



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:31 PM UTC

PDB ID : 8BNR / pdb\_00008bnr  
EMDB ID : EMD-16134  
Title : Escherichia coli anaerobic fatty acid beta oxidation trifunctional enzyme (anEcTFE) octameric complex  
Authors : Sah-Teli, S.K.; Pinkas, M.; Novacek, J.; Venkatesan, R.  
Deposited on : 2022-11-14  
Resolution : 10.30 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

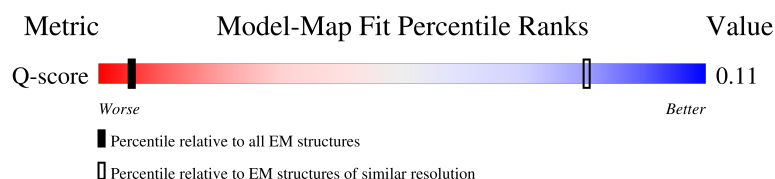
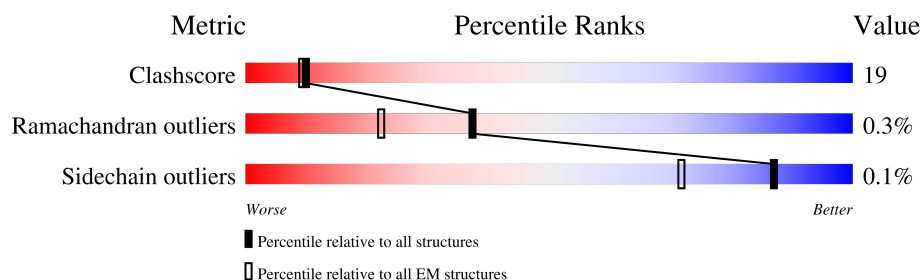
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.30 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                       | 116 ( 9.80 - 10.80 )                                     |

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     | 450    |                  |
| 1   | B     | 450    |                  |
| 1   | E     | 450    |                  |
| 1   | F     | 450    |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 2   | C     | 714    |  |
| 2   | D     | 714    |  |
| 2   | G     | 714    |  |
| 2   | H     | 714    |  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 33804 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 3-ketoacyl-CoA thiolase FadI.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 436      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3209  | 2018 | 581 | 593 | 17 |         |       |
| 1   | B     | 436      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3214  | 2020 | 583 | 594 | 17 |         |       |
| 1   | E     | 436      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3209  | 2018 | 581 | 593 | 17 |         |       |
| 1   | F     | 436      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3214  | 2020 | 583 | 594 | 17 |         |       |

There are 56 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | -13     | MET      | -      | initiating methionine | UNP P76503 |
| A     | -12     | GLY      | -      | expression tag        | UNP P76503 |
| A     | -11     | SER      | -      | expression tag        | UNP P76503 |
| A     | -10     | SER      | -      | expression tag        | UNP P76503 |
| A     | -9      | HIS      | -      | expression tag        | UNP P76503 |
| A     | -8      | HIS      | -      | expression tag        | UNP P76503 |
| A     | -7      | HIS      | -      | expression tag        | UNP P76503 |
| A     | -6      | HIS      | -      | expression tag        | UNP P76503 |
| A     | -5      | HIS      | -      | expression tag        | UNP P76503 |
| A     | -4      | HIS      | -      | expression tag        | UNP P76503 |
| A     | -3      | SER      | -      | expression tag        | UNP P76503 |
| A     | -2      | GLN      | -      | expression tag        | UNP P76503 |
| A     | -1      | ASP      | -      | expression tag        | UNP P76503 |
| A     | 0       | PRO      | -      | expression tag        | UNP P76503 |
| B     | -13     | MET      | -      | initiating methionine | UNP P76503 |
| B     | -12     | GLY      | -      | expression tag        | UNP P76503 |
| B     | -11     | SER      | -      | expression tag        | UNP P76503 |
| B     | -10     | SER      | -      | expression tag        | UNP P76503 |
| B     | -9      | HIS      | -      | expression tag        | UNP P76503 |
| B     | -8      | HIS      | -      | expression tag        | UNP P76503 |
| B     | -7      | HIS      | -      | expression tag        | UNP P76503 |
| B     | -6      | HIS      | -      | expression tag        | UNP P76503 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| B     | -5      | HIS      | -      | expression tag        | UNP P76503 |
| B     | -4      | HIS      | -      | expression tag        | UNP P76503 |
| B     | -3      | SER      | -      | expression tag        | UNP P76503 |
| B     | -2      | GLN      | -      | expression tag        | UNP P76503 |
| B     | -1      | ASP      | -      | expression tag        | UNP P76503 |
| B     | 0       | PRO      | -      | expression tag        | UNP P76503 |
| E     | -13     | MET      | -      | initiating methionine | UNP P76503 |
| E     | -12     | GLY      | -      | expression tag        | UNP P76503 |
| E     | -11     | SER      | -      | expression tag        | UNP P76503 |
| E     | -10     | SER      | -      | expression tag        | UNP P76503 |
| E     | -9      | HIS      | -      | expression tag        | UNP P76503 |
| E     | -8      | HIS      | -      | expression tag        | UNP P76503 |
| E     | -7      | HIS      | -      | expression tag        | UNP P76503 |
| E     | -6      | HIS      | -      | expression tag        | UNP P76503 |
| E     | -5      | HIS      | -      | expression tag        | UNP P76503 |
| E     | -4      | HIS      | -      | expression tag        | UNP P76503 |
| E     | -3      | SER      | -      | expression tag        | UNP P76503 |
| E     | -2      | GLN      | -      | expression tag        | UNP P76503 |
| E     | -1      | ASP      | -      | expression tag        | UNP P76503 |
| E     | 0       | PRO      | -      | expression tag        | UNP P76503 |
| F     | -13     | MET      | -      | initiating methionine | UNP P76503 |
| F     | -12     | GLY      | -      | expression tag        | UNP P76503 |
| F     | -11     | SER      | -      | expression tag        | UNP P76503 |
| F     | -10     | SER      | -      | expression tag        | UNP P76503 |
| F     | -9      | HIS      | -      | expression tag        | UNP P76503 |
| F     | -8      | HIS      | -      | expression tag        | UNP P76503 |
| F     | -7      | HIS      | -      | expression tag        | UNP P76503 |
| F     | -6      | HIS      | -      | expression tag        | UNP P76503 |
| F     | -5      | HIS      | -      | expression tag        | UNP P76503 |
| F     | -4      | HIS      | -      | expression tag        | UNP P76503 |
| F     | -3      | SER      | -      | expression tag        | UNP P76503 |
| F     | -2      | GLN      | -      | expression tag        | UNP P76503 |
| F     | -1      | ASP      | -      | expression tag        | UNP P76503 |
| F     | 0       | PRO      | -      | expression tag        | UNP P76503 |

- Molecule 2 is a protein called Fatty acid oxidation complex subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | C     | 710      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5204  | 3295 | 917 | 970 | 22 |         |       |
| 2   | D     | 710      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5275  | 3339 | 933 | 979 | 24 |         |       |

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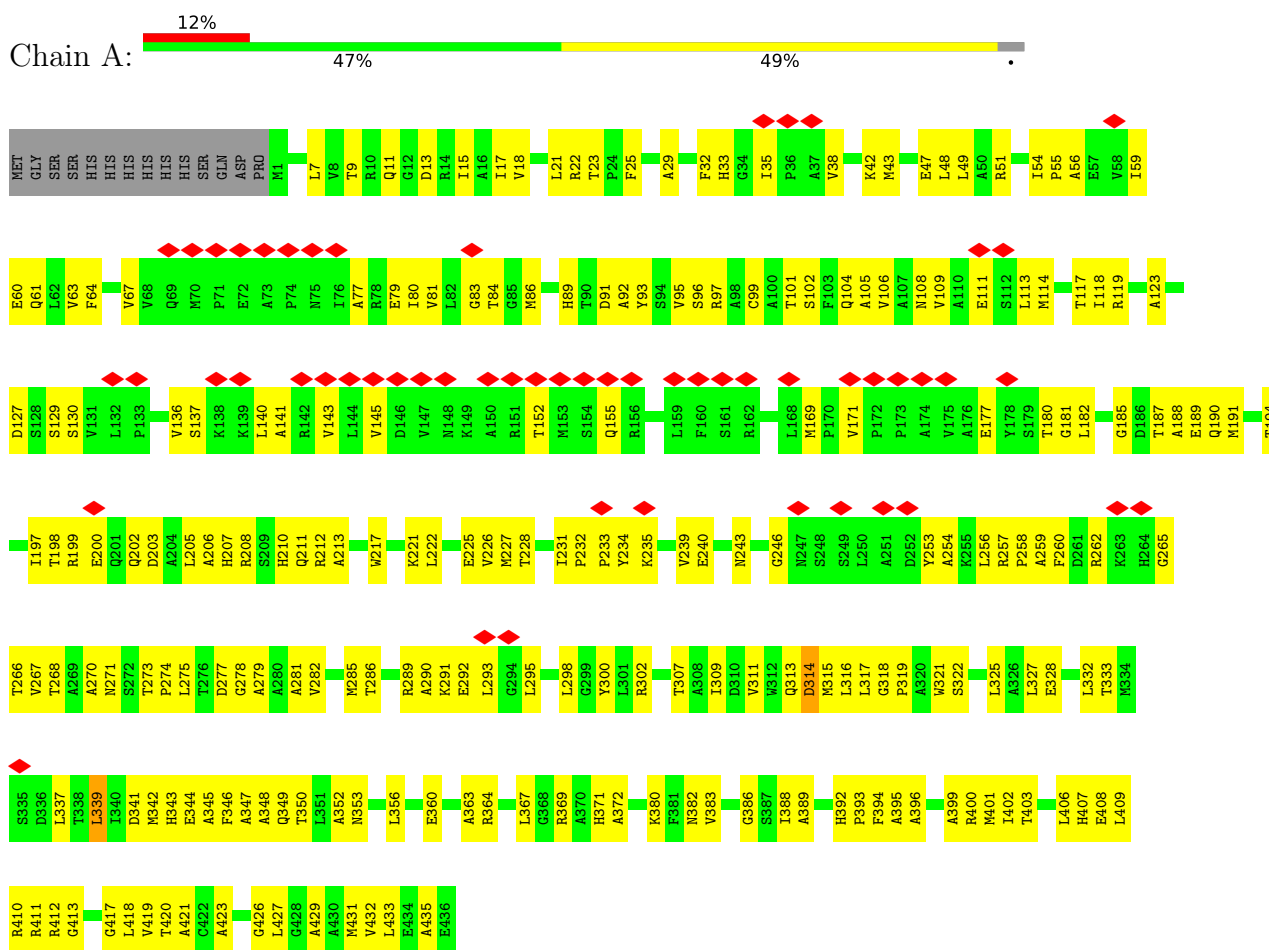
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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | G     | 710      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5204  | 3295 | 917 | 970 | 22 |         |       |
| 2   | H     | 710      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5275  | 3339 | 933 | 979 | 24 |         |       |

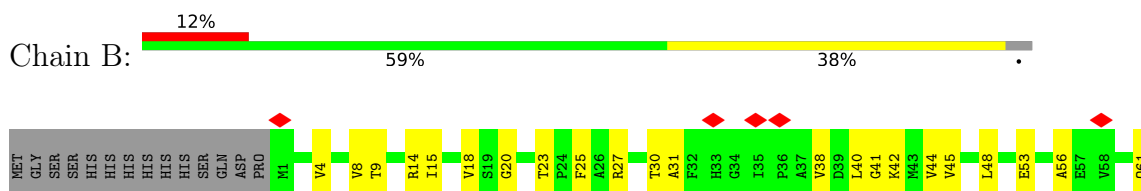
### 3 Residue-property plots

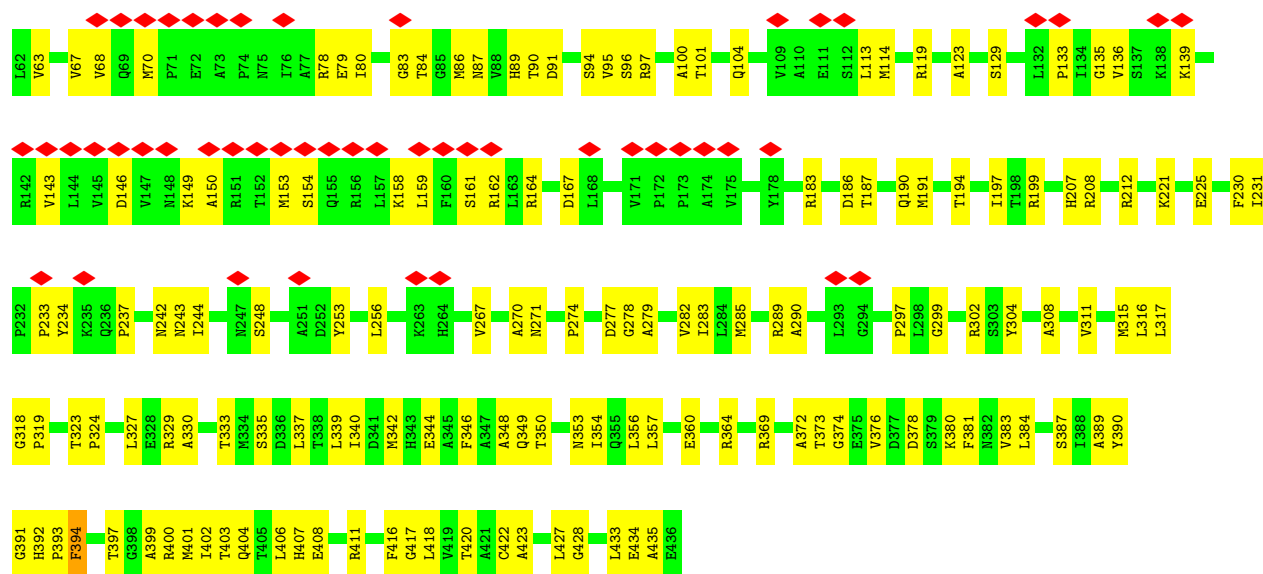
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 3-ketoacyl-CoA thiolase FadI

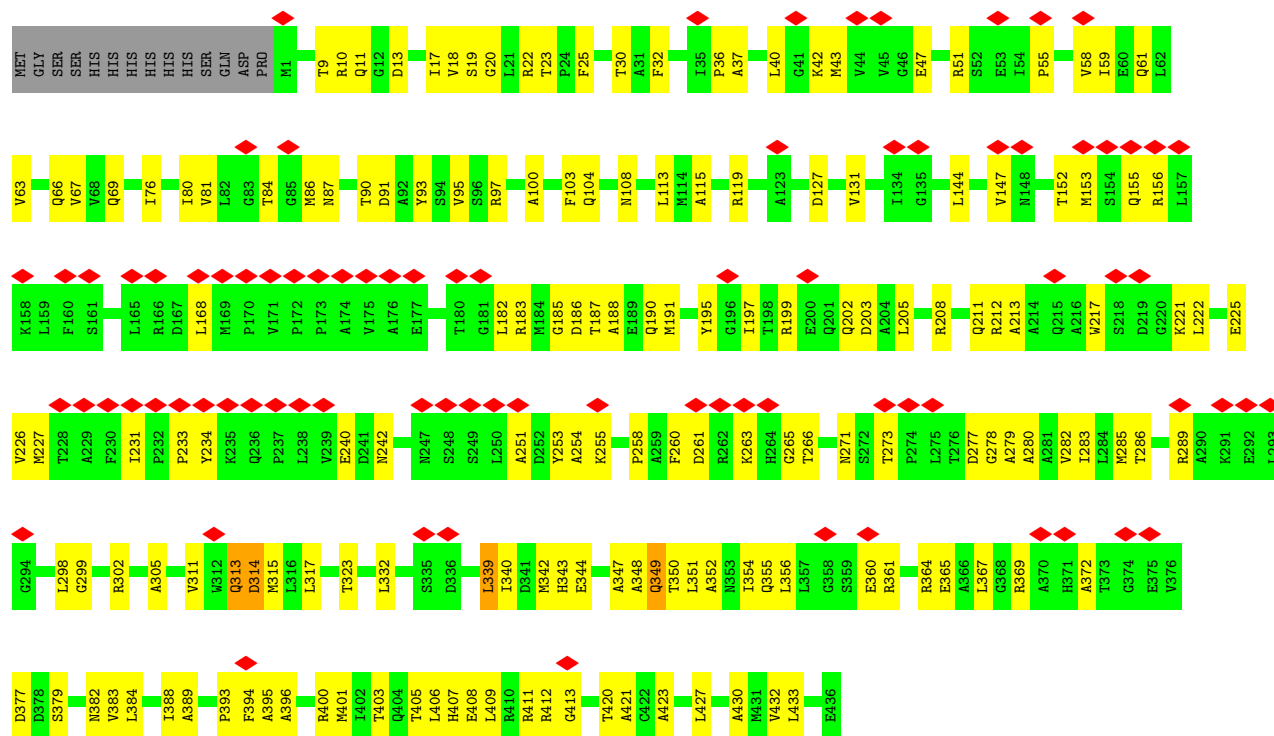


#### • Molecule 1: 3-ketoacyl-CoA thiolase FadI



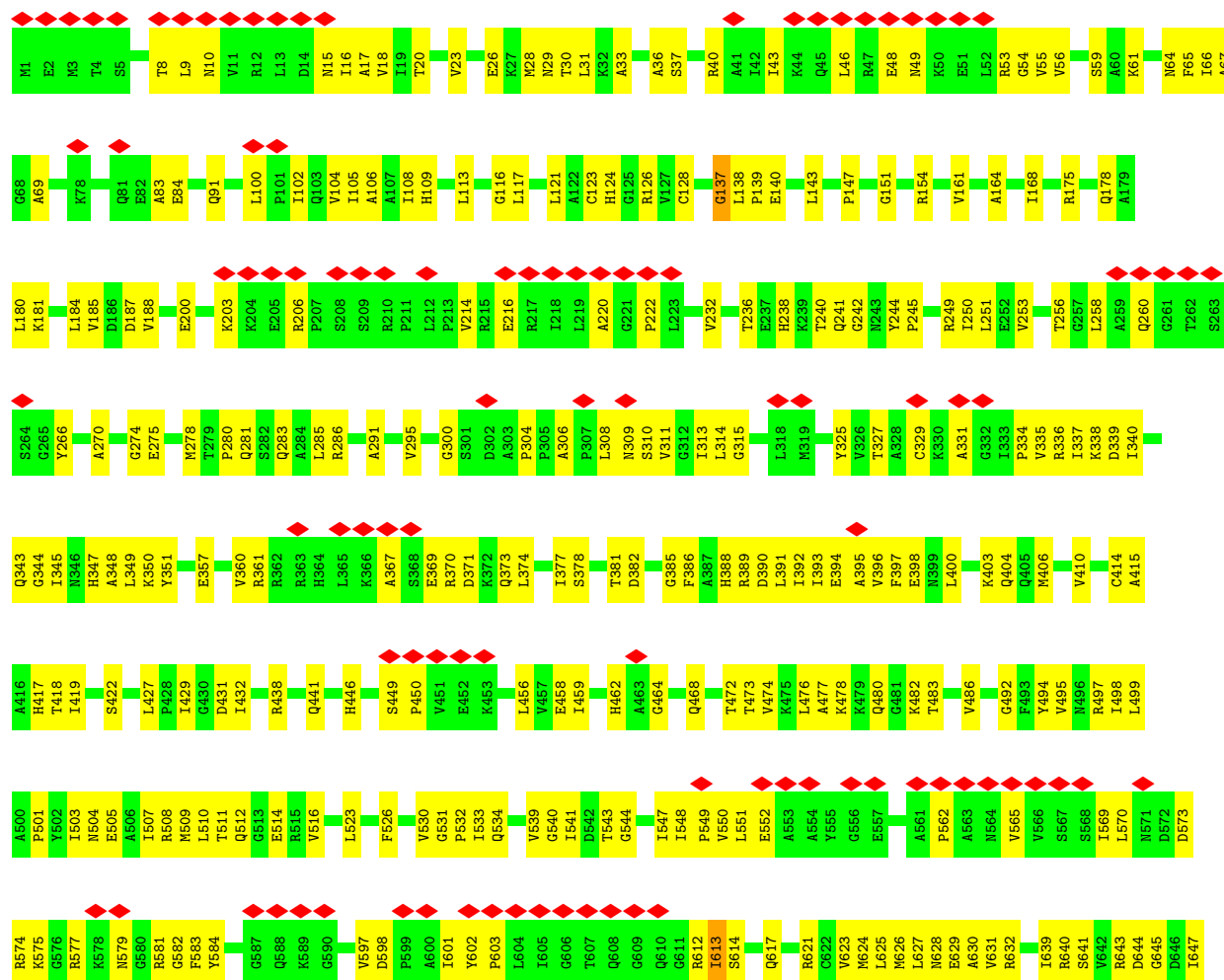


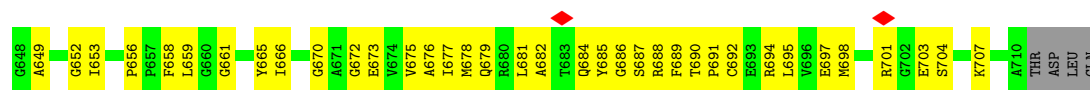
• Molecule 1: 3-ketoacyl-CoA thiolase FadI



