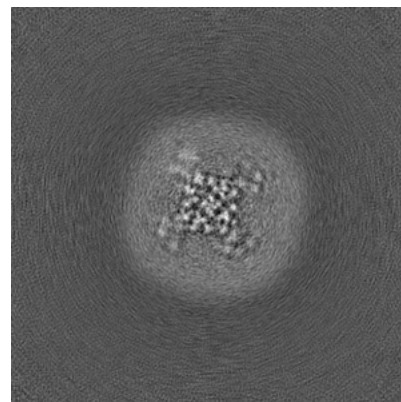
### 6.3.2 Raw map



X Index: 130



Y Index: 158



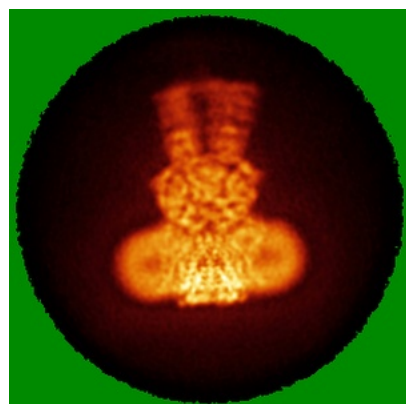
Z Index: 92

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

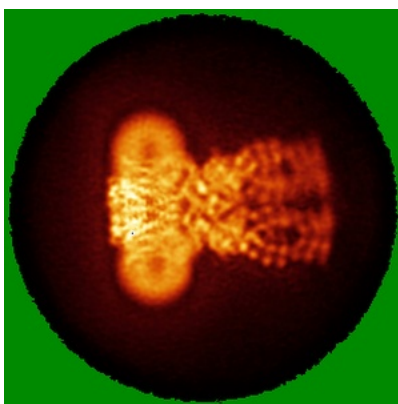


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

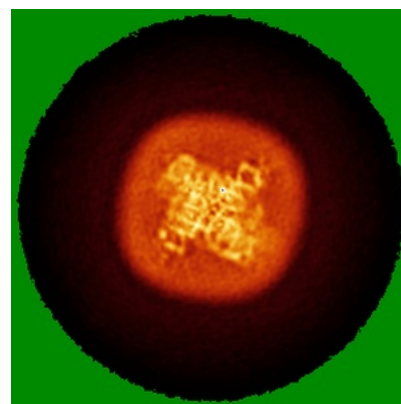
### 6.4.1 Primary map



X

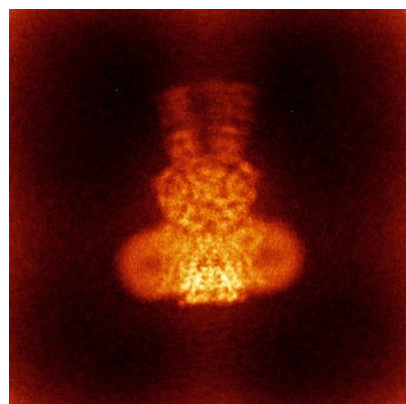