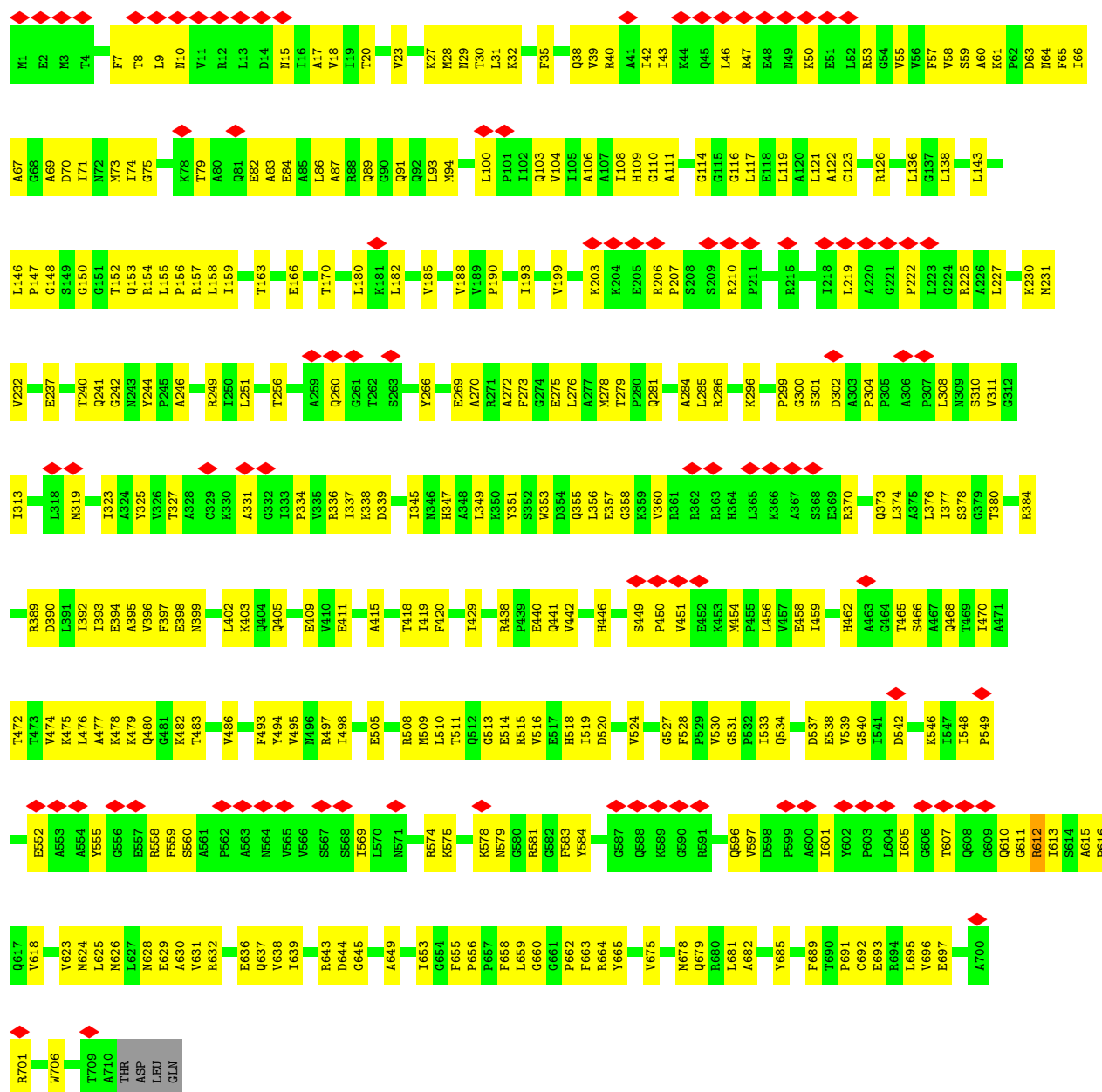
• Molecule 1: 3-ketoacyl-CoA thiolase FadI







• Molecule 2: Fatty acid oxidation complex subunit alpha



• Molecule 2: Fatty acid oxidation complex subunit alpha







## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 10184                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 48                                      | Depositor |
| Minimum defocus (nm)                 | 1200                                    | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 QUANTUM (4k x 4k)              | Depositor |
| Maximum map value                    | 0.227                                   | Depositor |
| Minimum map value                    | -0.018                                  | Depositor |
| Average map value                    | 0.005                                   | Depositor |
| Map value standard deviation         | 0.021                                   | Depositor |
| Recommended contour level            | 0.09                                    | Depositor |
| Map size (Å)                         | 298.08002, 298.08002, 298.08002         | wwPDB     |
| Map dimensions                       | 360, 360, 360                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.82800007, 0.82800007, 0.82800007      | Depositor |

## 5 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | A     | 0.16         | 0/3263  | 0.41        | 0/4427         |
| 1   | B     | 0.16         | 0/3268  | 0.39        | 0/4433         |
| 1   | E     | 0.13         | 0/3263  | 0.37        | 0/4427         |
| 1   | F     | 0.13         | 0/3268  | 0.34        | 0/4433         |
| 2   | C     | 0.15         | 0/5293  | 0.39        | 1/7193 (0.0%)  |
| 2   | D     | 0.15         | 0/5365  | 0.39        | 1/7276 (0.0%)  |
| 2   | G     | 0.12         | 0/5293  | 0.34        | 1/7193 (0.0%)  |
| 2   | H     | 0.12         | 0/5365  | 0.35        | 0/7276         |
| All | All   | 0.14         | 0/34378 | 0.37        | 3/46658 (0.0%) |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | C     | 137 | GLY  | N-CA-C  | 7.14  | 121.32      | 110.18   |
| 2   | G     | 137 | GLY  | N-CA-C  | 6.87  | 120.59      | 110.63   |
| 2   | D     | 493 | PHE  | CB-CA-C | -5.52 | 110.23      | 116.63   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3209  | 0        | 3238     | 181     | 0            |
| 1   | B     | 3214  | 0        | 3245     | 136     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | E     | 3209  | 0        | 3238     | 117     | 0            |
| 1   | F     | 3214  | 0        | 3245     | 90      | 0            |
| 2   | C     | 5204  | 0        | 5197     | 229     | 0            |
| 2   | D     | 5275  | 0        | 5329     | 236     | 0            |
| 2   | G     | 5204  | 0        | 5197     | 153     | 0            |
| 2   | H     | 5275  | 0        | 5329     | 197     | 0            |
| All | All   | 33804 | 0        | 34018    | 1319    | 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 19.

All (1319) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:29:ASN:H     | 2:D:64:ASN:HD21  | 1.24                     | 0.85              |
| 1:B:97:ARG:H     | 1:B:101:THR:HG22 | 1.43                     | 0.82              |
| 2:C:29:ASN:H     | 2:C:64:ASN:HD21  | 1.26                     | 0.81              |
| 2:D:446:HIS:HB3  | 2:D:458:GLU:HB2  | 1.62                     | 0.81              |
| 2:C:15:ASN:HB3   | 2:C:53:ARG:H     | 1.46                     | 0.80              |
| 1:F:30:THR:HG22  | 1:F:31:ALA:H     | 1.45                     | 0.80              |
| 1:F:190:GLN:NE2  | 1:F:191:MET:SD   | 2.55                     | 0.80              |
| 1:B:119:ARG:HH21 | 1:B:289:ARG:HD3  | 1.46                     | 0.79              |
| 1:A:339:LEU:HA   | 1:A:380:LYS:HB3  | 1.66                     | 0.78              |
| 1:E:231:ILE:HG22 | 1:E:233:PRO:HD2  | 1.64                     | 0.78              |
| 2:D:83:ALA:HB1   | 2:D:273:PHE:HB3  | 1.67                     | 0.77              |
| 2:D:574:ARG:HB2  | 2:D:581:ARG:HH21 | 1.48                     | 0.77              |
| 1:A:360:GLU:HA   | 1:A:372:ALA:HB2  | 1.66                     | 0.77              |
| 1:A:97:ARG:HD2   | 1:A:104:GLN:HB2  | 1.68                     | 0.76              |
| 1:F:81:VAL:HG21  | 1:F:90:THR:HG21  | 1.65                     | 0.76              |
| 2:H:29:ASN:H     | 2:H:64:ASN:HD21  | 1.34                     | 0.75              |
| 2:C:649:ALA:HA   | 2:C:653:ILE:HD13 | 1.68                     | 0.74              |
| 1:A:410:ARG:NH2  | 1:A:435:ALA:O    | 2.20                     | 0.74              |
| 1:B:56:ALA:HB1   | 1:B:86:MET:HA    | 1.68                     | 0.74              |
| 2:H:454:MET:O    | 2:H:482:LYS:NZ   | 2.21                     | 0.74              |
| 2:C:295:VAL:O    | 2:C:478:LYS:NZ   | 2.21                     | 0.73              |
| 1:E:212:ARG:HH21 | 1:E:383:VAL:HA   | 1.52                     | 0.73              |
| 2:C:83:ALA:HB3   | 2:C:274:GLY:HA2  | 1.71                     | 0.73              |
| 2:G:17:ALA:HB3   | 2:G:55:VAL:HG12  | 1.71                     | 0.73              |
| 1:A:60:GLU:HB2   | 1:A:118:ILE:HG23 | 1.71                     | 0.73              |
| 2:C:574:ARG:HB2  | 2:C:581:ARG:HH21 | 1.53                     | 0.73              |
| 1:F:97:ARG:H     | 1:F:101:THR:HG22 | 1.50                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:38:VAL:HG22  | 1:B:42:LYS:HZ3   | 1.54                     | 0.72              |
| 1:A:191:MET:HE1  | 1:A:316:LEU:HB2  | 1.71                     | 0.72              |
| 1:B:30:THR:HG22  | 1:B:31:ALA:H     | 1.52                     | 0.72              |
| 1:B:18:VAL:HA    | 1:B:297:PRO:HA   | 1.71                     | 0.72              |
| 1:F:5:LEU:HD23   | 1:F:329:ARG:HG2  | 1.72                     | 0.72              |
| 2:C:628:ASN:OD1  | 2:C:632:ARG:NH2  | 2.23                     | 0.72              |
| 2:G:15:ASN:HB3   | 2:G:53:ARG:H     | 1.54                     | 0.72              |
| 1:B:61:GLN:NE2   | 1:B:91:ASP:O     | 2.22                     | 0.71              |
| 2:D:497:ARG:NH1  | 2:D:636:GLU:OE2  | 2.21                     | 0.71              |
| 2:G:401:GLU:O    | 2:G:405:GLN:NE2  | 2.24                     | 0.71              |
| 2:D:249:ARG:HH12 | 2:D:275:GLU:HG3  | 1.56                     | 0.71              |
| 1:A:182:LEU:HD13 | 1:A:187:THR:HB   | 1.71                     | 0.71              |
| 2:D:91:GLN:NE2   | 2:D:269:GLU:OE2  | 2.23                     | 0.71              |
| 2:H:17:ALA:HB3   | 2:H:55:VAL:HG12  | 1.73                     | 0.71              |
| 1:B:208:ARG:NH2  | 1:B:381:PHE:O    | 2.24                     | 0.70              |
| 1:A:202:GLN:NE2  | 1:A:266:THR:O    | 2.25                     | 0.70              |
| 2:C:516:VAL:HG11 | 2:C:597:VAL:HG11 | 1.73                     | 0.70              |
| 1:A:346:PHE:HB2  | 1:A:349:GLN:HG2  | 1.74                     | 0.70              |
| 2:C:240:THR:HG23 | 2:C:242:GLY:H    | 1.55                     | 0.70              |
| 1:B:267:VAL:HA   | 1:B:271:ASN:HD21 | 1.56                     | 0.70              |
| 1:A:129:SER:N    | 1:A:277:ASP:OD1  | 2.25                     | 0.69              |
| 1:A:9:THR:HG23   | 1:A:11:GLN:H     | 1.56                     | 0.69              |
| 2:G:548:ILE:HA   | 2:G:551:LEU:HD23 | 1.73                     | 0.69              |
| 2:H:62:PRO:O     | 2:H:133:LYS:NZ   | 2.26                     | 0.69              |
| 2:C:508:ARG:O    | 2:C:512:GLN:NE2  | 2.25                     | 0.69              |
| 2:C:575:LYS:H    | 2:C:579:ASN:HD21 | 1.39                     | 0.69              |
| 1:E:222:LEU:HD23 | 1:E:384:LEU:HD23 | 1.73                     | 0.69              |
| 1:A:231:ILE:HG13 | 1:A:234:TYR:H    | 1.58                     | 0.69              |
| 2:D:8:THR:OG1    | 2:D:20:THR:OG1   | 2.10                     | 0.69              |
| 2:C:335:VAL:O    | 2:C:378:SER:OG   | 2.11                     | 0.69              |
| 2:D:411:GLU:OE1  | 2:D:438:ARG:NH1  | 2.25                     | 0.69              |
| 2:D:584:TYR:HA   | 2:D:597:VAL:HA   | 1.74                     | 0.69              |
| 1:F:59:ILE:HB    | 1:F:86:MET:HE1   | 1.75                     | 0.69              |
| 1:E:393:PRO:HB2  | 1:E:396:ALA:HB3  | 1.73                     | 0.69              |
| 2:G:310:SER:OG   | 2:G:388:HIS:O    | 2.11                     | 0.68              |
| 2:H:574:ARG:HB2  | 2:H:581:ARG:HH21 | 1.58                     | 0.68              |
| 2:D:249:ARG:NH2  | 2:D:275:GLU:OE2  | 2.24                     | 0.68              |
| 1:E:343:HIS:HA   | 1:E:401:MET:HE1  | 1.75                     | 0.68              |
| 2:C:632:ARG:HH21 | 2:C:692:CYS:HB2  | 1.56                     | 0.68              |
| 2:D:15:ASN:OD1   | 2:D:203:LYS:NZ   | 2.26                     | 0.68              |
| 2:H:359:LYS:HG2  | 2:H:362:ARG:HH21 | 1.59                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:510:LEU:HD21 | 2:D:519:ILE:HG21 | 1.75                     | 0.68              |
| 1:F:190:GLN:OE1  | 1:F:313:GLN:NE2  | 2.27                     | 0.68              |
| 2:C:577:ARG:NH2  | 2:C:584:TYR:O    | 2.26                     | 0.68              |
| 1:B:339:LEU:HA   | 1:B:380:LYS:HB2  | 1.76                     | 0.68              |
| 2:C:17:ALA:HB3   | 2:C:55:VAL:HG12  | 1.75                     | 0.68              |
| 2:H:504:ASN:ND2  | 2:H:558:ARG:O    | 2.26                     | 0.68              |
| 1:A:231:ILE:HD11 | 1:A:235:LYS:HG2  | 1.75                     | 0.67              |
| 1:B:311:VAL:HG23 | 1:B:315:MET:HG3  | 1.75                     | 0.67              |
| 2:D:17:ALA:HB3   | 2:D:55:VAL:HG12  | 1.75                     | 0.67              |
| 1:A:42:LYS:HE3   | 1:A:84:THR:HG23  | 1.75                     | 0.67              |
| 2:C:539:VAL:O    | 2:C:543:THR:OG1  | 2.12                     | 0.67              |
| 1:A:56:ALA:HB1   | 1:A:86:MET:HA    | 1.77                     | 0.67              |
| 1:A:198:THR:HG22 | 1:A:200:GLU:H    | 1.58                     | 0.67              |
| 1:A:339:LEU:H    | 1:A:380:LYS:HD2  | 1.59                     | 0.67              |
| 2:C:584:TYR:HE1  | 2:C:597:VAL:HG12 | 1.60                     | 0.67              |
| 2:G:240:THR:HG23 | 2:G:242:GLY:H    | 1.60                     | 0.67              |
| 2:C:446:HIS:HB3  | 2:C:458:GLU:HB2  | 1.77                     | 0.67              |
| 1:E:221:LYS:HB2  | 1:E:411:ARG:HH12 | 1.59                     | 0.66              |
| 1:A:61:GLN:HE22  | 1:A:63:VAL:HG23  | 1.59                     | 0.66              |
| 1:A:349:GLN:O    | 1:A:353:ASN:ND2  | 2.28                     | 0.66              |
| 1:A:360:GLU:OE2  | 1:A:364:ARG:NH2  | 2.28                     | 0.66              |
| 2:G:675:VAL:HA   | 2:G:678:MET:HE3  | 1.76                     | 0.66              |
| 1:A:273:THR:HB   | 1:A:388:ILE:HD13 | 1.76                     | 0.66              |
| 2:C:675:VAL:HG12 | 2:C:679:GLN:HE22 | 1.61                     | 0.66              |
| 2:C:43:ILE:HD11  | 2:C:100:LEU:HD11 | 1.78                     | 0.66              |
| 1:E:344:GLU:OE1  | 1:E:382:ASN:ND2  | 2.28                     | 0.66              |
| 2:G:577:ARG:NH2  | 2:G:584:TYR:O    | 2.29                     | 0.66              |
| 1:B:360:GLU:HA   | 1:B:372:ALA:HB2  | 1.77                     | 0.66              |
| 2:D:240:THR:HG23 | 2:D:242:GLY:H    | 1.61                     | 0.66              |
| 1:A:117:THR:HG23 | 1:B:329:ARG:HH22 | 1.60                     | 0.65              |
| 1:B:340:ILE:HG22 | 1:B:380:LYS:HG3  | 1.78                     | 0.65              |
| 1:A:80:ILE:O     | 1:A:84:THR:OG1   | 2.13                     | 0.65              |
| 2:D:227:LEU:HA   | 2:D:230:LYS:HE3  | 1.77                     | 0.65              |
| 1:E:153:MET:SD   | 1:E:156:ARG:NH1  | 2.69                     | 0.65              |
| 2:D:519:ILE:HG13 | 2:D:618:VAL:HG21 | 1.79                     | 0.65              |
| 2:C:56:VAL:HG12  | 2:C:105:ILE:HB   | 1.79                     | 0.65              |
| 2:H:449:SER:HB3  | 2:H:539:VAL:HG23 | 1.78                     | 0.65              |
| 1:A:205:LEU:HA   | 1:A:208:ARG:HG2  | 1.79                     | 0.65              |
| 2:C:300:GLY:HA3  | 2:C:474:VAL:HG11 | 1.78                     | 0.65              |
| 2:D:57:PHE:HB2   | 2:D:106:ALA:HA   | 1.79                     | 0.65              |
| 1:F:37:ALA:HA    | 1:F:40:LEU:HD12  | 1.77                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:573:ASP:O    | 2:G:581:ARG:NH1  | 2.28                     | 0.65              |
| 1:A:23:THR:HB    | 1:A:279:ALA:H    | 1.61                     | 0.65              |
| 1:A:348:ALA:O    | 1:A:349:GLN:HG3  | 1.97                     | 0.65              |
| 2:D:31:LEU:HB2   | 2:D:69:ALA:HA    | 1.77                     | 0.65              |
| 1:E:188:ALA:O    | 1:E:349:GLN:NE2  | 2.30                     | 0.65              |
| 2:C:547:ILE:O    | 2:C:550:VAL:HG12 | 1.97                     | 0.65              |
| 2:G:508:ARG:NH2  | 2:G:560:SER:O    | 2.30                     | 0.65              |
| 1:A:77:ALA:HB1   | 1:A:92:ALA:HB1   | 1.78                     | 0.65              |
| 1:B:191:MET:HE1  | 1:B:316:LEU:HB2  | 1.79                     | 0.65              |
| 1:A:18:VAL:HA    | 1:A:298:LEU:H    | 1.62                     | 0.64              |
| 2:D:40:ARG:HG3   | 2:D:93:LEU:HD13  | 1.79                     | 0.64              |
| 1:B:364:ARG:NH1  | 1:B:369:ARG:O    | 2.31                     | 0.64              |
| 2:C:371:ASP:HA   | 2:C:374:LEU:HB2  | 1.78                     | 0.64              |
| 2:C:534:GLN:HB3  | 2:C:584:TYR:HE2  | 1.61                     | 0.64              |
| 2:D:123:CYS:O    | 2:D:126:ARG:NH2  | 2.30                     | 0.64              |
| 1:A:102:SER:OG   | 1:A:395:ALA:O    | 2.12                     | 0.64              |
| 1:E:95:VAL:HG11  | 1:E:108:ASN:HD22 | 1.63                     | 0.64              |
| 1:E:183:ARG:HH22 | 1:E:260:PHE:HB3  | 1.62                     | 0.64              |
| 1:F:234:TYR:O    | 2:G:346:ASN:ND2  | 2.31                     | 0.64              |
| 2:G:138:LEU:HD23 | 2:G:147:PRO:HG2  | 1.79                     | 0.64              |
| 1:A:399:ALA:HA   | 1:A:402:ILE:HD12 | 1.78                     | 0.64              |
| 1:B:25:PHE:HE2   | 1:B:400:ARG:HD3  | 1.62                     | 0.64              |
| 1:B:337:LEU:HD11 | 1:B:418:LEU:HB2  | 1.79                     | 0.64              |
| 1:B:38:VAL:HG22  | 1:B:42:LYS:NZ    | 2.13                     | 0.64              |
| 2:D:64:ASN:HA    | 2:D:110:GLY:HA3  | 1.78                     | 0.64              |
| 1:F:197:ILE:HG21 | 1:F:348:ALA:HA   | 1.78                     | 0.64              |
| 2:D:308:LEU:HD11 | 2:D:472:THR:HB   | 1.80                     | 0.64              |
| 2:H:584:TYR:HA   | 2:H:597:VAL:HA   | 1.79                     | 0.64              |
| 2:D:626:MET:O    | 2:D:630:ALA:N    | 2.30                     | 0.64              |
| 2:H:53:ARG:HH21  | 2:H:203:LYS:HD2  | 1.63                     | 0.64              |
| 1:E:191:MET:HG2  | 1:E:314:ASP:CG   | 2.23                     | 0.64              |
| 2:H:519:ILE:HG13 | 2:H:618:VAL:HG21 | 1.79                     | 0.64              |
| 2:G:214:VAL:HG13 | 2:G:216:GLU:H    | 1.63                     | 0.63              |
| 2:D:180:LEU:HD22 | 2:D:188:VAL:HG22 | 1.78                     | 0.63              |
| 2:D:477:ALA:HB1  | 2:D:482:LYS:HB2  | 1.81                     | 0.63              |
| 1:E:199:ARG:NH1  | 1:E:254:ALA:O    | 2.31                     | 0.63              |
| 1:E:205:LEU:HA   | 1:E:208:ARG:HG2  | 1.80                     | 0.63              |
| 1:B:417:GLY:O    | 1:B:433:LEU:N    | 2.28                     | 0.63              |
| 2:D:374:LEU:HA   | 2:D:377:ILE:HD12 | 1.80                     | 0.63              |
| 2:C:281:GLN:HG3  | 2:C:658:PHE:HB2  | 1.80                     | 0.63              |
| 2:D:70:ASP:HB3   | 2:D:73:MET:HE1   | 1.81                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:37:ALA:HA    | 1:E:40:LEU:HD12  | 1.81                     | 0.63              |
| 2:H:442:VAL:HB   | 2:H:462:HIS:HE1  | 1.64                     | 0.63              |
| 1:B:42:LYS:HG3   | 1:B:84:THR:HG23  | 1.78                     | 0.63              |
| 1:F:208:ARG:NH2  | 1:F:381:PHE:O    | 2.24                     | 0.63              |
| 1:A:210:HIS:HB3  | 1:A:246:GLY:HA2  | 1.80                     | 0.63              |
| 2:C:314:LEU:O    | 2:C:395:ALA:N    | 2.29                     | 0.63              |
| 2:D:528:PHE:HE1  | 2:D:655:PHE:HA   | 1.64                     | 0.63              |
| 1:A:49:LEU:HD21  | 1:A:56:ALA:HB2   | 1.80                     | 0.63              |
| 2:C:360:VAL:HG21 | 2:C:370:ARG:HG3  | 1.80                     | 0.63              |
| 2:G:541:ILE:HB   | 2:G:575:LYS:HA   | 1.80                     | 0.63              |
| 2:H:405:GLN:NE2  | 2:H:409:GLU:OE1  | 2.32                     | 0.63              |
| 2:H:154:ARG:NH2  | 2:H:266:TYR:OH   | 2.31                     | 0.63              |
| 2:H:232:VAL:HG13 | 2:H:251:LEU:HD21 | 1.81                     | 0.63              |
| 2:C:369:GLU:O    | 2:C:373:GLN:NE2  | 2.32                     | 0.62              |
| 2:D:29:ASN:O     | 2:D:67:ALA:N     | 2.31                     | 0.62              |
| 2:C:84:GLU:HG3   | 2:C:274:GLY:HA3  | 1.81                     | 0.62              |
| 2:C:685:TYR:HB3  | 2:C:688:ARG:HH22 | 1.64                     | 0.62              |
| 2:C:357:GLU:O    | 2:C:361:ARG:N    | 2.26                     | 0.62              |
| 1:E:202:GLN:NE2  | 1:E:266:THR:O    | 2.33                     | 0.62              |
| 1:A:417:GLY:O    | 1:A:433:LEU:N    | 2.28                     | 0.62              |
| 1:E:190:GLN:NE2  | 1:E:191:MET:HG3  | 2.15                     | 0.62              |
| 2:D:20:THR:HB    | 2:D:60:ALA:HB2   | 1.81                     | 0.62              |
| 2:G:73:MET:HE2   | 2:G:86:LEU:HD11  | 1.80                     | 0.62              |
| 2:H:215:ARG:NH1  | 2:H:216:GLU:OE1  | 2.32                     | 0.62              |
| 2:C:509:MET:SD   | 2:C:510:LEU:HD22 | 2.39                     | 0.62              |
| 1:F:187:THR:HG22 | 1:F:191:MET:HE1  | 1.82                     | 0.62              |
| 2:G:497:ARG:NH1  | 2:G:629:GLU:OE2  | 2.32                     | 0.62              |
| 2:H:143:LEU:HD12 | 2:H:286:ARG:HG2  | 1.82                     | 0.62              |
| 1:F:343:HIS:HA   | 1:F:401:MET:HE1  | 1.82                     | 0.62              |
| 1:A:344:GLU:OE1  | 1:A:382:ASN:ND2  | 2.33                     | 0.62              |
| 2:C:26:GLU:HG2   | 2:C:28:MET:H     | 1.63                     | 0.62              |
| 2:D:32:LYS:H     | 2:D:35:PHE:HD2   | 1.47                     | 0.62              |
| 2:C:704:SER:OG   | 2:C:707:LYS:O    | 2.18                     | 0.62              |
| 2:D:497:ARG:NE   | 2:D:629:GLU:OE2  | 2.27                     | 0.62              |
| 1:E:19:SER:HA    | 1:E:298:LEU:HD22 | 1.82                     | 0.62              |
| 1:B:346:PHE:H    | 1:B:349:GLN:HE21 | 1.46                     | 0.61              |
| 2:C:415:ALA:O    | 2:C:438:ARG:NH1  | 2.27                     | 0.61              |
| 2:G:574:ARG:HG3  | 2:G:582:GLY:HA2  | 1.81                     | 0.61              |
| 2:H:157:ARG:NH1  | 2:H:262:THR:OG1  | 2.33                     | 0.61              |
| 1:B:80:ILE:O     | 1:B:84:THR:N     | 2.31                     | 0.61              |
| 1:B:349:GLN:O    | 1:B:353:ASN:ND2  | 2.34                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:449:SER:HB3  | 2:G:450:PRO:HD2  | 1.82                     | 0.61              |
| 2:D:459:ILE:HB   | 2:D:486:VAL:HA   | 1.82                     | 0.61              |
| 2:H:423:ASN:HD21 | 2:H:447:PHE:HB2  | 1.65                     | 0.61              |
| 2:H:240:THR:HG23 | 2:H:242:GLY:H    | 1.64                     | 0.61              |
| 2:C:505:GLU:OE2  | 2:C:621:ARG:NH2  | 2.34                     | 0.61              |
| 2:D:47:ARG:HH11  | 2:D:100:LEU:HD22 | 1.65                     | 0.61              |
| 2:H:206:ARG:HH21 | 2:H:210:ARG:H    | 1.46                     | 0.61              |
| 2:D:256:THR:OG1  | 2:D:260:GLN:NE2  | 2.33                     | 0.61              |
| 2:G:36:ALA:O     | 2:G:40:ARG:NE    | 2.33                     | 0.61              |
| 2:C:256:THR:OG1  | 2:C:260:GLN:NE2  | 2.34                     | 0.60              |
| 2:D:296:LYS:O    | 2:D:478:LYS:NZ   | 2.33                     | 0.60              |
| 2:H:488:ARG:HB3  | 2:H:638:VAL:HA   | 1.82                     | 0.60              |
| 2:C:65:PHE:HB2   | 2:C:109:HIS:H    | 1.65                     | 0.60              |
| 2:C:508:ARG:O    | 2:C:511:THR:OG1  | 2.18                     | 0.60              |
| 2:D:249:ARG:HG3  | 2:D:276:LEU:HD21 | 1.82                     | 0.60              |
| 1:F:231:ILE:HG13 | 1:F:234:TYR:H    | 1.67                     | 0.60              |
| 1:A:127:ASP:OD2  | 1:A:394:PHE:N    | 2.34                     | 0.60              |
| 1:A:352:ALA:O    | 1:A:356:LEU:N    | 2.31                     | 0.60              |
| 2:D:405:GLN:NE2  | 2:D:409:GLU:OE1  | 2.34                     | 0.60              |
| 2:D:477:ALA:HA   | 2:D:480:GLN:HB2  | 1.83                     | 0.60              |
| 2:C:499:LEU:HD21 | 2:C:653:ILE:HG12 | 1.82                     | 0.60              |
| 1:F:349:GLN:O    | 1:F:353:ASN:ND2  | 2.34                     | 0.60              |
| 2:C:29:ASN:HB2   | 2:C:66:ILE:HA    | 1.83                     | 0.60              |
| 2:D:514:GLU:HG3  | 2:D:611:GLY:HA2  | 1.84                     | 0.60              |
| 1:E:18:VAL:HB    | 1:E:283:ILE:HB   | 1.82                     | 0.60              |
| 2:C:497:ARG:NH1  | 2:C:629:GLU:OE2  | 2.34                     | 0.60              |
| 2:G:509:MET:HE1  | 2:G:618:VAL:HG13 | 1.84                     | 0.60              |
| 2:C:26:GLU:O     | 2:C:61:LYS:NZ    | 2.25                     | 0.59              |
| 1:E:251:ALA:O    | 1:E:255:LYS:NZ   | 2.35                     | 0.59              |
| 1:A:47:GLU:HB3   | 1:A:227:MET:HE1  | 1.83                     | 0.59              |
| 1:B:231:ILE:O    | 1:B:234:TYR:N    | 2.30                     | 0.59              |
| 2:G:423:ASN:HD21 | 2:G:447:PHE:HB2  | 1.67                     | 0.59              |
| 2:G:540:GLY:O    | 2:G:544:GLY:N    | 2.36                     | 0.59              |
| 1:A:123:ALA:O    | 1:A:282:VAL:N    | 2.34                     | 0.59              |
| 2:H:396:VAL:HG22 | 2:H:397:PHE:H    | 1.67                     | 0.59              |
| 1:A:342:MET:HG3  | 1:A:344:GLU:H    | 1.67                     | 0.59              |
| 2:C:180:LEU:HD22 | 2:C:188:VAL:HG22 | 1.85                     | 0.59              |
| 2:D:121:LEU:HD21 | 2:D:155:LEU:HD13 | 1.84                     | 0.59              |
| 1:E:348:ALA:O    | 1:E:350:THR:N    | 2.34                     | 0.59              |
| 2:H:47:ARG:HH11  | 2:H:100:LEU:HD22 | 1.66                     | 0.59              |
| 2:D:356:LEU:O    | 2:D:357:GLU:HG3  | 2.02                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:494:TYR:OH   | 2:D:645:GLY:O    | 2.16                     | 0.59              |
| 2:H:296:LYS:O    | 2:H:478:LYS:NZ   | 2.35                     | 0.59              |
| 1:B:302:ARG:NH2  | 1:B:330:ALA:O    | 2.36                     | 0.59              |
| 2:C:459:ILE:HB   | 2:C:486:VAL:HA   | 1.85                     | 0.59              |
| 2:D:415:ALA:O    | 2:D:438:ARG:NH1  | 2.36                     | 0.59              |
| 1:A:337:LEU:HD21 | 1:A:418:LEU:HD13 | 1.85                     | 0.58              |
| 1:E:217:TRP:HH2  | 1:E:226:VAL:HG11 | 1.67                     | 0.58              |
| 2:D:515:ARG:HB2  | 2:D:518:HIS:HD2  | 1.68                     | 0.58              |
| 2:G:337:ILE:O    | 2:G:380:THR:N    | 2.34                     | 0.58              |
| 1:A:33:HIS:ND1   | 1:A:130:SER:OG   | 2.32                     | 0.58              |
| 1:A:49:LEU:HD12  | 1:A:54:ILE:HG23  | 1.84                     | 0.58              |
| 1:A:289:ARG:HA   | 1:A:292:GLU:HG2  | 1.86                     | 0.58              |
| 2:C:220:ALA:O    | 2:C:222:PRO:HD2  | 2.02                     | 0.58              |
| 2:D:310:SER:HB3  | 2:D:389:ARG:HD3  | 1.85                     | 0.58              |
| 2:C:429:ILE:HB   | 2:C:462:HIS:HB3  | 1.85                     | 0.58              |
| 2:C:540:GLY:O    | 2:C:544:GLY:N    | 2.36                     | 0.58              |
| 2:D:222:PRO:HA   | 2:D:225:ARG:HG2  | 1.85                     | 0.58              |
| 2:D:611:GLY:O    | 2:D:613:ILE:N    | 2.35                     | 0.58              |
| 2:G:166:GLU:OE1  | 2:G:170:THR:OG1  | 2.22                     | 0.58              |
| 2:D:528:PHE:CE1  | 2:D:656:PRO:HD3  | 2.38                     | 0.58              |
| 1:F:339:LEU:HD22 | 1:F:405:THR:HG23 | 1.85                     | 0.58              |
| 2:G:140:GLU:HB2  | 2:G:147:PRO:HG3  | 1.86                     | 0.58              |
| 2:D:347:HIS:O    | 2:D:351:TYR:N    | 2.36                     | 0.57              |
| 2:D:396:VAL:HG22 | 2:D:397:PHE:H    | 1.69                     | 0.57              |
| 2:C:643:ARG:NH1  | 2:C:644:ASP:OD1  | 2.36                     | 0.57              |
| 1:A:267:VAL:HG23 | 1:A:347:ALA:HB3  | 1.86                     | 0.57              |
| 2:C:9:LEU:HD11   | 2:C:46:LEU:HD13  | 1.86                     | 0.57              |
| 1:F:120:ALA:HB1  | 1:F:285:MET:HE1  | 1.85                     | 0.57              |
| 2:H:64:ASN:HA    | 2:H:110:GLY:HA3  | 1.84                     | 0.57              |
| 1:A:343:HIS:HD2  | 1:A:345:ALA:HB2  | 1.70                     | 0.57              |
| 2:C:523:LEU:HG   | 2:C:532:PRO:HD3  | 1.86                     | 0.57              |
| 1:A:67:VAL:HG21  | 1:A:99:CYS:H     | 1.70                     | 0.57              |
| 1:A:136:VAL:HG12 | 1:B:136:VAL:HG13 | 1.85                     | 0.57              |