Y

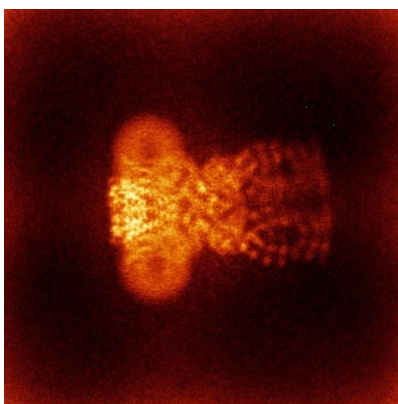


Z

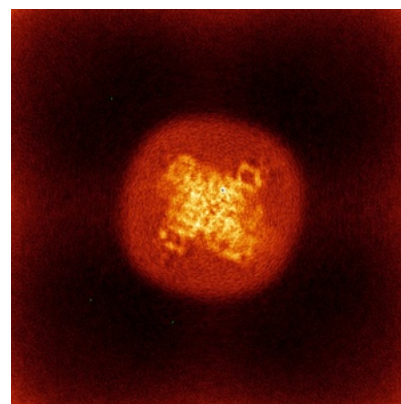
### 6.4.2 Raw map



X



Y

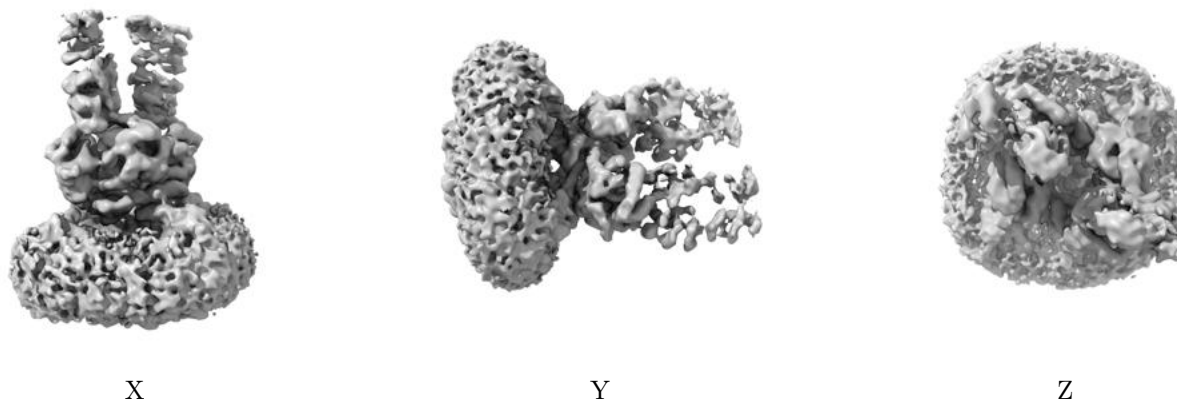


Z

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.

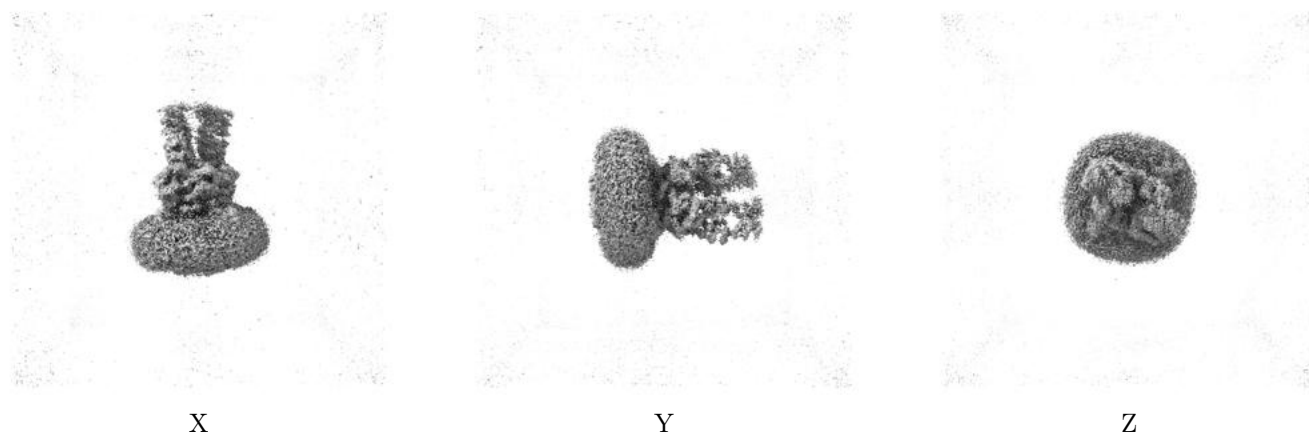
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.085. 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.