| 1:A:221:LYS:HB2  | 1:A:411:ARG:NH1  | 2.18                     | 0.57              |
| 2:C:404:GLN:NE2  | 2:C:431:ASP:O    | 2.37                     | 0.57              |
| 2:C:694:ARG:HA   | 2:C:697:GLU:HB3  | 1.85                     | 0.57              |
| 2:H:256:THR:OG1  | 2:H:260:GLN:NE2  | 2.38                     | 0.57              |
| 2:C:449:SER:HB3  | 2:C:450:PRO:HD2  | 1.86                     | 0.57              |
| 2:H:110:GLY:HA2  | 2:H:133:LYS:HE3  | 1.86                     | 0.57              |
| 2:H:631:VAL:HG21 | 2:H:695:LEU:HB2  | 1.86                     | 0.57              |
| 1:B:20:GLY:HA3   | 1:B:282:VAL:HG22 | 1.85                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:476:LEU:O    | 2:C:480:GLN:N    | 2.37                     | 0.57              |
| 2:C:624:MET:SD   | 2:C:625:LEU:HD22 | 2.44                     | 0.57              |
| 1:F:221:LYS:O    | 1:F:411:ARG:NH2  | 2.37                     | 0.57              |
| 2:H:8:THR:OG1    | 2:H:20:THR:OG1   | 2.23                     | 0.57              |
| 1:A:197:ILE:HG21 | 1:A:348:ALA:HB2  | 1.87                     | 0.57              |
| 1:B:319:PRO:O    | 1:B:323:THR:OG1  | 2.21                     | 0.57              |
| 2:C:31:LEU:HB2   | 2:C:69:ALA:HA    | 1.86                     | 0.57              |
| 2:G:220:ALA:O    | 2:G:222:PRO:HD2  | 2.03                     | 0.57              |
| 1:A:342:MET:SD   | 1:A:420:THR:OG1  | 2.58                     | 0.57              |
| 1:A:407:HIS:C    | 1:A:411:ARG:HE   | 2.12                     | 0.57              |
| 1:B:158:LYS:O    | 1:B:162:ARG:NH1  | 2.38                     | 0.57              |
| 1:A:199:ARG:NH1  | 1:A:254:ALA:O    | 2.38                     | 0.56              |
| 2:D:281:GLN:HG3  | 2:D:658:PHE:HB2  | 1.86                     | 0.56              |
| 2:D:664:ARG:HD2  | 2:D:706:TRP:HH2  | 1.70                     | 0.56              |
| 1:E:409:LEU:HA   | 1:E:412:ARG:HB2  | 1.87                     | 0.56              |
| 1:F:231:ILE:HD12 | 1:F:233:PRO:HG2  | 1.87                     | 0.56              |
| 2:G:154:ARG:NH2  | 2:G:266:TYR:OH   | 2.38                     | 0.56              |
| 1:A:9:THR:HG22   | 1:A:13:ASP:H     | 1.69                     | 0.56              |
| 2:C:281:GLN:N    | 2:C:281:GLN:OE1  | 2.38                     | 0.56              |
| 2:C:414:CYS:SG   | 2:C:415:ALA:N    | 2.78                     | 0.56              |
| 2:C:495:VAL:HG22 | 2:C:653:ILE:HD11 | 1.87                     | 0.56              |
| 1:B:67:VAL:HG21  | 1:B:394:PHE:HB3  | 1.87                     | 0.56              |
| 1:E:311:VAL:HA   | 1:E:315:MET:HG2  | 1.86                     | 0.56              |
| 2:G:311:VAL:HG11 | 2:G:327:THR:HG21 | 1.88                     | 0.56              |
| 2:H:386:PHE:HD1  | 2:H:389:ARG:HG3  | 1.70                     | 0.56              |
| 1:A:119:ARG:HE   | 1:A:289:ARG:HH11 | 1.53                     | 0.56              |
| 1:B:164:ARG:N    | 1:B:167:ASP:OD2  | 2.38                     | 0.56              |
| 2:H:32:LYS:H     | 2:H:35:PHE:HD2   | 1.54                     | 0.56              |
| 1:A:371:HIS:ND1  | 1:A:372:ALA:O    | 2.38                     | 0.56              |
| 2:D:59:SER:HA    | 2:D:65:PHE:HD1   | 1.70                     | 0.56              |
| 2:D:555:TYR:HB2  | 2:D:559:PHE:HE2  | 1.71                     | 0.56              |
| 1:E:9:THR:HG23   | 1:E:11:GLN:H     | 1.71                     | 0.56              |
| 1:E:55:PRO:HG2   | 1:E:58:VAL:HG13  | 1.88                     | 0.56              |
| 2:G:628:ASN:OD1  | 2:G:632:ARG:NH2  | 2.38                     | 0.56              |
| 2:H:126:ARG:NH1  | 2:H:184:LEU:O    | 2.35                     | 0.56              |
| 1:E:152:THR:HG23 | 1:E:155:GLN:H    | 1.71                     | 0.56              |
| 2:H:638:VAL:HG13 | 2:H:639:ILE:HG12 | 1.87                     | 0.56              |
| 1:A:169:MET:HE3  | 1:A:169:MET:HA   | 1.87                     | 0.56              |
| 2:D:558:ARG:NH1  | 2:D:629:GLU:OE1  | 2.39                     | 0.56              |
| 2:G:7:PHE:HB2    | 2:G:38:GLN:HE22  | 1.70                     | 0.56              |
| 2:H:420:PHE:HE1  | 2:H:422:SER:HB3  | 1.71                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:21:LEU:HB2   | 1:A:48:LEU:HD13  | 1.87                     | 0.56              |
| 1:B:53:GLU:HG2   | 2:C:385:GLY:HA2  | 1.88                     | 0.56              |
| 2:D:643:ARG:NH2  | 2:D:644:ASP:OD1  | 2.38                     | 0.56              |
| 2:D:649:ALA:HA   | 2:D:653:ILE:HD13 | 1.88                     | 0.56              |
| 2:H:328:ALA:HB1  | 2:H:376:LEU:HB2  | 1.87                     | 0.55              |
| 1:A:367:LEU:HD23 | 1:A:369:ARG:HE   | 1.71                     | 0.55              |
| 2:C:175:ARG:HB2  | 2:C:178:GLN:HG3  | 1.86                     | 0.55              |
| 2:C:569:ILE:O    | 2:C:575:LYS:NZ   | 2.39                     | 0.55              |
| 2:D:163:THR:HG21 | 2:D:182:LEU:HD11 | 1.89                     | 0.55              |
| 1:B:212:ARG:HH21 | 1:B:383:VAL:HA   | 1.72                     | 0.55              |
| 2:C:697:GLU:OE2  | 2:C:701:ARG:NH1  | 2.39                     | 0.55              |
| 2:D:637:GLN:NE2  | 2:D:639:ILE:O    | 2.39                     | 0.55              |
| 1:E:403:THR:O    | 1:E:407:HIS:ND1  | 2.39                     | 0.55              |
| 2:H:498:ILE:HA   | 2:H:629:GLU:HG2  | 1.88                     | 0.55              |
| 2:H:515:ARG:HB2  | 2:H:518:HIS:HD2  | 1.70                     | 0.55              |
| 2:H:574:ARG:HG3  | 2:H:582:GLY:HA2  | 1.87                     | 0.55              |
| 1:B:123:ALA:O    | 1:B:282:VAL:N    | 2.29                     | 0.55              |
| 2:C:161:VAL:HA   | 2:C:164:ALA:HB3  | 1.89                     | 0.55              |
| 2:C:180:LEU:HD13 | 2:C:187:ASP:HA   | 1.89                     | 0.55              |
| 2:C:612:ARG:HG3  | 2:C:613:ILE:HG23 | 1.89                     | 0.55              |
| 2:H:477:ALA:HB1  | 2:H:482:LYS:HB2  | 1.89                     | 0.55              |
| 2:G:624:MET:SD   | 2:G:625:LEU:HD22 | 2.47                     | 0.55              |
| 1:F:8:VAL:HA     | 1:F:14:ARG:HA    | 1.88                     | 0.55              |
| 1:B:25:PHE:CD1   | 1:B:278:GLY:HA3  | 2.42                     | 0.55              |
| 2:H:180:LEU:HD22 | 2:H:188:VAL:HG22 | 1.89                     | 0.55              |
| 2:H:494:TYR:CG   | 2:H:639:ILE:HD11 | 2.41                     | 0.55              |
| 2:C:477:ALA:HA   | 2:C:480:GLN:HB2  | 1.89                     | 0.55              |
| 2:D:154:ARG:NH2  | 2:D:266:TYR:OH   | 2.39                     | 0.55              |
| 1:A:423:ALA:HB3  | 1:A:427:LEU:HB2  | 1.88                     | 0.55              |
| 2:D:626:MET:HE1  | 2:D:662:PRO:HG3  | 1.88                     | 0.55              |
| 2:G:300:GLY:HA3  | 2:G:474:VAL:HG11 | 1.89                     | 0.55              |
| 2:G:360:VAL:HG23 | 2:G:370:ARG:HH21 | 1.71                     | 0.55              |
| 2:H:294:ASP:HB3  | 2:H:643:ARG:HH11 | 1.71                     | 0.55              |
| 1:A:180:THR:HG22 | 1:A:182:LEU:HG   | 1.87                     | 0.54              |
| 1:A:243:ASN:HD21 | 1:A:274:PRO:HG2  | 1.71                     | 0.54              |
| 1:B:357:LEU:O    | 1:B:373:THR:OG1  | 2.25                     | 0.54              |
| 2:D:494:TYR:CG   | 2:D:639:ILE:HD11 | 2.42                     | 0.54              |
| 1:E:273:THR:HB   | 1:E:388:ILE:HD13 | 1.89                     | 0.54              |
| 2:H:249:ARG:HG3  | 2:H:276:LEU:HD11 | 1.87                     | 0.54              |
| 2:H:310:SER:HB3  | 2:H:389:ARG:HD3  | 1.89                     | 0.54              |
| 2:H:506:ALA:HA   | 2:H:509:MET:HE2  | 1.88                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:67:VAL:HG23  | 1:A:395:ALA:HB2  | 1.89                     | 0.54              |
| 1:A:328:GLU:OE2  | 1:A:369:ARG:NH2  | 2.34                     | 0.54              |
| 2:G:282:SER:OG   | 2:G:286:ARG:NH1  | 2.39                     | 0.54              |
| 2:H:530:VAL:HG11 | 2:H:535:LEU:HD13 | 1.90                     | 0.54              |
| 2:G:117:LEU:HD11 | 2:G:137:GLY:H    | 1.72                     | 0.54              |
| 1:A:105:ALA:O    | 1:A:109:VAL:N    | 2.30                     | 0.54              |
| 1:A:152:THR:HG23 | 1:A:155:GLN:H    | 1.72                     | 0.54              |
| 1:B:161:SER:OG   | 1:B:162:ARG:NH1  | 2.41                     | 0.54              |
| 1:E:271:ASN:HB2  | 1:E:347:ALA:HB2  | 1.88                     | 0.54              |
| 2:H:83:ALA:HB1   | 2:H:273:PHE:HB3  | 1.87                     | 0.54              |
| 2:H:117:LEU:HD21 | 2:H:136:LEU:HB3  | 1.90                     | 0.54              |
| 2:D:237:GLU:HA   | 2:D:240:THR:HG22 | 1.89                     | 0.54              |
| 1:A:363:ALA:HB3  | 1:A:372:ALA:HA   | 1.90                     | 0.54              |
| 2:C:343:GLN:O    | 2:C:347:HIS:N    | 2.41                     | 0.54              |
| 2:D:31:LEU:HD21  | 2:D:66:ILE:HD11  | 1.90                     | 0.54              |
| 2:G:83:ALA:HB3   | 2:G:274:GLY:HA2  | 1.88                     | 0.54              |
| 2:C:37:SER:HA    | 2:C:40:ARG:HH21  | 1.73                     | 0.54              |
| 2:D:442:VAL:HB   | 2:D:462:HIS:HE1  | 1.72                     | 0.54              |
| 2:D:542:ASP:O    | 2:D:546:LYS:N    | 2.41                     | 0.54              |
| 1:A:227:MET:HG3  | 1:A:228:THR:N    | 2.22                     | 0.54              |
| 1:B:207:HIS:NE2  | 1:B:248:SER:O    | 2.37                     | 0.54              |
| 2:G:632:ARG:HH21 | 2:G:692:CYS:HB2  | 1.72                     | 0.54              |
| 2:H:625:LEU:HD21 | 2:H:689:PHE:HE1  | 1.73                     | 0.54              |
| 1:A:42:LYS:NZ    | 1:A:84:THR:H     | 2.05                     | 0.53              |
| 2:H:308:LEU:HD11 | 2:H:472:THR:HB   | 1.90                     | 0.53              |
| 1:A:29:ALA:HB2   | 1:B:149:LYS:NZ   | 2.23                     | 0.53              |
| 1:A:392:HIS:CE1  | 1:A:394:PHE:HA   | 2.44                     | 0.53              |
| 1:B:225:GLU:N    | 1:B:225:GLU:OE1  | 2.41                     | 0.53              |
| 1:F:392:HIS:ND1  | 1:F:397:THR:HG21 | 2.23                     | 0.53              |
| 2:H:356:LEU:O    | 2:H:357:GLU:HG3  | 2.09                     | 0.53              |
| 2:H:656:PRO:HB3  | 2:H:658:PHE:CE1  | 2.44                     | 0.53              |
| 2:C:516:VAL:HG23 | 2:C:533:ILE:HD11 | 1.88                     | 0.53              |
| 2:D:664:ARG:HD2  | 2:D:706:TRP:CH2  | 2.44                     | 0.53              |
| 2:H:231:MET:HE3  | 2:H:231:MET:O    | 2.07                     | 0.53              |
| 2:H:272:ALA:HB1  | 2:H:276:LEU:HD12 | 1.90                     | 0.53              |
| 1:B:354:ILE:HG23 | 1:B:376:VAL:HB   | 1.90                     | 0.53              |
| 2:C:314:LEU:HB2  | 2:C:394:GLU:HA   | 1.90                     | 0.53              |
| 1:F:187:THR:O    | 1:F:190:GLN:HG3  | 2.08                     | 0.53              |
| 1:B:324:PRO:HD3  | 1:B:373:THR:HG22 | 1.91                     | 0.53              |
| 2:D:281:GLN:OE1  | 2:D:281:GLN:N    | 2.38                     | 0.53              |
| 1:A:259:ALA:H    | 1:A:268:THR:HA   | 1.74                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:317:LEU:HD22 | 1:B:356:LEU:HD12 | 1.91                     | 0.53              |
| 2:D:334:PRO:HA   | 2:D:376:LEU:HD12 | 1.91                     | 0.53              |
| 1:A:271:ASN:HB2  | 1:A:347:ALA:HB2  | 1.89                     | 0.53              |
| 1:A:43:MET:SD    | 1:A:227:MET:HE3  | 2.49                     | 0.53              |
| 1:B:197:ILE:HG21 | 1:B:348:ALA:HA   | 1.89                     | 0.53              |
| 2:G:296:LYS:O    | 2:G:478:LYS:NZ   | 2.40                     | 0.53              |
| 2:G:650:VAL:HA   | 2:G:655:PHE:HB3  | 1.91                     | 0.53              |
| 2:H:84:GLU:O     | 2:H:88:ARG:N     | 2.38                     | 0.53              |
| 1:A:54:ILE:HD12  | 1:A:55:PRO:HD2   | 1.90                     | 0.53              |
| 1:A:61:GLN:HE21  | 1:A:93:TYR:HD2   | 1.57                     | 0.53              |
| 1:B:408:GLU:OE1  | 1:B:411:ARG:NH1  | 2.42                     | 0.53              |
| 2:C:414:CYS:SG   | 2:C:418:THR:HG21 | 2.49                     | 0.53              |
| 1:E:423:ALA:HB3  | 1:E:427:LEU:HB2  | 1.91                     | 0.53              |
| 1:F:284:LEU:O    | 1:F:285:MET:HE2  | 2.08                     | 0.53              |
| 2:G:219:LEU:HB2  | 2:G:224:GLY:HA3  | 1.91                     | 0.53              |
| 2:H:394:GLU:OE2  | 2:H:403:LYS:NZ   | 2.35                     | 0.53              |
| 2:C:639:ILE:HD13 | 2:C:645:GLY:HA2  | 1.89                     | 0.53              |
| 2:G:459:ILE:HD12 | 2:G:473:THR:HG22 | 1.89                     | 0.53              |
| 2:H:282:SER:OG   | 2:H:286:ARG:NH1  | 2.42                     | 0.53              |
| 2:C:627:LEU:HD22 | 2:C:666:ILE:HG23 | 1.90                     | 0.52              |
| 1:A:136:VAL:HG13 | 1:B:135:GLY:HA2  | 1.92                     | 0.52              |
| 2:C:126:ARG:NE   | 2:C:184:LEU:O    | 2.38                     | 0.52              |
| 2:D:10:ASN:HB2   | 2:D:18:VAL:HG13  | 1.92                     | 0.52              |
| 1:E:97:ARG:HD3   | 1:E:100:ALA:HB3  | 1.91                     | 0.52              |
| 2:G:542:ASP:OD1  | 2:G:542:ASP:N    | 2.42                     | 0.52              |
| 2:H:47:ARG:HE    | 2:H:50:LYS:HZ1   | 1.56                     | 0.52              |
| 2:H:459:ILE:HD12 | 2:H:473:THR:HG22 | 1.92                     | 0.52              |
| 2:C:140:GLU:HB2  | 2:C:147:PRO:HG3  | 1.91                     | 0.52              |
| 1:E:100:ALA:HB1  | 1:E:103:PHE:HB2  | 1.92                     | 0.52              |
| 2:H:663:PHE:HB2  | 2:H:706:TRP:CZ2  | 2.44                     | 0.52              |
| 1:A:51:ARG:HD3   | 2:D:384:ARG:HH21 | 1.74                     | 0.52              |
| 1:B:399:ALA:HA   | 1:B:402:ILE:HD12 | 1.91                     | 0.52              |
| 2:G:419:ILE:HA   | 2:G:441:GLN:HB3  | 1.90                     | 0.52              |
| 2:G:656:PRO:HB3  | 2:G:658:PHE:CE1  | 2.45                     | 0.52              |
| 2:H:43:ILE:HD11  | 2:H:100:LEU:HD11 | 1.89                     | 0.52              |
| 1:A:42:LYS:NZ    | 1:A:79:GLU:O     | 2.38                     | 0.52              |
| 1:A:348:ALA:C    | 1:A:350:THR:H    | 2.16                     | 0.52              |
| 1:B:30:THR:HG21  | 1:B:242:ASN:HD21 | 1.74                     | 0.52              |
| 2:C:29:ASN:O     | 2:C:67:ALA:N     | 2.35                     | 0.52              |
| 2:G:501:PRO:HB2  | 2:G:625:LEU:HD12 | 1.91                     | 0.52              |
| 2:D:301:SER:OG   | 2:D:302:ASP:N    | 2.42                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:514:GLU:HG3  | 2:H:611:GLY:HA2  | 1.90                     | 0.52              |
| 2:C:40:ARG:HA    | 2:C:43:ILE:HG22  | 1.92                     | 0.52              |
| 1:A:190:GLN:O    | 1:A:194:THR:N    | 2.37                     | 0.52              |
| 2:C:685:TYR:HB3  | 2:C:688:ARG:NH2  | 2.24                     | 0.52              |
| 2:G:175:ARG:HD2  | 2:G:177:LYS:HE2  | 1.91                     | 0.52              |
| 2:G:697:GLU:OE2  | 2:G:701:ARG:NH1  | 2.42                     | 0.52              |
| 2:D:117:LEU:HD21 | 2:D:136:LEU:HB3  | 1.90                     | 0.52              |
| 2:D:692:CYS:O    | 2:D:696:VAL:N    | 2.34                     | 0.52              |
| 1:E:59:ILE:HB    | 1:E:86:MET:HE1   | 1.92                     | 0.52              |
| 2:G:643:ARG:NH1  | 2:G:644:ASP:OD1  | 2.43                     | 0.52              |
| 1:B:199:ARG:NH2  | 1:B:253:TYR:O    | 2.43                     | 0.52              |
| 2:C:338:LYS:HB2  | 2:C:386:PHE:HE2  | 1.75                     | 0.52              |
| 2:C:54:GLY:HA2   | 2:C:102:ILE:HD12 | 1.92                     | 0.51              |
| 2:C:121:LEU:HD12 | 2:C:154:ARG:HB3  | 1.92                     | 0.51              |
| 2:H:40:ARG:HH11  | 2:H:93:LEU:HD13  | 1.75                     | 0.51              |
| 1:A:42:LYS:HZ1   | 1:A:83:GLY:CA    | 2.23                     | 0.51              |
| 1:B:199:ARG:NH2  | 1:B:256:LEU:O    | 2.43                     | 0.51              |
| 2:C:178:GLN:HA   | 2:C:181:LYS:HE3  | 1.92                     | 0.51              |
| 2:C:348:ALA:HA   | 2:C:351:TYR:HD2  | 1.74                     | 0.51              |
| 1:E:182:LEU:HD13 | 1:E:187:THR:HB   | 1.93                     | 0.51              |
| 1:F:55:PRO:HB2   | 1:F:58:VAL:HG23  | 1.93                     | 0.51              |
| 1:A:81:VAL:HA    | 1:A:86:MET:HE2   | 1.92                     | 0.51              |
| 2:D:58:VAL:HG12  | 2:D:60:ALA:H     | 1.74                     | 0.51              |
| 2:D:308:LEU:HD23 | 2:D:390:ASP:HB3  | 1.92                     | 0.51              |
| 2:D:357:GLU:HA   | 2:D:360:VAL:HB   | 1.93                     | 0.51              |
| 1:E:258:PRO:HB3  | 1:E:265:GLY:HA3  | 1.92                     | 0.51              |
| 1:F:332:LEU:HD12 | 1:F:432:VAL:HG11 | 1.91                     | 0.51              |
| 2:G:508:ARG:O    | 2:G:511:THR:OG1  | 2.28                     | 0.51              |
| 2:G:541:ILE:HG21 | 2:G:569:ILE:HG21 | 1.92                     | 0.51              |
| 2:H:256:THR:O    | 2:H:264:SER:OG   | 2.28                     | 0.51              |
| 1:A:38:VAL:O     | 1:A:42:LYS:HG2   | 2.10                     | 0.51              |
| 2:C:573:ASP:O    | 2:C:581:ARG:NE   | 2.44                     | 0.51              |
| 2:D:374:LEU:HD13 | 2:D:377:ILE:HD12 | 1.92                     | 0.51              |
| 2:G:486:VAL:HB   | 2:G:640:ARG:HE   | 1.76                     | 0.51              |
| 2:D:419:ILE:HG22 | 2:D:441:GLN:HG2  | 1.93                     | 0.51              |
| 2:G:565:VAL:HG12 | 2:G:605:ILE:HG23 | 1.92                     | 0.51              |
| 2:H:232:VAL:O    | 2:H:236:THR:N    | 2.34                     | 0.51              |
| 2:D:510:LEU:HD13 | 2:D:516:VAL:HG22 | 1.91                     | 0.51              |
| 2:D:612:ARG:NH1  | 2:D:685:TYR:OH   | 2.44                     | 0.51              |
| 2:G:250:ILE:HA   | 2:G:253:VAL:HG12 | 1.92                     | 0.51              |
| 2:C:631:VAL:HG11 | 2:C:695:LEU:HD12 | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:333:THR:HG22 | 1:B:335:SER:H    | 1.76                     | 0.51              |
| 1:A:212:ARG:HH21 | 1:A:383:VAL:HA   | 1.76                     | 0.51              |
| 1:A:386:GLY:HA2  | 1:A:401:MET:HE1  | 1.93                     | 0.51              |
| 1:B:337:LEU:HD21 | 1:B:418:LEU:HB3  | 1.93                     | 0.51              |
| 1:F:9:THR:HG23   | 1:F:11:GLN:H     | 1.76                     | 0.51              |
| 1:B:423:ALA:HB3  | 1:B:427:LEU:HB2  | 1.93                     | 0.51              |
| 2:C:374:LEU:HA   | 2:C:377:ILE:HD13 | 1.93                     | 0.51              |
| 2:G:146:LEU:HD23 | 2:G:276:LEU:HD13 | 1.93                     | 0.51              |
| 1:A:129:SER:HB3  | 1:A:275:LEU:HG   | 1.93                     | 0.50              |
| 1:A:409:LEU:O    | 1:A:413:GLY:N    | 2.44                     | 0.50              |
| 1:B:318:GLY:HA3  | 1:B:428:GLY:HA3  | 1.92                     | 0.50              |
| 1:B:384:LEU:O    | 1:B:390:TYR:OH   | 2.29                     | 0.50              |
| 2:D:339:ASP:HB2  | 2:D:345:ILE:HG13 | 1.93                     | 0.50              |
| 2:H:91:GLN:HA    | 2:H:94:MET:HE2   | 1.93                     | 0.50              |
| 2:D:199:VAL:O    | 2:D:203:LYS:HG2  | 2.12                     | 0.50              |
| 1:E:352:ALA:O    | 1:E:356:LEU:N    | 2.40                     | 0.50              |
| 1:F:22:ARG:HD2   | 1:F:25:PHE:CZ    | 2.46                     | 0.50              |
| 1:F:70:MET:HE3   | 1:F:71:PRO:HD2   | 1.93                     | 0.50              |
| 2:C:26:GLU:HG3   | 2:C:28:MET:HE2   | 1.93                     | 0.50              |
| 2:C:295:VAL:HG11 | 2:C:483:THR:HG23 | 1.93                     | 0.50              |
| 2:D:528:PHE:CE1  | 2:D:655:PHE:HA   | 2.45                     | 0.50              |
| 2:D:663:PHE:HB2  | 2:D:706:TRP:CZ2  | 2.46                     | 0.50              |
| 2:G:121:LEU:HD12 | 2:G:154:ARG:HB3  | 1.92                     | 0.50              |
| 1:A:108:ASN:O    | 1:A:111:GLU:HG2  | 2.11                     | 0.50              |
| 1:A:290:ALA:O    | 1:A:295:LEU:N    | 2.40                     | 0.50              |
| 2:C:65:PHE:N     | 2:C:109:HIS:O    | 2.43                     | 0.50              |
| 2:C:280:PRO:HA   | 2:C:283:GLN:NE2  | 2.26                     | 0.50              |
| 2:D:531:GLY:H    | 2:D:534:GLN:HE21 | 1.59                     | 0.50              |
| 2:D:537:ASP:OD1  | 2:D:538:GLU:N    | 2.45                     | 0.50              |
| 1:E:313:GLN:O    | 1:E:314:ASP:C    | 2.54                     | 0.50              |
| 2:C:403:LYS:HA   | 2:C:406:MET:HE2  | 1.93                     | 0.50              |
| 2:G:9:LEU:HD11   | 2:G:46:LEU:HD13  | 1.94                     | 0.50              |
| 2:D:643:ARG:HH21 | 2:D:644:ASP:CG   | 2.19                     | 0.50              |
| 1:E:119:ARG:HE   | 1:E:289:ARG:HH21 | 1.59                     | 0.50              |
| 2:G:91:GLN:NE2   | 2:G:266:TYR:O    | 2.45                     | 0.50              |
| 2:G:486:VAL:HG11 | 2:G:640:ARG:HH21 | 1.76                     | 0.50              |
| 2:H:153:GLN:NE2  | 2:H:269:GLU:OE2  | 2.42                     | 0.50              |
| 2:H:611:GLY:O    | 2:H:613:ILE:N    | 2.45                     | 0.50              |
| 1:A:341:ASP:HB3  | 1:A:419:VAL:HG13 | 1.94                     | 0.50              |
| 1:B:95:VAL:HG22  | 1:B:96:SER:H     | 1.76                     | 0.50              |
| 2:C:548:ILE:HA   | 2:C:551:LEU:HD23 | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:230:LYS:NZ   | 2:D:231:MET:HE3  | 2.26                     | 0.50              |
| 2:G:56:VAL:HG12  | 2:G:105:ILE:HB   | 1.93                     | 0.50              |
| 1:A:32:PHE:HA    | 1:A:35:ILE:HD13  | 1.94                     | 0.50              |
| 2:C:308:LEU:HD13 | 2:C:390:ASP:HB2  | 1.93                     | 0.50              |
| 1:E:36:PRO:HA    | 1:E:131:VAL:HG21 | 1.92                     | 0.50              |
| 2:G:446:HIS:HB3  | 2:G:458:GLU:HB2  | 1.92                     | 0.50              |
| 2:H:29:ASN:HB2   | 2:H:66:ILE:HA    | 1.94                     | 0.50              |
| 2:H:664:ARG:HD2  | 2:H:706:TRP:CH2  | 2.46                     | 0.50              |
| 1:B:40:LEU:HB3   | 1:B:279:ALA:HB2  | 1.94                     | 0.49              |
| 2:C:23:VAL:HG22  | 2:C:29:ASN:HD22  | 1.77                     | 0.49              |
| 2:C:691:PRO:HB3  | 2:C:695:LEU:HD22 | 1.93                     | 0.49              |
| 2:G:232:VAL:HG23 | 2:G:251:LEU:HD21 | 1.93                     | 0.49              |
| 2:H:138:LEU:HD23 | 2:H:167:MET:HE1  | 1.93                     | 0.49              |
| 2:H:146:LEU:HB2  | 2:H:147:PRO:HD2  | 1.93                     | 0.49              |
| 2:H:620:GLU:O    | 2:H:624:MET:HG2  | 2.11                     | 0.49              |
| 1:A:257:ARG:HD2  | 1:A:258:PRO:O    | 2.12                     | 0.49              |
| 1:A:400:ARG:O    | 1:A:403:THR:OG1  | 2.29                     | 0.49              |
| 2:C:311:VAL:C    | 2:C:389:ARG:HD2  | 2.37                     | 0.49              |
| 2:C:398:GLU:HA   | 2:C:403:LYS:NZ   | 2.27                     | 0.49              |
| 2:G:423:ASN:ND2  | 2:G:447:PHE:HB2  | 2.26                     | 0.49              |
| 2:G:613:ILE:HD12 | 2:G:617:GLN:HB2  | 1.95                     | 0.49              |
| 1:A:199:ARG:NH2  | 1:A:256:LEU:O    | 2.45                     | 0.49              |
| 1:B:14:ARG:NH1   | 1:B:434:GLU:OE2  | 2.46                     | 0.49              |
| 1:B:15:ILE:HD12  | 1:B:113:LEU:HD11 | 1.93                     | 0.49              |
| 2:C:419:ILE:HA   | 2:C:441:GLN:HB3  | 1.94                     | 0.49              |
| 2:D:240:THR:OG1  | 2:D:244:TYR:HB2  | 2.11                     | 0.49              |
| 1:E:234:TYR:HB3  | 2:H:346:ASN:OD1  | 2.11                     | 0.49              |
| 2:G:337:ILE:N    | 2:G:378:SER:O    | 2.44                     | 0.49              |
| 2:G:406:MET:HE1  | 2:G:420:PHE:HZ   | 1.76                     | 0.49              |
| 2:C:400:LEU:HD13 | 2:C:427:LEU:HG   | 1.95                     | 0.49              |
| 2:D:84:GLU:HG2   | 2:D:270:ALA:O    | 2.11                     | 0.49              |
| 1:E:187:THR:HG21 | 1:E:315:MET:HE1  | 1.92                     | 0.49              |
| 2:C:291:ALA:HB3  | 2:C:647:ILE:HD13 | 1.93                     | 0.49              |
| 2:D:300:GLY:HA3  | 2:D:474:VAL:HG11 | 1.95                     | 0.49              |
| 2:D:596:GLN:NE2  | 2:D:597:VAL:HG22 | 2.28                     | 0.49              |
| 1:F:406:LEU:HD13 | 1:F:435:ALA:HB2  | 1.95                     | 0.49              |
| 2:G:40:ARG:HA    | 2:G:43:ILE:HG22  | 1.94                     | 0.49              |
| 2:H:359:LYS:HB2  | 2:H:370:ARG:NH2  | 2.28                     | 0.49              |
| 1:B:340:ILE:HG21 | 1:B:376:VAL:HG13 | 1.95                     | 0.49              |
| 2:C:343:GLN:C    | 2:C:347:HIS:HD1  | 2.20                     | 0.49              |
| 1:E:420:THR:HG22 | 1:E:430:ALA:HA   | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:674:VAL:HA   | 2:G:677:ILE:HD12 | 1.94                     | 0.49              |
| 2:H:356:LEU:HG   | 2:H:357:GLU:H    | 1.78                     | 0.49              |
| 1:A:64:PHE:HZ    | 1:A:281:ALA:HB2  | 1.77                     | 0.49              |
| 1:A:350:THR:HA   | 1:A:353:ASN:HD22 | 1.76                     | 0.49              |
| 1:B:342:MET:HE1  | 1:B:350:THR:HA   | 1.95                     | 0.49              |
| 2:C:10:ASN:N     | 2:C:18:VAL:O     | 2.43                     | 0.49              |
| 2:C:498:ILE:HG13 | 2:C:499:LEU:HD22 | 1.95                     | 0.49              |
| 2:C:340:ILE:HA   | 2:C:381:THR:OG1  | 2.13                     | 0.49              |
| 1:F:377:ASP:HB3  | 1:F:380:LYS:HG2  | 1.94                     | 0.49              |
| 2:H:28:MET:HE2   | 2:H:30:THR:HG22  | 1.95                     | 0.49              |
| 1:B:48:LEU:HD21  | 1:B:283:ILE:HD11 | 1.93                     | 0.49              |
| 2:D:527:GLY:HA3  | 2:D:656:PRO:HG3  | 1.94                     | 0.49              |
| 2:D:533:ILE:HG13 | 2:D:534:GLN:N    | 2.28                     | 0.49              |
| 1:E:47:GLU:OE1   | 1:E:51:ARG:NH2   | 2.46                     | 0.49              |
| 1:B:406:LEU:HD13 | 1:B:435:ALA:HB2  | 1.95                     | 0.49              |
| 2:C:394:GLU:HG3  | 2:C:422:SER:HA   | 1.95                     | 0.49              |
| 2:C:396:VAL:HG22 | 2:C:397:PHE:H    | 1.77                     | 0.49              |
| 2:D:57:PHE:CD2   | 2:D:119:LEU:HD21 | 2.48                     | 0.49              |
| 2:D:152:THR:OG1  | 2:D:153:GLN:OE1  | 2.24                     | 0.49              |
| 2:G:84:GLU:HG2   | 2:G:270:ALA:O    | 2.13                     | 0.49              |
| 2:H:153:GLN:HB3  | 2:H:257:GLY:HA3  | 1.94                     | 0.49              |
| 2:H:314:LEU:HD22 | 2:H:406:MET:HE2  | 1.95                     | 0.49              |
| 1:A:337:LEU:HD11 | 1:A:418:LEU:HB2  | 1.95                     | 0.48              |
| 2:D:419:ILE:HA   | 2:D:441:GLN:HB3  | 1.95                     | 0.48              |
| 1:E:286:THR:HG23 | 1:E:289:ARG:H    | 1.78                     | 0.48              |
| 2:G:343:GLN:O    | 2:G:347:HIS:ND1  | 2.46                     | 0.48              |
| 1:A:211:GLN:C    | 1:A:213:ALA:H    | 2.21                     | 0.48              |
| 2:D:47:ARG:HH21  | 2:D:50:LYS:HZ1   | 1.61                     | 0.48              |
| 2:D:678:MET:HA   | 2:D:681:LEU:HD12 | 1.95                     | 0.48              |
| 1:E:18:VAL:HG21  | 1:E:285:MET:HE3  | 1.95                     | 0.48              |
| 1:F:212:ARG:HE   | 1:F:383:VAL:HA   | 1.78                     | 0.48              |
| 2:D:94:MET:HG2   | 2:D:122:ALA:HB2  | 1.95                     | 0.48              |
| 2:G:477:ALA:HB1  | 2:G:482:LYS:HB2  | 1.94                     | 0.48              |
| 2:H:459:ILE:HG13 | 2:H:474:VAL:HG22 | 1.95                     | 0.48              |
| 2:H:644:ASP:HA   | 2:H:647:ILE:HG22 | 1.93                     | 0.48              |
| 1:A:7:LEU:O      | 1:A:15:ILE:HG12  | 2.13                     | 0.48              |
| 1:A:104:GLN:NE2  | 1:A:108:ASN:OD1  | 2.45                     | 0.48              |
| 1:B:183:ARG:NE   | 1:B:186:ASP:OD2  | 2.34                     | 0.48              |
| 1:B:384:LEU:HD22 | 1:B:404:GLN:HB3  | 1.94                     | 0.48              |
| 2:D:631:VAL:HG11 | 2:D:695:LEU:HD12 | 1.94                     | 0.48              |
| 2:D:693:GLU:O    | 2:D:697:GLU:N    | 2.41                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:339:LEU:HD22 | 1:E:405:THR:HG23 | 1.94                     | 0.48              |
| 1:F:166:ARG:HA   | 1:F:169:MET:HE1  | 1.96                     | 0.48              |
| 2:C:472:THR:O    | 2:C:476:LEU:HG   | 2.14                     | 0.48              |
| 2:D:656:PRO:HG2  | 2:D:659:LEU:HD12 | 1.95                     | 0.48              |
| 1:E:408:GLU:OE1  | 1:E:411:ARG:NH2  | 2.46                     | 0.48              |
| 2:G:621:ARG:HA   | 2:G:624:MET:HG3  | 1.96                     | 0.48              |
| 2:C:336:ARG:NH1  | 2:C:385:GLY:HA3  | 2.29                     | 0.48              |
| 2:H:337:ILE:N    | 2:H:378:SER:O    | 2.44                     | 0.48              |
| 2:C:84:GLU:HG2   | 2:C:270:ALA:O    | 2.13                     | 0.48              |
| 2:C:473:THR:HA   | 2:C:476:LEU:HD12 | 1.95                     | 0.48              |
| 2:C:681:LEU:HA   | 2:C:684:GLN:HG2  | 1.95                     | 0.48              |
| 2:D:691:PRO:HB2  | 2:D:696:VAL:HG23 | 1.96                     | 0.48              |
| 1:E:43:MET:HE2   | 1:E:227:MET:SD   | 2.54                     | 0.48              |
| 1:F:144:LEU:HA   | 1:F:147:VAL:HG22 | 1.94                     | 0.48              |
| 2:H:150:GLY:O    | 2:H:154:ARG:HG2  | 2.13                     | 0.48              |
| 2:C:236:THR:O    | 2:C:240:THR:N    | 2.27                     | 0.48              |
| 2:C:573:ASP:OD1  | 2:C:573:ASP:N    | 2.47                     | 0.48              |
| 2:D:505:GLU:HG3  | 2:D:509:MET:HE2  | 1.96                     | 0.48              |
| 1:E:76:ILE:O     | 1:E:80:ILE:HG12  | 2.14                     | 0.48              |
| 1:F:176:ALA:HB1  | 1:F:181:GLY:HA2  | 1.94                     | 0.48              |
| 2:H:555:TYR:HB2  | 2:H:559:PHE:HE2  | 1.79                     | 0.48              |
| 2:H:663:PHE:HB2  | 2:H:706:TRP:CH2  | 2.47                     | 0.48              |
| 2:C:338:LYS:HB2  | 2:C:386:PHE:CE2  | 2.49                     | 0.48              |
| 2:D:697:GLU:HG2  | 2:D:701:ARG:HE   | 1.79                     | 0.48              |
| 1:E:23:THR:HB    | 1:E:279:ALA:H    | 1.77                     | 0.48              |
| 1:F:187:THR:HG23 | 1:F:315:MET:HE2  | 1.96                     | 0.48              |
| 1:F:360:GLU:OE1  | 1:F:372:ALA:N    | 2.47                     | 0.48              |
| 2:G:54:GLY:HA2   | 2:G:102:ILE:HD12 | 1.96                     | 0.48              |
| 1:A:102:SER:O    | 1:A:106:VAL:HG23 | 2.13                     | 0.48              |
| 1:A:289:ARG:HE   | 1:A:293:LEU:HD23 | 1.78                     | 0.48              |
| 1:A:319:PRO:HG2  | 1:A:342:MET:HE1  | 1.96                     | 0.48              |
| 1:B:234:TYR:CE2  | 2:C:349:LEU:HB3  | 2.48                     | 0.48              |
| 2:C:240:THR:OG1  | 2:C:244:TYR:HB2  | 2.13                     | 0.48              |
| 2:D:399:ASN:HB3  | 2:D:402:LEU:HB3  | 1.95                     | 0.48              |
| 2:G:393:ILE:HG13 | 2:G:421:ALA:HB3  | 1.95                     | 0.48              |
| 1:A:177:GLU:O    | 1:A:181:GLY:N    | 2.30                     | 0.47              |
| 1:B:70:MET:HA    | 1:B:133:PRO:HG3  | 1.94                     | 0.47              |
| 2:C:250:ILE:HA   | 2:C:253:VAL:HG12 | 1.96                     | 0.47              |
| 2:C:686:GLY:HA3  | 2:C:688:ARG:HH12 | 1.77                     | 0.47              |
| 1:E:315:MET:SD   | 1:E:315:MET:N    | 2.86                     | 0.47              |
| 1:F:16:ALA:HA    | 1:F:300:TYR:HA   | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:610:GLN:H    | 2:G:612:ARG:NH1  | 2.12                     | 0.47              |
| 2:H:300:GLY:HA3  | 2:H:474:VAL:HG11 | 1.96                     | 0.47              |
| 2:H:406:MET:HA   | 2:H:409:GLU:HG2  | 1.94                     | 0.47              |
| 2:H:697:GLU:HG2  | 2:H:701:ARG:HE   | 1.78                     | 0.47              |
| 2:C:245:PRO:HD3  | 2:C:281:GLN:HE21 | 1.79                     | 0.47              |
| 2:C:692:CYS:HB3  | 2:C:695:LEU:HB2  | 1.96                     | 0.47              |
| 2:D:628:ASN:OD1  | 2:D:632:ARG:NH2  | 2.47                     | 0.47              |
| 2:D:659:LEU:HD13 | 2:D:665:TYR:CD2  | 2.49                     | 0.47              |
| 1:E:113:LEU:HD21 | 1:E:286:THR:HB   | 1.96                     | 0.47              |
| 2:G:29:ASN:HB2   | 2:G:66:ILE:HA    | 1.94                     | 0.47              |
| 2:G:462:HIS:NE2  | 2:G:464:GLY:O    | 2.47                     | 0.47              |
| 2:G:686:GLY:HA3  | 2:G:688:ARG:HH12 | 1.77                     | 0.47              |
| 2:H:420:PHE:CE1  | 2:H:422:SER:HB3  | 2.49                     | 0.47              |
| 2:C:117:LEU:HD11 | 2:C:137:GLY:H    | 1.78                     | 0.47              |
| 1:E:87:ASN:HB3   | 1:E:90:THR:HG23  | 1.96                     | 0.47              |
| 1:E:348:ALA:HA   | 1:E:351:LEU:HB2  | 1.96                     | 0.47              |
| 1:F:52:SER:O     | 1:F:53:GLU:HG3   | 2.14                     | 0.47              |
| 2:H:27:LYS:O     | 2:H:61:LYS:NZ    | 2.43                     | 0.47              |
| 1:A:9:THR:HA     | 1:A:114:MET:HE1  | 1.96                     | 0.47              |
| 1:A:325:LEU:HA   | 1:A:328:GLU:HG2  | 1.96                     | 0.47              |
| 2:C:313:ILE:HG13 | 2:C:393:ILE:HG23 | 1.95                     | 0.47              |
| 2:D:624:MET:O    | 2:D:628:ASN:N    | 2.25                     | 0.47              |
| 1:E:30:THR:OG1   | 1:E:242:ASN:ND2  | 2.47                     | 0.47              |
| 1:E:367:LEU:HD23 | 1:E:369:ARG:HE   | 1.79                     | 0.47              |
| 1:F:25:PHE:CD1   | 1:F:278:GLY:HA3  | 2.48                     | 0.47              |
| 2:G:238:HIS:O    | 2:G:241:GLN:NE2  | 2.48                     | 0.47              |
| 2:G:311:VAL:C    | 2:G:389:ARG:HD2  | 2.40                     | 0.47              |
| 2:G:536:LEU:HB3  | 2:G:541:ILE:HD13 | 1.96                     | 0.47              |
| 2:H:394:GLU:CD   | 2:H:403:LYS:HZ2  | 2.21                     | 0.47              |
| 1:B:97:ARG:HH12  | 1:B:100:ALA:HB3  | 1.79                     | 0.47              |
| 2:C:33:ALA:O     | 2:C:37:SER:N     | 2.46                     | 0.47              |
| 1:F:122:ILE:HG12 | 1:F:283:ILE:HG23 | 1.96                     | 0.47              |
| 2:G:281:GLN:OE1  | 2:G:281:GLN:N    | 2.48                     | 0.47              |
| 2:G:316:GLY:N    | 2:G:339:ASP:OD2  | 2.48                     | 0.47              |
| 2:G:400:LEU:HD13 | 2:G:427:LEU:HG   | 1.96                     | 0.47              |
| 2:G:577:ARG:HH22 | 2:G:584:TYR:HB2  | 1.79                     | 0.47              |
| 2:H:528:PHE:HE1  | 2:H:655:PHE:HA   | 1.79                     | 0.47              |
| 2:H:551:LEU:HB3  | 2:H:559:PHE:CD2  | 2.50                     | 0.47              |
| 2:H:552:GLU:OE2  | 2:H:560:SER:N    | 2.48                     | 0.47              |
| 1:A:97:ARG:O     | 1:A:101:THR:OG1  | 2.24                     | 0.47              |
| 1:A:285:MET:HE1  | 1:A:290:ALA:N    | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:9:THR:HA     | 1:B:114:MET:SD   | 2.53                     | 0.47              |
| 1:B:285:MET:HE1  | 1:B:290:ALA:N    | 2.30                     | 0.47              |
| 2:C:143:LEU:HD12 | 2:C:285:LEU:HB3  | 1.95                     | 0.47              |
| 1:E:211:GLN:C    | 1:E:213:ALA:H    | 2.22                     | 0.47              |
| 1:F:298:LEU:HD21 | 1:F:407:HIS:CE1  | 2.49                     | 0.47              |
| 2:H:540:GLY:HA2  | 2:H:578:LYS:NZ   | 2.30                     | 0.47              |
| 2:H:646:ASP:O    | 2:H:650:VAL:HG12 | 2.14                     | 0.47              |
| 1:A:140:LEU:HD12 | 1:A:143:VAL:HG21 | 1.96                     | 0.47              |
| 1:A:409:LEU:HA   | 1:A:412:ARG:HB2  | 1.97                     | 0.47              |
| 1:B:15:ILE:HD12  | 1:B:113:LEU:CD1  | 2.45                     | 0.47              |
| 1:B:23:THR:HB    | 1:B:279:ALA:H    | 1.80                     | 0.47              |
| 2:C:367:ALA:O    | 2:C:370:ARG:HB2  | 2.15                     | 0.47              |
| 2:D:71:ILE:HA    | 2:D:74:ILE:HD13  | 1.97                     | 0.47              |
| 2:D:114:GLY:HA2  | 2:D:138:LEU:HD13 | 1.96                     | 0.47              |
| 2:D:356:LEU:C    | 2:D:358:GLY:H    | 2.23                     | 0.47              |
| 1:E:191:MET:SD   | 1:E:314:ASP:HA   | 2.55                     | 0.47              |
| 2:G:65:PHE:CD2   | 2:G:66:ILE:HG22  | 2.50                     | 0.47              |
| 2:H:485:ILE:HG23 | 2:H:644:ASP:HB3  | 1.97                     | 0.47              |
| 2:H:501:PRO:HA   | 2:H:504:ASN:HB3  | 1.97                     | 0.47              |
| 2:H:573:ASP:O    | 2:H:579:ASN:ND2  | 2.47                     | 0.47              |
| 2:C:613:ILE:HD12 | 2:C:617:GLN:HB2  | 1.97                     | 0.47              |
| 2:D:153:GLN:C    | 2:D:156:PRO:HD2  | 2.40                     | 0.47              |
| 1:E:9:THR:HG22   | 1:E:13:ASP:H     | 1.78                     | 0.47              |
| 1:E:61:GLN:HB2   | 1:E:91:ASP:HB2   | 1.97                     | 0.47              |
| 1:E:67:VAL:HG23  | 1:E:395:ALA:HB2  | 1.97                     | 0.47              |
| 2:H:462:HIS:NE2  | 2:H:464:GLY:O    | 2.48                     | 0.47              |
| 1:A:313:GLN:O    | 1:A:314:ASP:C    | 2.56                     | 0.47              |
| 1:B:234:TYR:HD2  | 2:C:350:LYS:HA   | 1.80                     | 0.47              |
| 2:D:126:ARG:HG3  | 2:D:185:VAL:HA   | 1.96                     | 0.47              |
| 1:E:42:LYS:HG3   | 1:E:80:ILE:HD13  | 1.96                     | 0.47              |
| 1:F:327:LEU:O    | 1:F:331:GLY:N    | 2.48                     | 0.47              |
| 2:H:114:GLY:H    | 2:H:139:PRO:HD2  | 1.80                     | 0.47              |
| 1:B:44:VAL:HG13  | 1:B:45:VAL:HG13  | 1.97                     | 0.47              |
| 1:B:323:THR:HB   | 1:B:373:THR:HG21 | 1.97                     | 0.47              |
| 2:C:504:ASN:C    | 2:C:508:ARG:HE   | 2.22                     | 0.47              |
| 1:E:81:VAL:HG22  | 1:E:86:MET:HG2   | 1.97                     | 0.47              |
| 1:E:225:GLU:OE2  | 1:E:407:HIS:ND1  | 2.48                     | 0.47              |
| 1:F:287:GLU:HB3  | 1:F:300:TYR:HE1  | 1.80                     | 0.47              |
| 2:H:40:ARG:HA    | 2:H:43:ILE:HG22  | 1.97                     | 0.47              |
| 1:A:231:ILE:HB   | 1:A:233:PRO:HD2  | 1.97                     | 0.46              |
| 2:D:66:ILE:HG23  | 2:D:116:GLY:HA2  | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:520:ASP:OD2  | 2:D:531:GLY:HA3  | 2.15                     | 0.46              |
| 2:H:281:GLN:OE1  | 2:H:281:GLN:N    | 2.48                     | 0.46              |
| 2:H:343:GLN:HA   | 2:H:346:ASN:HB3  | 1.96                     | 0.46              |
| 1:A:22:ARG:N     | 1:A:225:GLU:O    | 2.40                     | 0.46              |
| 1:A:234:TYR:CE1  | 2:D:349:LEU:HB3  | 2.50                     | 0.46              |
| 1:A:339:LEU:N    | 1:A:380:LYS:HD2  | 2.28                     | 0.46              |
| 1:A:408:GLU:O    | 1:A:412:ARG:N    | 2.38                     | 0.46              |
| 1:B:67:VAL:HG12  | 1:B:68:VAL:H     | 1.80                     | 0.46              |
| 2:C:214:VAL:HG13 | 2:C:216:GLU:H    | 1.80                     | 0.46              |
| 2:D:65:PHE:HB2   | 2:D:109:HIS:H    | 1.80                     | 0.46              |
| 2:D:311:VAL:C    | 2:D:389:ARG:HD2  | 2.41                     | 0.46              |
| 1:E:63:VAL:HA    | 1:E:93:TYR:O     | 2.15                     | 0.46              |
| 1:E:299:GLY:HA3  | 1:E:406:LEU:HD12 | 1.96                     | 0.46              |
| 1:A:258:PRO:HB3  | 1:A:265:GLY:HA3  | 1.97                     | 0.46              |
| 1:A:307:THR:HG21 | 1:A:321:TRP:HB3  | 1.97                     | 0.46              |
| 1:B:397:THR:HG22 | 1:B:400:ARG:HH21 | 1.79                     | 0.46              |
| 2:C:462:HIS:NE2  | 2:C:464:GLY:O    | 2.49                     | 0.46              |
| 2:C:494:TYR:CG   | 2:C:639:ILE:HD11 | 2.50                     | 0.46              |
| 2:D:370:ARG:HA   | 2:D:373:GLN:HE22 | 1.79                     | 0.46              |
| 2:D:392:ILE:HG13 | 2:D:420:PHE:HA   | 1.97                     | 0.46              |
| 2:D:429:ILE:HB   | 2:D:462:HIS:HB3  | 1.96                     | 0.46              |
| 2:D:451:VAL:O    | 2:D:482:LYS:NZ   | 2.49                     | 0.46              |
| 1:F:30:THR:HG22  | 1:F:31:ALA:N     | 2.23                     | 0.46              |
| 2:H:338:LYS:HA   | 2:H:380:THR:O    | 2.14                     | 0.46              |
| 1:A:61:GLN:HG2   | 1:A:91:ASP:O     | 2.16                     | 0.46              |
| 1:A:185:GLY:HA3  | 1:A:260:PHE:CZ   | 2.50                     | 0.46              |
| 2:D:40:ARG:HA    | 2:D:43:ILE:HG22  | 1.97                     | 0.46              |
| 1:E:97:ARG:HD2   | 1:E:104:GLN:HB2  | 1.97                     | 0.46              |
| 1:F:36:PRO:HB2   | 1:F:38:VAL:HG12  | 1.96                     | 0.46              |
| 1:F:423:ALA:HB3  | 1:F:427:LEU:HB2  | 1.98                     | 0.46              |
| 2:G:414:CYS:SG   | 2:G:415:ALA:N    | 2.84                     | 0.46              |
| 1:B:373:THR:OG1  | 1:B:374:GLY:N    | 2.49                     | 0.46              |
| 1:F:400:ARG:NH2  | 1:F:401:MET:HE3  | 2.30                     | 0.46              |
| 2:G:180:LEU:HD22 | 2:G:188:VAL:HG22 | 1.96                     | 0.46              |
| 1:A:56:ALA:O     | 1:A:59:ILE:HG22  | 2.15                     | 0.46              |
| 1:A:332:LEU:HD12 | 1:A:432:VAL:HG11 | 1.98                     | 0.46              |
| 1:B:139:LYS:O    | 1:B:143:VAL:HG23 | 2.15                     | 0.46              |
| 1:B:423:ALA:N    | 1:B:427:LEU:O    | 2.46                     | 0.46              |
| 2:C:661:GLY:O    | 2:C:665:TYR:N    | 2.42                     | 0.46              |
| 2:D:449:SER:HB3  | 2:D:539:VAL:HG23 | 1.98                     | 0.46              |
| 2:G:583:PHE:HB3  | 2:G:601:ILE:HG21 | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:304:PRO:O    | 2:H:468:GLN:HG3  | 2.15                     | 0.46              |
| 2:H:398:GLU:HA   | 2:H:403:LYS:NZ   | 2.31                     | 0.46              |
| 2:C:583:PHE:HB2  | 2:C:601:ILE:HD13 | 1.97                     | 0.46              |
| 2:D:27:LYS:HB3   | 2:D:63:ASP:OD2   | 2.15                     | 0.46              |
| 2:D:675:VAL:O    | 2:D:679:GLN:N    | 2.40                     | 0.46              |
| 1:E:197:ILE:HG21 | 1:E:348:ALA:HB2  | 1.97                     | 0.46              |
| 1:E:361:ARG:O    | 1:E:365:GLU:HG3  | 2.16                     | 0.46              |
| 1:F:383:VAL:HG21 | 1:F:412:ARG:HH22 | 1.80                     | 0.46              |
| 2:G:523:LEU:O    | 2:G:528:PHE:HB2  | 2.15                     | 0.46              |
| 2:G:548:ILE:HG13 | 2:G:549:PRO:HD3  | 1.98                     | 0.46              |
| 2:G:574:ARG:NH2  | 2:G:598:ASP:OD2  | 2.48                     | 0.46              |
| 2:H:419:ILE:HD12 | 2:H:469:THR:HG23 | 1.98                     | 0.46              |
| 2:H:460:ILE:HD13 | 2:H:493:PHE:CE1  | 2.51                     | 0.46              |
| 2:H:495:VAL:HG13 | 2:H:653:ILE:HD11 | 1.97                     | 0.46              |
| 1:A:51:ARG:O     | 2:D:384:ARG:HG2  | 2.16                     | 0.46              |
| 1:B:221:LYS:HB2  | 1:B:411:ARG:NH2  | 2.31                     | 0.46              |
| 1:B:316:LEU:HD22 | 1:B:422:CYS:SG   | 2.56                     | 0.46              |
| 2:C:531:GLY:H    | 2:C:534:GLN:HE21 | 1.63                     | 0.46              |
| 2:C:666:ILE:O    | 2:C:670:GLY:N    | 2.49                     | 0.46              |
| 2:D:552:GLU:OE2  | 2:D:560:SER:N    | 2.48                     | 0.46              |
| 1:E:22:ARG:HA    | 1:E:280:ALA:HA   | 1.98                     | 0.46              |
| 1:F:76:ILE:O     | 1:F:80:ILE:HG12  | 2.16                     | 0.46              |
| 1:F:339:LEU:HB3  | 1:F:409:LEU:HD11 | 1.96                     | 0.46              |
| 1:B:344:GLU:O    | 1:B:387:SER:HB2  | 2.16                     | 0.46              |
| 2:C:65:PHE:HD2   | 2:C:66:ILE:HG22  | 1.81                     | 0.46              |
| 2:C:673:GLU:O    | 2:C:677:ILE:HG12 | 2.16                     | 0.46              |
| 2:D:497:ARG:HH21 | 2:D:558:ARG:HH22 | 1.64                     | 0.46              |
| 1:E:188:ALA:HA   | 1:E:191:MET:HE3  | 1.97                     | 0.46              |
| 2:G:283:GLN:HA   | 2:G:286:ARG:HB2  | 1.97                     | 0.46              |
| 2:G:426:SER:HB3  | 2:G:547:ILE:HG12 | 1.98                     | 0.46              |
| 2:H:308:LEU:HD23 | 2:H:390:ASP:HB3  | 1.97                     | 0.46              |
| 1:A:318:GLY:O    | 1:A:322:SER:N    | 2.45                     | 0.46              |