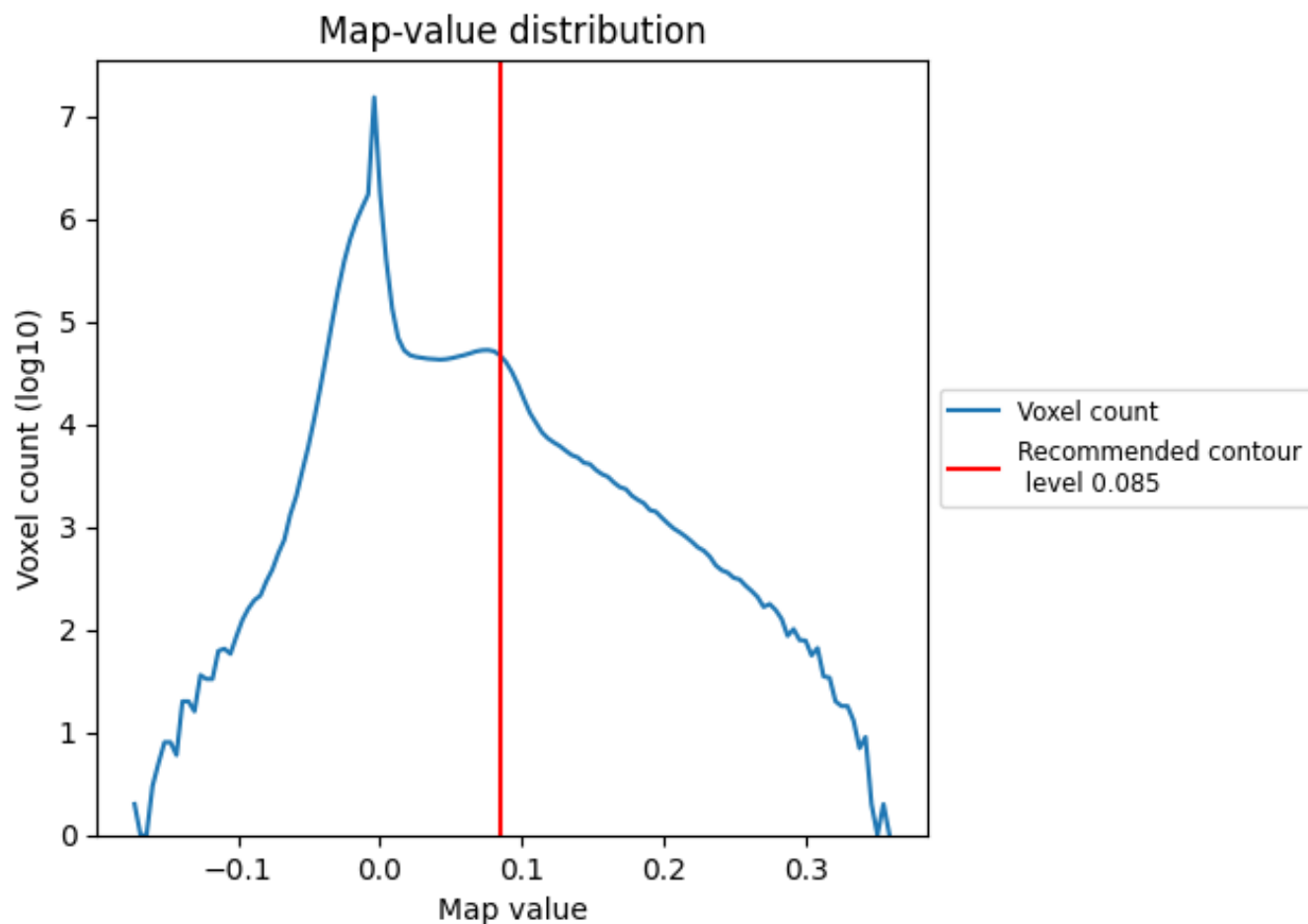
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