| 1:B:231:ILE:HG22 | 1:B:233:PRO:HD2  | 1.98                     | 0.46              |
| 2:C:569:ILE:HG22 | 2:C:575:LYS:HZ3  | 1.81                     | 0.46              |
| 2:C:698:MET:HA   | 2:C:703:GLU:HB2  | 1.97                     | 0.46              |
| 2:D:79:THR:C     | 2:D:278:MET:HE3  | 2.41                     | 0.46              |
| 2:D:313:ILE:CD1  | 2:D:393:ILE:HG23 | 2.46                     | 0.46              |
| 2:D:555:TYR:HB3  | 2:D:558:ARG:HH21 | 1.81                     | 0.46              |
| 2:D:625:LEU:HD21 | 2:D:689:PHE:CE1  | 2.51                     | 0.46              |
| 1:E:186:ASP:OD1  | 1:E:187:THR:N    | 2.50                     | 0.46              |
| 1:E:195:TYR:HE1  | 1:E:314:ASP:OD2  | 1.99                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:343:HIS:HB2  | 1:E:421:ALA:HA   | 1.98                     | 0.46              |
| 2:G:685:TYR:HB3  | 2:G:688:ARG:HH22 | 1.82                     | 0.46              |
| 1:A:9:THR:HG23   | 1:A:11:GLN:N     | 2.29                     | 0.45              |
| 1:A:199:ARG:HA   | 1:A:202:GLN:HG2  | 1.97                     | 0.45              |
| 1:B:41:GLY:O     | 1:B:45:VAL:HG22  | 2.16                     | 0.45              |
| 2:D:32:LYS:HE2   | 2:D:35:PHE:CE2   | 2.51                     | 0.45              |
| 2:D:313:ILE:HD11 | 2:D:395:ALA:HB2  | 1.97                     | 0.45              |
| 2:D:584:TYR:CD1  | 2:D:597:VAL:HG12 | 2.51                     | 0.45              |
| 1:E:340:ILE:HD12 | 1:E:342:MET:HE3  | 1.98                     | 0.45              |
| 1:F:361:ARG:O    | 1:F:365:GLU:HG3  | 2.16                     | 0.45              |
| 2:G:547:ILE:O    | 2:G:550:VAL:HG12 | 2.16                     | 0.45              |
| 2:H:601:ILE:O    | 2:H:605:ILE:HG12 | 2.16                     | 0.45              |
| 2:C:311:VAL:HG23 | 2:C:391:LEU:HB3  | 1.97                     | 0.45              |
| 2:C:672:GLY:O    | 2:C:676:ALA:N    | 2.42                     | 0.45              |
| 2:D:275:GLU:HG2  | 2:D:276:LEU:N    | 2.32                     | 0.45              |
| 2:D:454:MET:O    | 2:D:482:LYS:NZ   | 2.29                     | 0.45              |
| 2:G:10:ASN:HB3   | 2:G:18:VAL:HG13  | 1.96                     | 0.45              |
| 2:G:166:GLU:O    | 2:G:170:THR:N    | 2.43                     | 0.45              |
| 2:G:644:ASP:HA   | 2:G:647:ILE:HG22 | 1.98                     | 0.45              |
| 2:H:494:TYR:OH   | 2:H:645:GLY:O    | 2.27                     | 0.45              |
| 2:C:151:GLY:HA2  | 2:C:154:ARG:HD2  | 1.99                     | 0.45              |
| 1:E:42:LYS:HG2   | 1:E:84:THR:HG23  | 1.98                     | 0.45              |
| 1:E:361:ARG:O    | 1:E:364:ARG:HG3  | 2.16                     | 0.45              |
| 1:F:139:LYS:O    | 1:F:143:VAL:HG23 | 2.17                     | 0.45              |
| 1:F:183:ARG:NH2  | 1:F:186:ASP:OD1  | 2.40                     | 0.45              |
| 2:H:311:VAL:C    | 2:H:389:ARG:HD2  | 2.40                     | 0.45              |
| 1:A:232:PRO:HB3  | 2:D:353:TRP:CH2  | 2.51                     | 0.45              |
| 1:A:239:VAL:HG13 | 1:A:240:GLU:HG3  | 1.99                     | 0.45              |
| 1:B:4:VAL:HA     | 1:B:329:ARG:HA   | 1.99                     | 0.45              |
| 2:D:157:ARG:NH1  | 2:D:158:LEU:HB2  | 2.31                     | 0.45              |
| 2:D:440:GLU:HA   | 2:D:465:THR:HA   | 1.99                     | 0.45              |
| 2:G:28:MET:HE2   | 2:G:30:THR:HG22  | 1.98                     | 0.45              |
| 2:G:317:GLY:H    | 2:G:348:ALA:HB2  | 1.82                     | 0.45              |
| 2:G:573:ASP:OD1  | 2:G:573:ASP:N    | 2.49                     | 0.45              |
| 2:H:447:PHE:HD2  | 2:H:451:VAL:HG11 | 1.80                     | 0.45              |
| 1:A:89:HIS:HA    | 1:B:308:ALA:HB3  | 1.99                     | 0.45              |
| 1:B:400:ARG:O    | 1:B:403:THR:OG1  | 2.33                     | 0.45              |
| 1:B:400:ARG:NH1  | 1:B:401:MET:HE3  | 2.31                     | 0.45              |
| 2:C:10:ASN:HB2   | 2:C:18:VAL:HG13  | 1.99                     | 0.45              |
| 2:D:656:PRO:HB3  | 2:D:658:PHE:CZ   | 2.51                     | 0.45              |
| 2:G:386:PHE:HD1  | 2:G:389:ARG:HG3  | 1.82                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:313:ILE:HD12 | 2:H:324:ALA:HB2  | 1.99                     | 0.45              |
| 2:H:596:GLN:NE2  | 2:H:597:VAL:HG22 | 2.31                     | 0.45              |
| 1:A:29:ALA:HB2   | 1:B:149:LYS:HZ1  | 1.82                     | 0.45              |
| 2:C:200:GLU:O    | 2:C:203:LYS:HG2  | 2.17                     | 0.45              |
| 2:D:30:THR:OG1   | 2:D:32:LYS:NZ    | 2.48                     | 0.45              |
| 1:E:406:LEU:HD21 | 1:E:433:LEU:HD22 | 1.98                     | 0.45              |
| 1:F:212:ARG:HH21 | 1:F:383:VAL:HA   | 1.81                     | 0.45              |
| 2:G:502:TYR:CE1  | 2:G:622:CYS:HB3  | 2.51                     | 0.45              |
| 2:H:610:GLN:HG3  | 2:H:611:GLY:H    | 1.82                     | 0.45              |
| 1:A:25:PHE:HA    | 1:A:277:ASP:O    | 2.17                     | 0.45              |
| 1:A:317:LEU:HD13 | 1:A:356:LEU:HD11 | 1.99                     | 0.45              |
| 1:B:342:MET:HA   | 1:B:420:THR:O    | 2.17                     | 0.45              |
| 2:C:8:THR:HB     | 2:C:20:THR:OG1   | 2.16                     | 0.45              |
| 2:C:91:GLN:HE21  | 2:C:266:TYR:HD1  | 1.65                     | 0.45              |
| 2:C:497:ARG:HH12 | 2:C:632:ARG:HG3  | 1.82                     | 0.45              |
| 1:E:332:LEU:HD12 | 1:E:432:VAL:HG11 | 1.97                     | 0.45              |
| 2:G:156:PRO:HB2  | 2:G:258:LEU:HD21 | 1.97                     | 0.45              |
| 1:A:119:ARG:NH2  | 1:A:292:GLU:OE2  | 2.49                     | 0.45              |
| 2:C:124:HIS:CD2  | 2:C:206:ARG:HH22 | 2.35                     | 0.45              |
| 2:C:499:LEU:HD13 | 2:C:626:MET:HE1  | 1.99                     | 0.45              |
| 2:D:533:ILE:HD12 | 2:D:583:PHE:HB3  | 1.98                     | 0.45              |
| 1:E:25:PHE:HE2   | 1:E:400:ARG:HD3  | 1.81                     | 0.45              |
| 1:E:311:VAL:HG23 | 1:E:315:MET:HG2  | 1.97                     | 0.45              |
| 2:H:156:PRO:HB2  | 2:H:258:LEU:HD21 | 1.99                     | 0.45              |
| 2:D:449:SER:HB2  | 2:D:450:PRO:HD2  | 1.99                     | 0.45              |
| 2:H:15:ASN:HD21  | 2:H:53:ARG:NH1   | 2.14                     | 0.45              |
| 2:H:114:GLY:N    | 2:H:139:PRO:HD2  | 2.32                     | 0.45              |
| 2:H:642:VAL:HB   | 2:H:706:TRP:HE1  | 1.81                     | 0.45              |
| 1:A:231:ILE:HG13 | 1:A:234:TYR:N    | 2.30                     | 0.45              |
| 2:D:32:LYS:HE2   | 2:D:35:PHE:HE2   | 1.81                     | 0.45              |
| 2:D:53:ARG:HH21  | 2:D:203:LYS:HD2  | 1.81                     | 0.45              |
| 2:D:398:GLU:HA   | 2:D:403:LYS:NZ   | 2.31                     | 0.45              |
| 1:F:192:ALA:HB2  | 1:F:348:ALA:HB1  | 1.99                     | 0.45              |
| 1:F:361:ARG:O    | 1:F:364:ARG:HG3  | 2.17                     | 0.45              |
| 2:G:584:TYR:HE1  | 2:G:597:VAL:HG12 | 1.82                     | 0.45              |
| 1:A:243:ASN:ND2  | 1:A:274:PRO:HG2  | 2.32                     | 0.44              |
| 1:B:159:LEU:HD23 | 1:B:162:ARG:HH22 | 1.81                     | 0.44              |
| 1:B:274:PRO:HD2  | 1:B:391:GLY:HA2  | 1.98                     | 0.44              |
| 2:D:150:GLY:O    | 2:D:154:ARG:HG2  | 2.17                     | 0.44              |
| 2:D:206:ARG:HH21 | 2:D:210:ARG:H    | 1.65                     | 0.44              |
| 1:F:217:TRP:HH2  | 1:F:226:VAL:HG11 | 1.81                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:350:LYS:NZ   | 2:G:354:ASP:OD2  | 2.43                     | 0.44              |
| 2:H:352:SER:HA   | 2:H:355:GLN:HE21 | 1.82                     | 0.44              |
| 2:H:674:VAL:HG23 | 2:H:677:ILE:HD11 | 1.99                     | 0.44              |
| 1:A:117:THR:HG1  | 1:B:304:TYR:HH   | 1.65                     | 0.44              |
| 1:A:137:SER:HA   | 1:A:171:VAL:HG23 | 1.98                     | 0.44              |
| 1:A:309:ILE:HA   | 1:B:89:HIS:CE1   | 2.52                     | 0.44              |
| 1:A:327:LEU:HD12 | 1:A:333:THR:N    | 2.32                     | 0.44              |
| 1:B:392:HIS:NE2  | 1:B:394:PHE:HA   | 2.33                     | 0.44              |
| 2:C:249:ARG:NH2  | 2:C:275:GLU:OE2  | 2.45                     | 0.44              |
| 2:C:278:MET:SD   | 2:C:278:MET:N    | 2.90                     | 0.44              |
| 2:D:656:PRO:HB3  | 2:D:658:PHE:CE2  | 2.52                     | 0.44              |
| 2:D:675:VAL:HG22 | 2:D:695:LEU:HD21 | 2.00                     | 0.44              |
| 1:E:25:PHE:CD1   | 1:E:278:GLY:HA3  | 2.52                     | 0.44              |
| 1:E:203:ASP:O    | 1:E:253:TYR:OH   | 2.29                     | 0.44              |
| 2:H:275:GLU:O    | 2:H:279:THR:OG1  | 2.36                     | 0.44              |
| 2:H:502:TYR:CG   | 2:H:626:MET:HE3  | 2.53                     | 0.44              |
| 2:H:613:ILE:HG21 | 2:H:621:ARG:HH21 | 1.83                     | 0.44              |
| 2:C:220:ALA:HB1  | 2:C:258:LEU:HD13 | 1.98                     | 0.44              |
| 2:D:39:VAL:HA    | 2:D:42:ILE:HB    | 1.98                     | 0.44              |
| 2:H:380:THR:OG1  | 2:H:382:ASP:OD1  | 2.36                     | 0.44              |
| 2:C:602:TYR:HB2  | 2:C:603:PRO:HD3  | 1.98                     | 0.44              |
| 2:C:682:ALA:HB2  | 2:C:689:PHE:HB2  | 2.00                     | 0.44              |
| 1:E:339:LEU:HB3  | 1:E:409:LEU:HD11 | 2.00                     | 0.44              |
| 1:F:342:MET:SD   | 1:F:350:THR:HG23 | 2.57                     | 0.44              |
| 2:G:84:GLU:HG3   | 2:G:274:GLY:HA3  | 2.00                     | 0.44              |
| 2:H:528:PHE:CE1  | 2:H:656:PRO:HD3  | 2.53                     | 0.44              |
| 2:H:613:ILE:HG12 | 2:H:621:ARG:HH22 | 1.82                     | 0.44              |
| 2:H:633:CYS:SG   | 2:H:634:VAL:N    | 2.90                     | 0.44              |
| 2:H:691:PRO:HB2  | 2:H:696:VAL:HG23 | 2.00                     | 0.44              |
| 1:A:42:LYS:HZ1   | 1:A:83:GLY:HA3   | 1.82                     | 0.44              |
| 1:E:32:PHE:HD2   | 1:E:277:ASP:HB2  | 1.82                     | 0.44              |
| 1:E:305:ALA:N    | 1:E:430:ALA:O    | 2.48                     | 0.44              |
| 1:E:409:LEU:O    | 1:E:413:GLY:N    | 2.51                     | 0.44              |
| 1:F:199:ARG:NH2  | 1:F:253:TYR:O    | 2.50                     | 0.44              |
| 2:G:304:PRO:HA   | 2:G:305:PRO:HD3  | 1.84                     | 0.44              |
| 2:H:446:HIS:HB3  | 2:H:458:GLU:HB2  | 1.99                     | 0.44              |
| 1:A:203:ASP:O    | 1:A:253:TYR:OH   | 2.19                     | 0.44              |
| 1:A:342:MET:HG2  | 1:A:350:THR:OG1  | 2.18                     | 0.44              |
| 2:D:299:PRO:HA   | 2:D:478:LYS:HE3  | 2.00                     | 0.44              |
| 2:D:456:LEU:HD23 | 2:D:483:THR:HB   | 1.99                     | 0.44              |
| 2:H:87:ALA:O     | 2:H:91:GLN:HG2   | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:173:GLN:HB2  | 2:H:175:ARG:NH1  | 2.33                     | 0.44              |
| 1:A:117:THR:HG23 | 1:B:329:ARG:NH2  | 2.32                     | 0.44              |
| 1:A:311:VAL:HG13 | 1:A:315:MET:HG2  | 1.99                     | 0.44              |
| 1:B:360:GLU:O    | 1:B:364:ARG:HG2  | 2.17                     | 0.44              |
| 2:C:113:LEU:HD12 | 2:C:139:PRO:HG3  | 2.00                     | 0.44              |
| 2:D:336:ARG:HB2  | 2:D:389:ARG:NH2  | 2.32                     | 0.44              |
| 2:D:438:ARG:HD2  | 2:D:441:GLN:OE1  | 2.18                     | 0.44              |
| 2:D:516:VAL:HG11 | 2:D:533:ILE:HD13 | 1.99                     | 0.44              |
| 2:D:528:PHE:CZ   | 2:D:623:VAL:HG12 | 2.52                     | 0.44              |
| 1:E:217:TRP:CE3  | 1:E:240:GLU:HG2  | 2.53                     | 0.44              |
| 2:G:474:VAL:HG13 | 2:G:484:PRO:HB2  | 2.00                     | 0.44              |
| 2:H:219:LEU:HD23 | 2:H:219:LEU:H    | 1.81                     | 0.44              |
| 1:A:17:ILE:HG23  | 1:A:298:LEU:O    | 2.17                     | 0.44              |
| 1:A:203:ASP:OD1  | 1:A:271:ASN:ND2  | 2.33                     | 0.44              |
| 1:B:104:GLN:O    | 1:B:104:GLN:NE2  | 2.51                     | 0.44              |
| 2:C:143:LEU:HD11 | 2:C:286:ARG:HA   | 2.00                     | 0.44              |
| 2:C:309:ASN:O    | 2:C:334:PRO:HD2  | 2.18                     | 0.44              |
| 2:D:7:PHE:HE2    | 2:D:35:PHE:HB3   | 1.83                     | 0.44              |
| 2:D:35:PHE:HA    | 2:D:38:GLN:HE21  | 1.83                     | 0.44              |
| 1:E:311:VAL:O    | 1:E:311:VAL:HG13 | 2.16                     | 0.44              |
| 1:F:22:ARG:HD3   | 1:F:400:ARG:HB2  | 1.99                     | 0.44              |
| 1:F:360:GLU:HA   | 1:F:372:ALA:HB2  | 1.99                     | 0.44              |
| 2:C:541:ILE:HG21 | 2:C:569:ILE:HG21 | 1.99                     | 0.44              |
| 2:D:166:GLU:O    | 2:D:170:THR:N    | 2.45                     | 0.44              |
| 2:D:639:ILE:HG21 | 2:D:645:GLY:N    | 2.33                     | 0.44              |
| 2:G:249:ARG:HH21 | 2:G:272:ALA:HA   | 1.83                     | 0.44              |
| 2:G:488:ARG:HA   | 2:G:488:ARG:HD2  | 1.85                     | 0.44              |
| 2:H:643:ARG:HH21 | 2:H:644:ASP:CG   | 2.26                     | 0.44              |
| 1:A:217:TRP:CZ3  | 1:A:240:GLU:HA   | 2.53                     | 0.43              |
| 1:B:244:ILE:HD11 | 1:B:390:TYR:CD1  | 2.53                     | 0.43              |
| 2:C:313:ILE:HG23 | 2:C:337:ILE:HD13 | 1.99                     | 0.43              |
| 2:C:336:ARG:HH12 | 2:C:385:GLY:HA3  | 1.83                     | 0.43              |
| 2:D:508:ARG:O    | 2:D:511:THR:HG22 | 2.18                     | 0.43              |
| 1:E:352:ALA:HA   | 1:E:355:GLN:HB3  | 2.00                     | 0.43              |
| 1:F:63:VAL:HA    | 1:F:93:TYR:O     | 2.17                     | 0.43              |
| 1:F:234:TYR:CZ   | 2:G:349:LEU:HD23 | 2.53                     | 0.43              |
| 2:G:524:VAL:HA   | 2:G:528:PHE:O    | 2.18                     | 0.43              |
| 2:H:199:VAL:O    | 2:H:203:LYS:HG2  | 2.18                     | 0.43              |
| 1:B:15:ILE:HG23  | 1:B:113:LEU:HD11 | 2.00                     | 0.43              |
| 1:B:146:ASP:O    | 1:B:150:ALA:N    | 2.51                     | 0.43              |
| 1:B:187:THR:O    | 1:B:190:GLN:HG3  | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:416:PHE:CD1  | 1:B:434:GLU:HA   | 2.53                     | 0.43              |
| 2:C:59:SER:HA    | 2:C:65:PHE:HA    | 2.00                     | 0.43              |
| 2:C:106:ALA:HB2  | 2:C:123:CYS:SG   | 2.59                     | 0.43              |
| 2:C:232:VAL:O    | 2:C:236:THR:OG1  | 2.34                     | 0.43              |
| 2:D:29:ASN:N     | 2:D:64:ASN:HD21  | 2.05                     | 0.43              |
| 1:F:66:GLN:HG2   | 1:F:76:ILE:HD13  | 2.01                     | 0.43              |
| 2:G:383:TYR:HA   | 2:G:386:PHE:HD2  | 1.83                     | 0.43              |
| 2:H:127:VAL:HG21 | 2:H:198:ALA:HB2  | 1.99                     | 0.43              |
| 2:H:244:TYR:CE1  | 2:H:658:PHE:HB3  | 2.53                     | 0.43              |
| 2:H:639:ILE:HG21 | 2:H:645:GLY:N    | 2.33                     | 0.43              |
| 1:A:108:ASN:HA   | 1:A:111:GLU:CD   | 2.43                     | 0.43              |
| 2:C:392:ILE:HG21 | 2:C:410:VAL:HG21 | 2.00                     | 0.43              |
| 2:C:492:GLY:HA3  | 2:C:551:LEU:HD11 | 1.99                     | 0.43              |
| 1:E:203:ASP:OD1  | 1:E:271:ASN:ND2  | 2.24                     | 0.43              |
| 2:G:639:ILE:HD13 | 2:G:645:GLY:HA2  | 2.01                     | 0.43              |
| 2:H:438:ARG:HD3  | 2:H:441:GLN:HB2  | 2.00                     | 0.43              |
| 2:H:643:ARG:NH2  | 2:H:644:ASP:OD1  | 2.51                     | 0.43              |
| 1:A:191:MET:HE3  | 1:A:314:ASP:HA   | 2.01                     | 0.43              |
| 1:A:343:HIS:CD2  | 1:A:345:ALA:HB2  | 2.52                     | 0.43              |
| 2:C:238:HIS:O    | 2:C:241:GLN:NE2  | 2.52                     | 0.43              |
| 2:C:494:TYR:CD1  | 2:C:639:ILE:HD11 | 2.53                     | 0.43              |
| 2:D:337:ILE:HG22 | 2:D:378:SER:O    | 2.18                     | 0.43              |
| 2:D:370:ARG:O    | 2:D:374:LEU:HD23 | 2.18                     | 0.43              |
| 2:D:610:GLN:HG3  | 2:D:611:GLY:H    | 1.83                     | 0.43              |
| 1:E:212:ARG:HB3  | 1:E:383:VAL:O    | 2.18                     | 0.43              |
| 2:G:404:GLN:HG2  | 2:G:435:HIS:CE1  | 2.54                     | 0.43              |
| 2:G:601:ILE:O    | 2:G:605:ILE:HG12 | 2.18                     | 0.43              |
| 2:H:222:PRO:HA   | 2:H:225:ARG:HG2  | 1.99                     | 0.43              |
| 2:H:311:VAL:HG12 | 2:H:335:VAL:HG23 | 2.00                     | 0.43              |
| 2:H:443:ILE:HG21 | 2:H:473:THR:OG1  | 2.18                     | 0.43              |
| 2:C:345:ILE:O    | 2:C:349:LEU:HD13 | 2.18                     | 0.43              |
| 2:C:574:ARG:HG3  | 2:C:582:GLY:HA2  | 1.99                     | 0.43              |
| 2:D:57:PHE:HD2   | 2:D:119:LEU:HD21 | 1.83                     | 0.43              |
| 2:D:319:MET:SD   | 2:D:319:MET:N    | 2.92                     | 0.43              |
| 1:E:95:VAL:HG11  | 1:E:108:ASN:ND2  | 2.31                     | 0.43              |
| 2:G:498:ILE:HA   | 2:G:629:GLU:HG2  | 2.00                     | 0.43              |
| 2:H:253:VAL:HG21 | 2:H:269:GLU:HB3  | 2.01                     | 0.43              |
| 1:B:87:ASN:O     | 1:B:90:THR:OG1   | 2.32                     | 0.43              |
| 2:C:344:GLY:HA2  | 2:C:347:HIS:HB2  | 2.00                     | 0.43              |
| 2:C:477:ALA:HB1  | 2:C:482:LYS:HB2  | 2.01                     | 0.43              |
| 2:D:159:ILE:HD11 | 2:D:182:LEU:HG   | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:127:ASP:OD2  | 1:E:394:PHE:N    | 2.51                     | 0.43              |
| 1:E:168:LEU:H    | 1:E:168:LEU:HD23 | 1.84                     | 0.43              |
| 1:F:141:ALA:O    | 1:F:145:VAL:HG23 | 2.19                     | 0.43              |
| 1:F:199:ARG:HH22 | 1:F:256:LEU:H    | 1.65                     | 0.43              |
| 2:H:310:SER:HB2  | 2:H:389:ARG:HA   | 2.01                     | 0.43              |
| 1:A:113:LEU:HD21 | 1:A:286:THR:HB   | 2.00                     | 0.43              |
| 2:C:675:VAL:O    | 2:C:678:MET:HG3  | 2.19                     | 0.43              |
| 1:E:360:GLU:HA   | 1:E:372:ALA:HB2  | 2.00                     | 0.43              |
| 2:G:338:LYS:HB2  | 2:G:386:PHE:CZ   | 2.53                     | 0.43              |
| 2:G:545:THR:O    | 2:G:548:ILE:HG12 | 2.18                     | 0.43              |
| 2:G:551:LEU:HB3  | 2:G:559:PHE:CD2  | 2.53                     | 0.43              |
| 1:A:206:ALA:HA   | 1:A:388:ILE:HG21 | 2.01                     | 0.43              |
| 1:B:129:SER:N    | 1:B:277:ASP:OD1  | 2.39                     | 0.43              |
| 2:C:569:ILE:HG22 | 2:C:575:LYS:NZ   | 2.33                     | 0.43              |
| 2:D:319:MET:O    | 2:D:323:ILE:HG12 | 2.19                     | 0.43              |
| 2:D:475:LYS:HB2  | 2:D:479:LYS:HZ3  | 1.84                     | 0.43              |
| 1:F:14:ARG:NH1   | 1:F:434:GLU:OE2  | 2.52                     | 0.43              |
| 2:H:523:LEU:HD13 | 2:H:619:ALA:HA   | 2.00                     | 0.43              |
| 1:A:188:ALA:HA   | 1:A:191:MET:SD   | 2.59                     | 0.43              |
| 1:A:286:THR:HG23 | 1:A:289:ARG:H    | 1.84                     | 0.43              |
| 1:B:407:HIS:O    | 1:B:411:ARG:N    | 2.45                     | 0.43              |
| 2:D:61:LYS:HG3   | 2:D:63:ASP:H     | 1.83                     | 0.43              |
| 2:D:148:GLY:HA2  | 2:D:273:PHE:CE2  | 2.53                     | 0.43              |
| 2:D:246:ALA:HA   | 2:D:249:ARG:HB2  | 2.01                     | 0.43              |
| 2:D:394:GLU:CD   | 2:D:403:LYS:HZ2  | 2.26                     | 0.43              |
| 1:E:317:LEU:HD22 | 1:E:356:LEU:HD12 | 2.01                     | 0.43              |
| 1:A:61:GLN:NE2   | 1:A:63:VAL:HG23  | 2.31                     | 0.43              |
| 1:A:101:THR:HB   | 1:A:395:ALA:HB1  | 2.01                     | 0.43              |
| 2:C:91:GLN:NE2   | 2:C:266:TYR:O    | 2.48                     | 0.43              |
| 2:C:641:SER:HB3  | 2:C:643:ARG:HG3  | 2.00                     | 0.43              |
| 2:D:219:LEU:H    | 2:D:219:LEU:HD23 | 1.84                     | 0.43              |
| 2:D:304:PRO:O    | 2:D:468:GLN:HG3  | 2.19                     | 0.43              |
| 2:D:575:LYS:HB2  | 2:D:579:ASN:HB2  | 2.00                     | 0.43              |
| 1:F:217:TRP:CE3  | 1:F:240:GLU:HG2  | 2.54                     | 0.43              |
| 2:H:529:PRO:HD2  | 2:H:654:GLY:O    | 2.18                     | 0.43              |
| 1:B:299:GLY:HA3  | 1:B:435:ALA:HA   | 2.01                     | 0.42              |
| 1:B:327:LEU:HD12 | 1:B:333:THR:N    | 2.34                     | 0.42              |
| 2:C:510:LEU:HA   | 2:C:514:GLU:HB2  | 2.00                     | 0.42              |
| 2:D:87:ALA:O     | 2:D:91:GLN:HG2   | 2.19                     | 0.42              |
| 1:E:183:ARG:NH2  | 1:E:186:ASP:HB3  | 2.34                     | 0.42              |
| 2:G:236:THR:HA   | 2:G:239:LYS:HG2  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:240:THR:OG1  | 2:H:244:TYR:HB2  | 2.19                     | 0.42              |
| 1:A:309:ILE:HG12 | 1:A:426:GLY:O    | 2.18                     | 0.42              |
| 1:A:421:ALA:N    | 1:A:429:ALA:O    | 2.49                     | 0.42              |
| 1:B:53:GLU:CG    | 2:C:385:GLY:HA2  | 2.49                     | 0.42              |
| 1:B:97:ARG:NE    | 1:B:104:GLN:HB2  | 2.34                     | 0.42              |
| 2:C:403:LYS:HD3  | 2:C:432:ILE:HG12 | 2.01                     | 0.42              |
| 2:C:503:ILE:O    | 2:C:507:ILE:HG12 | 2.19                     | 0.42              |
| 2:C:583:PHE:HA   | 2:C:598:ASP:OD2  | 2.19                     | 0.42              |
| 2:D:9:LEU:HD11   | 2:D:46:LEU:HD12  | 2.01                     | 0.42              |
| 2:D:555:TYR:HB2  | 2:D:559:PHE:CE2  | 2.53                     | 0.42              |
| 1:E:17:ILE:O     | 1:E:298:LEU:N    | 2.51                     | 0.42              |