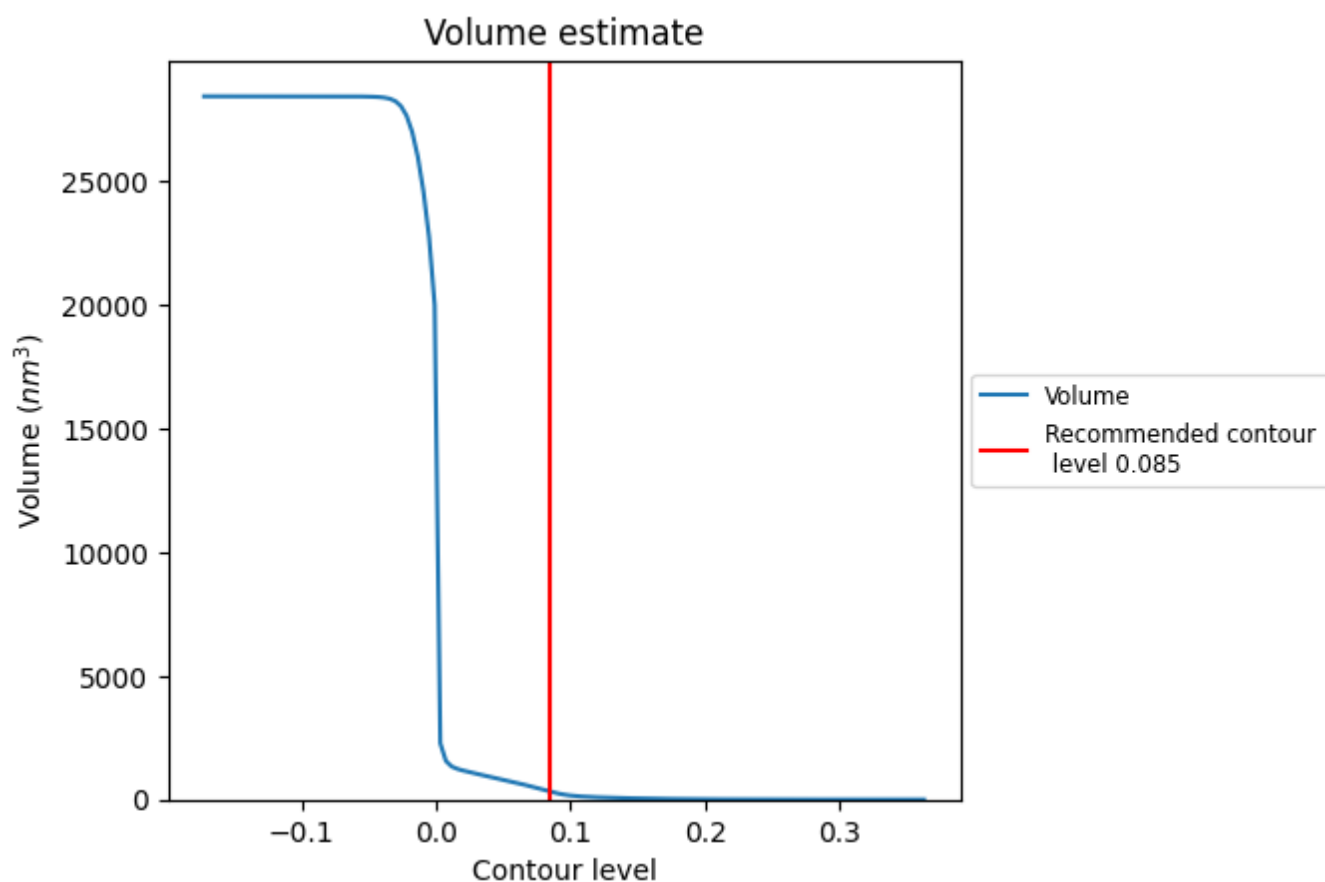
This section contains the results of statistical analysis of the map.

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



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

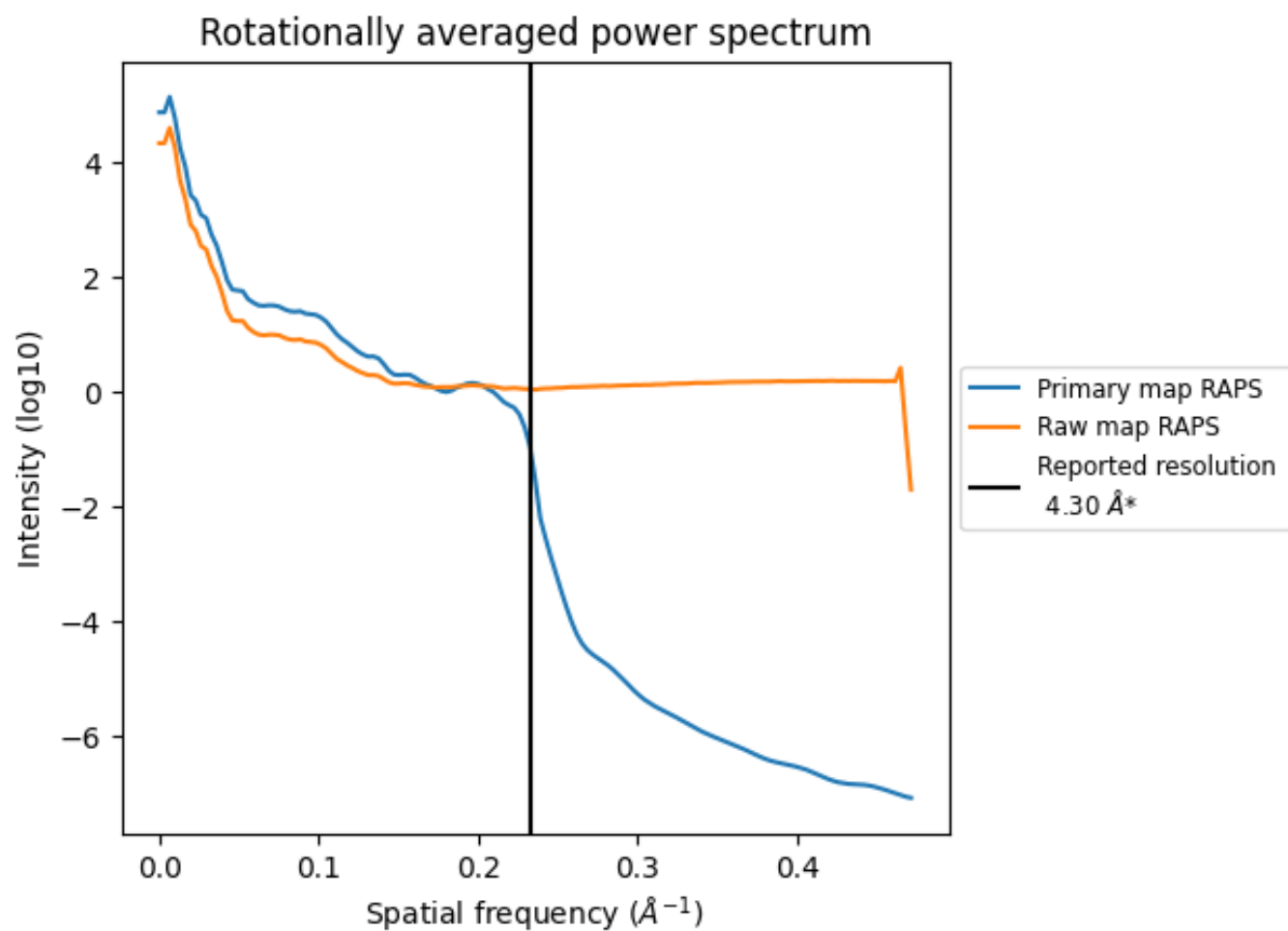
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 321 nm<sup>3</sup>; this corresponds to an approximate mass of 290 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 ⓘ