| 1:E:356:LEU:HD23 | 1:E:356:LEU:HA   | 1.85                     | 0.42              |
| 2:G:43:ILE:HD11  | 2:G:100:LEU:HD11 | 2.01                     | 0.42              |
| 2:G:117:LEU:HD22 | 2:G:138:LEU:CD1  | 2.49                     | 0.42              |
| 2:G:488:ARG:HB2  | 2:G:638:VAL:HA   | 2.00                     | 0.42              |
| 2:G:681:LEU:HA   | 2:G:684:GLN:HG2  | 1.99                     | 0.42              |
| 2:H:117:LEU:HD11 | 2:H:136:LEU:HB3  | 2.00                     | 0.42              |
| 2:H:345:ILE:HG22 | 2:H:349:LEU:HD13 | 2.01                     | 0.42              |
| 2:C:36:ALA:O     | 2:C:40:ARG:NE    | 2.44                     | 0.42              |
| 2:C:339:ASP:HB3  | 2:C:345:ILE:HG12 | 2.00                     | 0.42              |
| 2:C:621:ARG:O    | 2:C:624:MET:HG3  | 2.19                     | 0.42              |
| 2:D:108:ILE:HG21 | 2:D:136:LEU:HD21 | 2.01                     | 0.42              |
| 2:D:601:ILE:O    | 2:D:605:ILE:HG12 | 2.19                     | 0.42              |
| 1:E:191:MET:HG2  | 1:E:314:ASP:OD2  | 2.19                     | 0.42              |
| 1:F:15:ILE:HD12  | 1:F:113:LEU:HD11 | 2.01                     | 0.42              |
| 2:G:91:GLN:HE21  | 2:G:266:TYR:HD1  | 1.68                     | 0.42              |
| 2:G:131:ASP:O    | 2:G:134:THR:HG22 | 2.20                     | 0.42              |
| 2:H:40:ARG:NH1   | 2:H:92:GLN:HE22  | 2.18                     | 0.42              |
| 2:H:461:PRO:HB3  | 2:H:465:THR:HG21 | 2.00                     | 0.42              |
| 1:A:189:GLU:OE2  | 1:A:260:PHE:HB2  | 2.19                     | 0.42              |
| 1:B:25:PHE:HD1   | 1:B:278:GLY:HA3  | 1.85                     | 0.42              |
| 1:B:79:GLU:O     | 1:B:83:GLY:N     | 2.52                     | 0.42              |
| 1:B:101:THR:HA   | 1:B:104:GLN:HB3  | 2.00                     | 0.42              |
| 1:B:244:ILE:HD11 | 1:B:390:TYR:CE1  | 2.53                     | 0.42              |
| 2:C:48:GLU:OE2   | 2:C:49:ASN:N     | 2.48                     | 0.42              |
| 2:C:306:ALA:H    | 2:C:472:THR:HG22 | 1.84                     | 0.42              |
| 2:C:310:SER:OG   | 2:C:388:HIS:O    | 2.27                     | 0.42              |
| 2:D:392:ILE:HG23 | 2:D:418:THR:HG21 | 2.02                     | 0.42              |
| 2:D:472:THR:O    | 2:D:476:LEU:HG   | 2.19                     | 0.42              |
| 1:F:25:PHE:N     | 1:F:241:ASP:OD1  | 2.52                     | 0.42              |
| 2:H:301:SER:OG   | 2:H:302:ASP:N    | 2.53                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:486:VAL:HB   | 2:C:640:ARG:HE   | 1.84                     | 0.42              |
| 2:C:501:PRO:HB2  | 2:C:625:LEU:HB3  | 2.01                     | 0.42              |
| 2:C:526:PHE:HE2  | 2:C:623:VAL:HG21 | 1.84                     | 0.42              |
| 2:D:143:LEU:HA   | 2:D:285:LEU:HB3  | 2.01                     | 0.42              |
| 2:D:520:ASP:OD2  | 2:D:534:GLN:NE2  | 2.52                     | 0.42              |
| 2:G:37:SER:HA    | 2:G:40:ARG:HH21  | 1.83                     | 0.42              |
| 2:G:159:ILE:HG23 | 2:G:164:ALA:HB2  | 2.01                     | 0.42              |
| 2:H:10:ASN:O     | 2:H:18:VAL:N     | 2.46                     | 0.42              |
| 2:H:449:SER:HB2  | 2:H:450:PRO:HD2  | 2.01                     | 0.42              |
| 2:H:456:LEU:HD23 | 2:H:651:PHE:HD2  | 1.84                     | 0.42              |
| 1:A:257:ARG:HD3  | 1:A:262:ARG:HG2  | 2.02                     | 0.42              |
| 1:B:212:ARG:HE   | 1:B:383:VAL:HA   | 1.85                     | 0.42              |
| 1:B:230:PHE:CE1  | 1:B:237:PRO:HB3  | 2.55                     | 0.42              |
| 1:B:399:ALA:O    | 1:B:403:THR:HG23 | 2.19                     | 0.42              |
| 1:B:402:ILE:O    | 1:B:406:LEU:HD23 | 2.19                     | 0.42              |
| 2:C:31:LEU:HD21  | 2:C:66:ILE:HD11  | 2.01                     | 0.42              |
| 2:C:659:LEU:HD13 | 2:C:665:TYR:CD1  | 2.55                     | 0.42              |
| 2:D:38:GLN:O     | 2:D:42:ILE:N     | 2.45                     | 0.42              |
| 1:F:323:THR:HG22 | 1:F:334:MET:HE1  | 2.02                     | 0.42              |
| 1:A:95:VAL:HG22  | 1:A:96:SER:H     | 1.85                     | 0.42              |
| 1:B:97:ARG:NH2   | 1:B:100:ALA:O    | 2.52                     | 0.42              |
| 1:B:392:HIS:ND1  | 1:B:397:THR:HG21 | 2.35                     | 0.42              |
| 2:C:562:PRO:HG2  | 2:C:565:VAL:HG21 | 2.01                     | 0.42              |
| 2:C:678:MET:SD   | 2:C:691:PRO:HG3  | 2.59                     | 0.42              |
| 2:D:29:ASN:H     | 2:D:64:ASN:ND2   | 2.04                     | 0.42              |
| 2:D:79:THR:N     | 2:D:82:GLU:OE1   | 2.36                     | 0.42              |
| 2:G:692:CYS:O    | 2:G:696:VAL:HG22 | 2.19                     | 0.42              |
| 2:H:9:LEU:HA     | 2:H:19:ILE:HD13  | 2.01                     | 0.42              |
| 2:H:407:VAL:HA   | 2:H:410:VAL:HG12 | 2.01                     | 0.42              |
| 2:H:583:PHE:O    | 2:H:598:ASP:N    | 2.35                     | 0.42              |
| 2:H:650:VAL:HA   | 2:H:655:PHE:HB3  | 2.01                     | 0.42              |
| 2:H:698:MET:HG2  | 2:H:705:PHE:HE1  | 1.84                     | 0.42              |
| 1:A:207:HIS:O    | 1:A:211:GLN:HG2  | 2.19                     | 0.42              |
| 1:A:217:TRP:CD2  | 1:A:222:LEU:HD11 | 2.54                     | 0.42              |
| 1:B:25:PHE:CE2   | 1:B:400:ARG:HD3  | 2.48                     | 0.42              |
| 1:B:153:MET:SD   | 1:B:154:SER:N    | 2.93                     | 0.42              |
| 2:C:327:THR:O    | 2:C:331:ALA:HB3  | 2.20                     | 0.42              |
| 2:D:275:GLU:O    | 2:D:279:THR:OG1  | 2.38                     | 0.42              |
| 2:D:336:ARG:NH1  | 2:D:384:ARG:O    | 2.36                     | 0.42              |
| 1:F:18:VAL:HA    | 1:F:297:PRO:HA   | 2.01                     | 0.42              |
| 1:F:316:LEU:HD22 | 1:F:422:CYS:SG   | 2.59                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:494:TYR:CG   | 2:G:639:ILE:HD11 | 2.55                     | 0.42              |
| 1:B:27:ARG:CZ    | 1:B:243:ASN:HA   | 2.49                     | 0.42              |
| 2:C:456:LEU:HD13 | 2:C:652:GLY:HA3  | 2.01                     | 0.42              |
| 2:C:495:VAL:O    | 2:C:499:LEU:HD23 | 2.20                     | 0.42              |
| 2:C:497:ARG:HH12 | 2:C:632:ARG:CG   | 2.32                     | 0.42              |
| 2:D:23:VAL:HG23  | 2:D:29:ASN:HD22  | 1.84                     | 0.42              |
| 2:D:148:GLY:HA2  | 2:D:273:PHE:CZ   | 2.54                     | 0.42              |
| 2:D:540:GLY:HA2  | 2:D:578:LYS:NZ   | 2.35                     | 0.42              |
| 2:D:558:ARG:HH12 | 2:D:629:GLU:CD   | 2.28                     | 0.42              |
| 2:G:317:GLY:HA2  | 2:G:347:HIS:HB3  | 2.02                     | 0.42              |
| 2:H:225:ARG:HH12 | 2:H:258:LEU:C    | 2.28                     | 0.42              |
| 2:H:528:PHE:CZ   | 2:H:623:VAL:HG12 | 2.55                     | 0.42              |
| 1:B:190:GLN:O    | 1:B:194:THR:N    | 2.51                     | 0.42              |
| 2:C:128:CYS:SG   | 2:C:185:VAL:HG21 | 2.60                     | 0.42              |
| 2:C:486:VAL:HG11 | 2:C:640:ARG:HH21 | 1.85                     | 0.42              |
| 2:D:190:PRO:HD2  | 2:D:193:ILE:HD11 | 2.01                     | 0.42              |
| 1:E:144:LEU:HA   | 1:E:147:VAL:HG12 | 2.02                     | 0.42              |
| 1:E:348:ALA:O    | 1:E:350:THR:HG22 | 2.20                     | 0.42              |
| 1:E:377:ASP:OD2  | 1:E:379:SER:OG   | 2.32                     | 0.42              |
| 2:G:175:ARG:HH21 | 2:G:362:ARG:HH12 | 1.67                     | 0.42              |
| 2:H:89:GLN:O     | 2:H:92:GLN:NE2   | 2.53                     | 0.42              |
| 2:H:309:ASN:N    | 2:H:390:ASP:OD2  | 2.46                     | 0.42              |
| 2:H:409:GLU:O    | 2:H:413:ASN:N    | 2.51                     | 0.42              |
| 1:A:311:VAL:HA   | 1:A:315:MET:CG   | 2.49                     | 0.41              |
| 1:A:418:LEU:HG   | 1:A:431:MET:O    | 2.20                     | 0.41              |
| 1:B:8:VAL:HA     | 1:B:14:ARG:HA    | 2.01                     | 0.41              |
| 1:B:267:VAL:HA   | 1:B:271:ASN:ND2  | 2.29                     | 0.41              |
| 2:C:104:VAL:HG12 | 2:C:123:CYS:SG   | 2.60                     | 0.41              |
| 2:D:28:MET:SD    | 2:D:28:MET:N     | 2.93                     | 0.41              |
| 1:E:20:GLY:HA3   | 1:E:282:VAL:HG22 | 2.01                     | 0.41              |
| 1:F:113:LEU:HD13 | 1:F:286:THR:HB   | 2.02                     | 0.41              |
| 1:F:343:HIS:NE2  | 1:F:345:ALA:HB2  | 2.35                     | 0.41              |
| 2:G:438:ARG:HD2  | 2:G:438:ARG:O    | 2.20                     | 0.41              |
| 2:G:672:GLY:HA2  | 2:G:675:VAL:HG23 | 2.02                     | 0.41              |
| 1:A:418:LEU:HD12 | 1:A:432:VAL:HG22 | 2.02                     | 0.41              |
| 1:B:63:VAL:HG13  | 1:B:94:SER:HA    | 2.01                     | 0.41              |
| 1:B:337:LEU:HD23 | 1:B:340:ILE:HB   | 2.00                     | 0.41              |
| 2:D:64:ASN:HA    | 2:D:111:ALA:H    | 1.85                     | 0.41              |
| 2:D:615:ALA:HB3  | 2:D:616:PRO:HD3  | 2.02                     | 0.41              |
| 1:E:302:ARG:HA   | 1:E:302:ARG:HD2  | 1.83                     | 0.41              |
| 1:F:108:ASN:O    | 1:F:111:GLU:HG2  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:424:THR:O    | 2:G:446:HIS:HD2  | 2.03                     | 0.41              |
| 2:H:338:LYS:HB2  | 2:H:386:PHE:CZ   | 2.55                     | 0.41              |
| 2:H:501:PRO:HB3  | 2:H:625:LEU:HD12 | 2.02                     | 0.41              |
| 1:A:221:LYS:HB2  | 1:A:411:ARG:HH12 | 1.83                     | 0.41              |
| 1:B:285:MET:SD   | 1:B:290:ALA:HB2  | 2.60                     | 0.41              |
| 2:C:232:VAL:HG23 | 2:C:251:LEU:HD21 | 2.02                     | 0.41              |
| 2:C:614:SER:H    | 2:C:617:GLN:HG3  | 1.86                     | 0.41              |
| 2:C:626:MET:O    | 2:C:630:ALA:N    | 2.40                     | 0.41              |
| 2:C:687:SER:O    | 2:C:690:THR:HG23 | 2.20                     | 0.41              |
| 2:D:325:TYR:CE2  | 2:D:355:GLN:HB2  | 2.54                     | 0.41              |
| 1:F:333:THR:HG22 | 1:F:335:SER:H    | 1.85                     | 0.41              |
| 2:H:228:LEU:O    | 2:H:232:VAL:HG12 | 2.21                     | 0.41              |
| 2:H:253:VAL:HA   | 2:H:256:THR:HG22 | 2.02                     | 0.41              |
| 2:H:533:ILE:HG13 | 2:H:534:GLN:N    | 2.35                     | 0.41              |
| 1:A:141:ALA:O    | 1:A:145:VAL:HG23 | 2.20                     | 0.41              |
| 1:A:222:LEU:HD13 | 1:A:226:VAL:HG21 | 2.03                     | 0.41              |
| 1:A:393:PRO:HB2  | 1:A:396:ALA:HB3  | 2.02                     | 0.41              |
| 2:C:570:LEU:HA   | 2:C:575:LYS:NZ   | 2.35                     | 0.41              |
| 2:D:15:ASN:HD21  | 2:D:53:ARG:NH1   | 2.19                     | 0.41              |
| 2:D:86:LEU:O     | 2:D:89:GLN:HG3   | 2.20                     | 0.41              |
| 2:D:143:LEU:HD12 | 2:D:286:ARG:HA   | 2.02                     | 0.41              |
| 1:E:10:ARG:HH21  | 1:E:115:ALA:HA   | 1.84                     | 0.41              |
| 1:F:233:PRO:HB2  | 1:F:235:LYS:HG2  | 2.02                     | 0.41              |
| 2:G:146:LEU:HA   | 2:G:147:PRO:HD3  | 1.86                     | 0.41              |
| 2:G:391:LEU:HD11 | 2:G:421:ALA:HB2  | 2.02                     | 0.41              |
| 2:G:617:GLN:H    | 2:G:617:GLN:HG2  | 1.73                     | 0.41              |
| 2:H:163:THR:HG21 | 2:H:182:LEU:HD11 | 2.02                     | 0.41              |
| 2:H:585:LEU:HD23 | 2:H:596:GLN:O    | 2.21                     | 0.41              |
| 1:A:91:ASP:HB3   | 1:A:93:TYR:CE2   | 2.56                     | 0.41              |
| 2:C:164:ALA:O    | 2:C:168:ILE:HG12 | 2.20                     | 0.41              |
| 2:C:398:GLU:HA   | 2:C:403:LYS:HZ3  | 1.85                     | 0.41              |
| 2:D:495:VAL:HG13 | 2:D:653:ILE:HD11 | 2.02                     | 0.41              |
| 2:D:513:GLY:HA2  | 2:D:607:THR:OG1  | 2.20                     | 0.41              |
| 1:E:32:PHE:CD2   | 1:E:277:ASP:HB2  | 2.56                     | 0.41              |
| 1:F:25:PHE:HD1   | 1:F:278:GLY:HA3  | 1.85                     | 0.41              |
| 2:G:48:GLU:OE2   | 2:G:49:ASN:N     | 2.50                     | 0.41              |
| 2:C:23:VAL:HG23  | 2:C:61:LYS:HZ1   | 1.85                     | 0.41              |
| 2:C:338:LYS:HE2  | 2:C:382:ASP:C    | 2.46                     | 0.41              |
| 2:C:549:PRO:HA   | 2:C:552:GLU:OE1  | 2.20                     | 0.41              |
| 2:D:284:ALA:HB1  | 2:D:660:GLY:CA   | 2.50                     | 0.41              |
| 1:E:153:MET:HA   | 1:E:156:ARG:HH11 | 1.84                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:35:ILE:O     | 1:F:35:ILE:HG13  | 2.20                     | 0.41              |
| 2:H:311:VAL:H    | 2:H:389:ARG:HH11 | 1.68                     | 0.41              |
| 1:A:327:LEU:HD12 | 1:A:332:LEU:C    | 2.45                     | 0.41              |
| 2:C:325:TYR:O    | 2:C:329:CYS:N    | 2.54                     | 0.41              |
| 2:D:65:PHE:N     | 2:D:109:HIS:O    | 2.54                     | 0.41              |
| 2:D:75:GLY:HA2   | 2:D:286:ARG:HH21 | 1.86                     | 0.41              |
| 2:D:146:LEU:HD21 | 2:D:272:ALA:HB1  | 2.03                     | 0.41              |
| 1:E:202:GLN:HB2  | 1:E:347:ALA:HB1  | 2.01                     | 0.41              |
| 1:F:267:VAL:HA   | 1:F:271:ASN:HD21 | 1.85                     | 0.41              |
| 1:F:307:THR:HG21 | 1:F:321:TRP:HB3  | 2.02                     | 0.41              |
| 2:H:488:ARG:HG3  | 2:H:490:LYS:HG2  | 2.02                     | 0.41              |
| 1:A:25:PHE:CD1   | 1:A:278:GLY:HA3  | 2.56                     | 0.41              |
| 1:A:291:LYS:NZ   | 1:A:300:TYR:OH   | 2.48                     | 0.41              |
| 2:C:304:PRO:O    | 2:C:468:GLN:HG3  | 2.21                     | 0.41              |
| 2:D:29:ASN:HB2   | 2:D:66:ILE:HA    | 2.02                     | 0.41              |
| 2:D:313:ILE:HD12 | 2:D:393:ILE:HG23 | 2.02                     | 0.41              |
| 1:E:18:VAL:HG12  | 1:E:19:SER:H     | 1.84                     | 0.41              |
| 2:G:504:ASN:ND2  | 2:G:560:SER:O    | 2.41                     | 0.41              |
| 2:H:462:HIS:CD2  | 2:H:464:GLY:H    | 2.38                     | 0.41              |
| 1:A:406:LEU:O    | 1:A:410:ARG:HG2  | 2.21                     | 0.41              |
| 1:B:80:ILE:O     | 1:B:84:THR:OG1   | 2.37                     | 0.41              |
| 1:B:253:TYR:CD1  | 1:B:270:ALA:HB1  | 2.56                     | 0.41              |
| 1:B:378:ASP:HA   | 1:B:381:PHE:HB3  | 2.03                     | 0.41              |
| 2:C:30:THR:HA    | 2:C:67:ALA:HB3   | 2.03                     | 0.41              |
| 2:C:65:PHE:CD2   | 2:C:108:ILE:HG22 | 2.55                     | 0.41              |
| 1:E:350:THR:O    | 1:E:354:ILE:HD12 | 2.20                     | 0.41              |
| 1:F:15:ILE:HD11  | 1:F:114:MET:SD   | 2.60                     | 0.41              |
| 1:F:81:VAL:HG22  | 1:F:86:MET:HG2   | 2.02                     | 0.41              |
| 2:G:426:SER:CB   | 2:G:547:ILE:HG12 | 2.51                     | 0.41              |
| 2:G:449:SER:O    | 2:G:450:PRO:C    | 2.63                     | 0.41              |
| 2:G:516:VAL:HG21 | 2:G:597:VAL:HG11 | 2.03                     | 0.41              |
| 2:G:691:PRO:HB3  | 2:G:695:LEU:HD22 | 2.02                     | 0.41              |
| 2:H:27:LYS:HB3   | 2:H:63:ASP:OD2   | 2.21                     | 0.41              |
| 2:H:449:SER:O    | 2:H:450:PRO:C    | 2.64                     | 0.41              |
| 2:H:500:ALA:HB3  | 2:H:501:PRO:HD3  | 2.03                     | 0.41              |
| 2:H:537:ASP:OD1  | 2:H:538:GLU:HG3  | 2.20                     | 0.41              |
| 2:H:558:ARG:NH1  | 2:H:629:GLU:OE1  | 2.54                     | 0.41              |
| 1:A:15:ILE:HD12  | 1:A:113:LEU:HD22 | 2.03                     | 0.41              |
| 1:B:78:ARG:HA    | 1:B:78:ARG:HD2   | 1.81                     | 0.41              |
| 2:C:417:HIS:O    | 2:C:441:GLN:NE2  | 2.54                     | 0.41              |
| 2:C:449:SER:O    | 2:C:450:PRO:C    | 2.63                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:583:PHE:HB3  | 2:C:601:ILE:HG21 | 2.03                     | 0.41              |
| 2:D:47:ARG:HH21  | 2:D:50:LYS:NZ    | 2.19                     | 0.41              |
| 2:D:55:VAL:HG23  | 2:D:104:VAL:HA   | 2.02                     | 0.41              |
| 2:D:59:SER:OG    | 2:D:64:ASN:O     | 2.39                     | 0.41              |
| 1:F:81:VAL:HG13  | 1:F:86:MET:HB3   | 2.03                     | 0.41              |
| 1:F:340:ILE:HG21 | 1:F:376:VAL:HG13 | 2.02                     | 0.41              |
| 2:G:246:ALA:HB2  | 2:G:276:LEU:HD11 | 2.03                     | 0.41              |
| 2:G:575:LYS:H    | 2:G:579:ASN:ND2  | 2.19                     | 0.41              |
| 2:H:475:LYS:HA   | 2:H:478:LYS:HD2  | 2.01                     | 0.41              |
| 2:H:675:VAL:HG21 | 2:H:699:GLY:HA3  | 2.02                     | 0.41              |
| 2:C:392:ILE:HD11 | 2:C:414:CYS:SG   | 2.61                     | 0.40              |
| 2:C:499:LEU:HD21 | 2:C:653:ILE:CG2  | 2.51                     | 0.40              |
| 2:D:466:SER:O    | 2:D:470:ILE:HD12 | 2.22                     | 0.40              |
| 2:D:505:GLU:N    | 2:D:508:ARG:HH21 | 2.19                     | 0.40              |
| 1:E:66:GLN:NE2   | 1:E:69:GLN:HA    | 2.35                     | 0.40              |
| 1:E:183:ARG:C    | 1:E:185:GLY:H    | 2.28                     | 0.40              |
| 1:F:97:ARG:HH22  | 1:F:306:PHE:HB3  | 1.85                     | 0.40              |
| 1:F:193:LYS:NZ   | 1:F:261:ASP:OD2  | 2.40                     | 0.40              |
| 1:F:303:SER:HB2  | 1:F:330:ALA:HB2  | 2.03                     | 0.40              |
| 2:H:43:ILE:HD12  | 2:H:43:ILE:HA    | 1.89                     | 0.40              |
| 2:H:84:GLU:HG2   | 2:H:270:ALA:O    | 2.21                     | 0.40              |
| 2:H:356:LEU:C    | 2:H:358:GLY:H    | 2.29                     | 0.40              |
| 2:H:610:GLN:O    | 2:H:612:ARG:HG2  | 2.20                     | 0.40              |
| 1:A:268:THR:HG23 | 1:A:270:ALA:H    | 1.86                     | 0.40              |
| 1:A:285:MET:SD   | 1:A:290:ALA:HB2  | 2.61                     | 0.40              |
| 1:A:408:GLU:N    | 1:A:411:ARG:HH21 | 2.18                     | 0.40              |
| 2:C:16:ILE:HD13  | 2:C:16:ILE:HA    | 1.99                     | 0.40              |
| 2:C:200:GLU:HB2  | 2:C:203:LYS:NZ   | 2.36                     | 0.40              |
| 2:C:656:PRO:HB3  | 2:C:658:PHE:CZ   | 2.56                     | 0.40              |
| 2:D:449:SER:O    | 2:D:450:PRO:C    | 2.64                     | 0.40              |
| 1:E:323:THR:OG1  | 1:E:420:THR:HG21 | 2.20                     | 0.40              |
| 2:G:534:GLN:HB3  | 2:G:584:TYR:HE2  | 1.86                     | 0.40              |
| 1:A:182:LEU:HD23 | 1:A:182:LEU:HA   | 1.85                     | 0.40              |
| 2:C:66:ILE:HD13  | 2:C:116:GLY:HA2  | 2.04                     | 0.40              |
| 2:C:367:ALA:HB1  | 2:C:370:ARG:HH21 | 1.87                     | 0.40              |
| 2:D:338:LYS:HA   | 2:D:380:THR:O    | 2.21                     | 0.40              |
| 2:D:569:ILE:HG22 | 2:D:574:ARG:O    | 2.21                     | 0.40              |
| 2:D:682:ALA:HB2  | 2:D:689:PHE:HB2  | 2.04                     | 0.40              |
| 2:G:337:ILE:HB   | 2:G:379:GLY:HA2  | 2.03                     | 0.40              |
| 2:C:315:GLY:C    | 2:C:337:ILE:HD11 | 2.46                     | 0.40              |
| 2:D:241:GLN:HG3  | 2:D:524:VAL:O    | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:327:THR:O    | 2:D:331:ALA:HB3  | 2.21                     | 0.40              |
| 2:D:498:ILE:HG22 | 2:D:629:GLU:HB3  | 2.04                     | 0.40              |
| 2:G:212:LEU:HD23 | 2:G:212:LEU:H    | 1.86                     | 0.40              |
| 2:H:697:GLU:HG2  | 2:H:701:ARG:HH21 | 1.86                     | 0.40              |
| 1:A:302:ARG:HA   | 1:A:302:ARG:HD2  | 1.82                     | 0.40              |
| 1:B:25:PHE:CE2   | 1:B:393:PRO:HG2  | 2.57                     | 0.40              |
| 2:C:697:GLU:HG2  | 2:C:701:ARG:HH12 | 1.86                     | 0.40              |
| 2:D:103:GLN:NE2  | 2:D:207:PRO:HA   | 2.36                     | 0.40              |
| 2:D:146:LEU:HB2  | 2:D:147:PRO:HD2  | 2.03                     | 0.40              |
| 2:D:232:VAL:HG23 | 2:D:251:LEU:HD21 | 2.03                     | 0.40              |
| 2:D:548:ILE:HB   | 2:D:549:PRO:HD3  | 2.03                     | 0.40              |
| 2:D:638:VAL:HG13 | 2:D:639:ILE:HG12 | 2.02                     | 0.40              |
| 1:E:261:ASP:C    | 1:E:263:LYS:H    | 2.29                     | 0.40              |
| 1:F:231:ILE:HG13 | 1:F:234:TYR:N    | 2.35                     | 0.40              |
| 2:G:130:ASP:OD1  | 2:G:190:PRO:HA   | 2.21                     | 0.40              |
| 2:G:425:SER:HA   | 2:G:493:PHE:HE2  | 1.86                     | 0.40              |
| 2:H:23:VAL:HG12  | 2:H:25:GLY:H     | 1.86                     | 0.40              |
| 2:H:232:VAL:HA   | 2:H:235:LYS:HB3  | 2.04                     | 0.40              |
| 2:H:235:LYS:HG3  | 2:H:239:LYS:NZ   | 2.37                     | 0.40              |
| 2:H:462:HIS:HD2  | 2:H:464:GLY:H    | 1.69                     | 0.40              |
| 2:H:516:VAL:HG11 | 2:H:533:ILE:HD13 | 2.02                     | 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     | 434/450 (96%) | 397 (92%) | 35 (8%) | 2 (0%)   | 24          | 63 |
| 1   | B     | 434/450 (96%) | 403 (93%) | 29 (7%) | 2 (0%)   | 24          | 63 |
| 1   | E     | 434/450 (96%) | 400 (92%) | 31 (7%) | 3 (1%)   | 18          | 56 |
| 1   | F     | 434/450 (96%) | 413 (95%) | 20 (5%) | 1 (0%)   | 43          | 78 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 2   | C     | 708/714 (99%)   | 660 (93%)  | 46 (6%)  | 2 (0%)   | 36          | 72 |
| 2   | D     | 708/714 (99%)   | 659 (93%)  | 47 (7%)  | 2 (0%)   | 36          | 72 |
| 2   | G     | 708/714 (99%)   | 654 (92%)  | 52 (7%)  | 2 (0%)   | 36          | 72 |
| 2   | H     | 708/714 (99%)   | 662 (94%)  | 45 (6%)  | 1 (0%)   | 48          | 83 |
| All | All   | 4568/4656 (98%) | 4248 (93%) | 305 (7%) | 15 (0%)  | 37          | 72 |