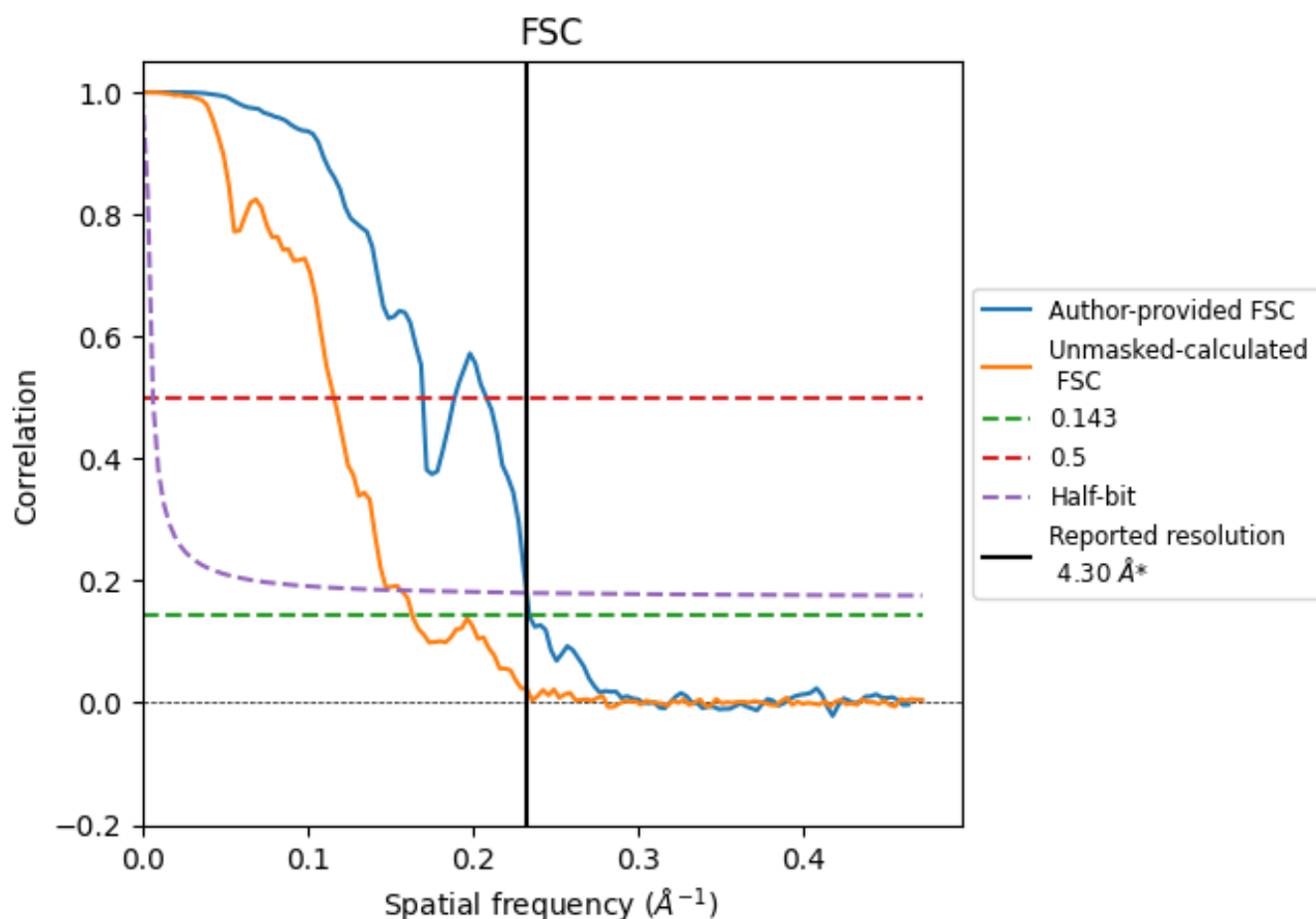


\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 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  $0.233 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.30                               | -    | -        |
| Author-provided FSC curve | 4.27                               | 5.89 | 4.30     |
| Unmasked-calculated*      | 6.12                               | 8.62 | 6.38     |

\*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 6.12 differs from the reported value 4.3 by more than 10 %

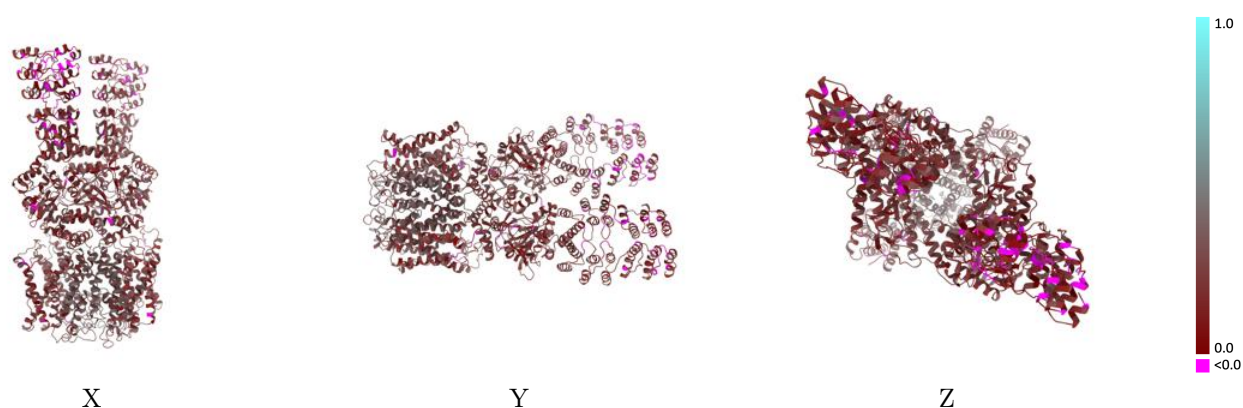
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37500 and PDB model 8WFZ. Per-residue inclusion information can be found in section [3](#) on page [4](#).

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

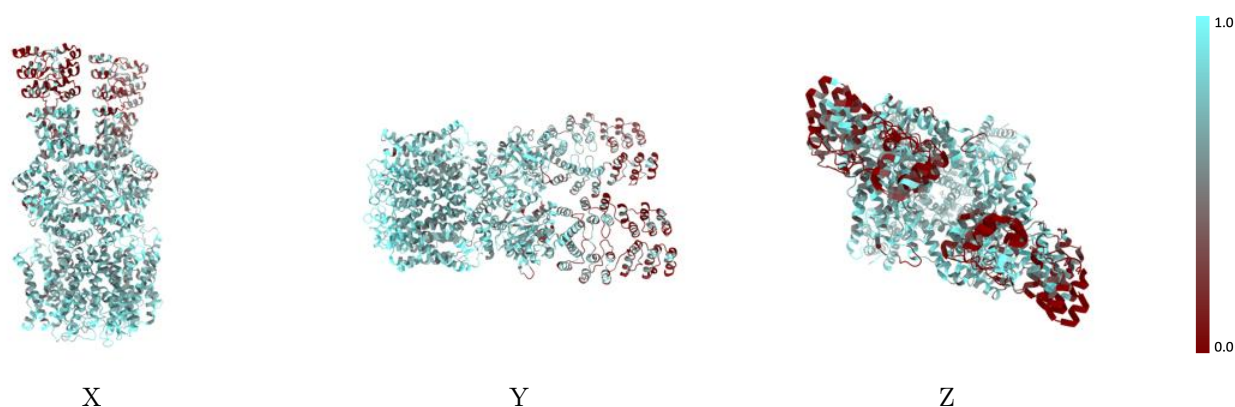
This section was not generated.

### 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.

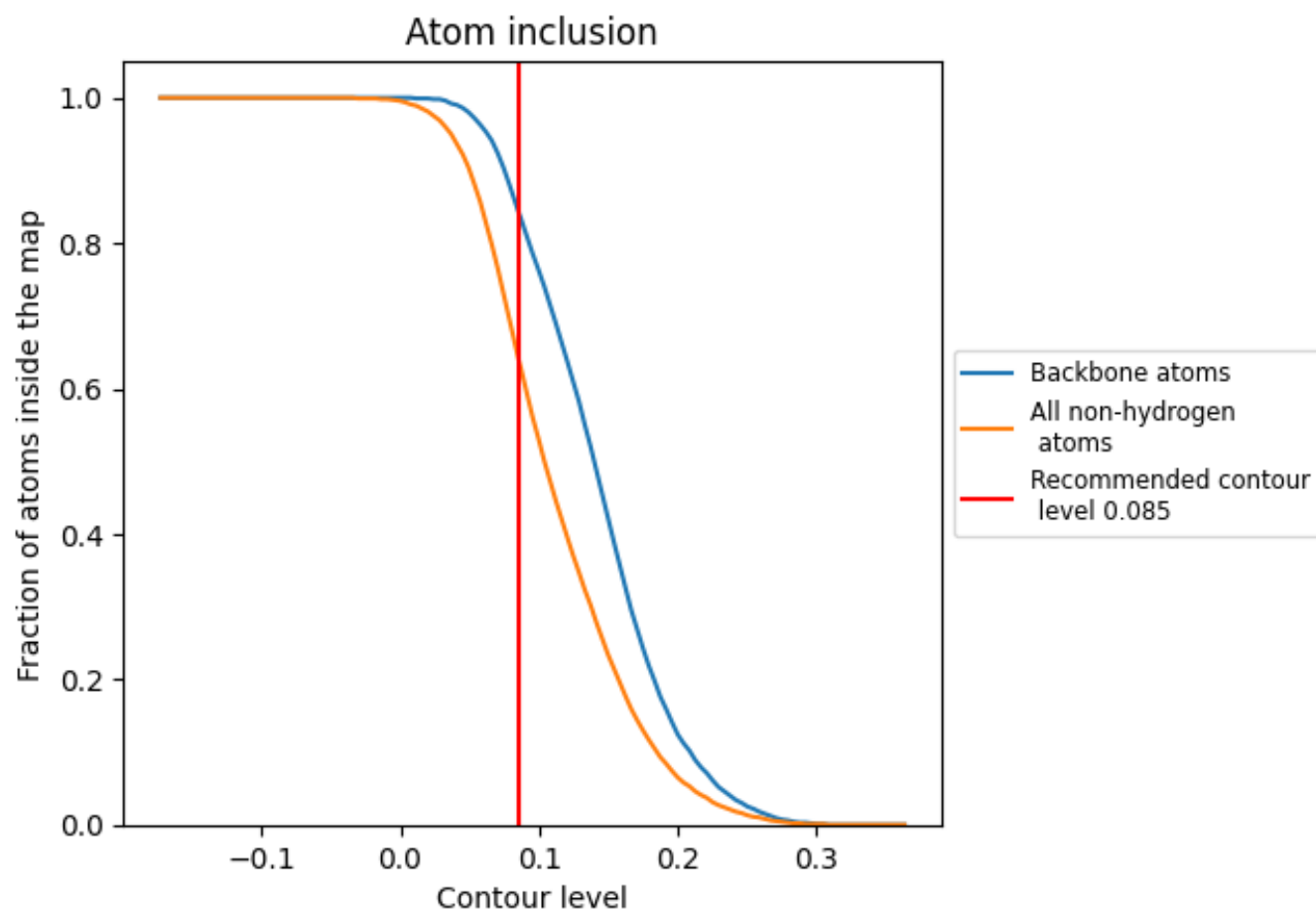
### 9.3 Atom inclusion mapped to coordinate model [i](#)





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 (0.085).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 64% 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 (0.085) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.6420 | <div></div> 0.2330 |
| A     | <div></div> 0.6580 | <div></div> 0.2300 |
| B     | <div></div> 0.6370 | <div></div> 0.2330 |
| C     | <div></div> 0.6230 | <div></div> 0.2430 |
| D     | <div></div> 0.6480 | <div></div> 0.2280 |