All (15) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 389 | ALA  |
| 1   | B     | 389 | ALA  |
| 2   | C     | 530 | VAL  |
| 2   | C     | 613 | ILE  |
| 2   | D     | 530 | VAL  |
| 1   | E     | 349 | GLN  |
| 1   | E     | 389 | ALA  |
| 1   | F     | 389 | ALA  |
| 2   | G     | 530 | VAL  |
| 2   | G     | 613 | ILE  |
| 2   | H     | 530 | VAL  |
| 1   | B     | 394 | PHE  |
| 1   | E     | 339 | LEU  |
| 1   | A     | 339 | LEU  |
| 2   | D     | 612 | ARG  |

### 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     | 320/347 (92%) | 319 (100%) | 1 (0%)   | 86          | 86  |
| 1   | B     | 321/347 (92%) | 321 (100%) | 0        | 100         | 100 |
| 1   | E     | 320/347 (92%) | 318 (99%)  | 2 (1%)   | 78          | 83  |
| 1   | F     | 321/347 (92%) | 321 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 2   | C     | 524/570 (92%)   | 523 (100%)  | 1 (0%)   | 87          | 87  |
| 2   | D     | 540/570 (95%)   | 540 (100%)  | 0        | 100         | 100 |
| 2   | G     | 524/570 (92%)   | 523 (100%)  | 1 (0%)   | 87          | 87  |
| 2   | H     | 540/570 (95%)   | 540 (100%)  | 0        | 100         | 100 |
| All | All   | 3410/3668 (93%) | 3405 (100%) | 5 (0%)   | 87          | 89  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 314 | ASP  |
| 2   | C     | 138 | LEU  |
| 1   | E     | 313 | GLN  |
| 1   | E     | 314 | ASP  |
| 2   | G     | 138 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 61  | GLN  |
| 1   | A     | 75  | ASN  |
| 1   | A     | 190 | GLN  |
| 1   | A     | 202 | GLN  |
| 1   | A     | 243 | ASN  |
| 1   | A     | 264 | HIS  |
| 1   | A     | 343 | HIS  |
| 1   | B     | 75  | ASN  |
| 1   | B     | 104 | GLN  |
| 1   | B     | 201 | GLN  |
| 1   | B     | 215 | GLN  |
| 1   | B     | 264 | HIS  |
| 1   | B     | 353 | ASN  |
| 1   | B     | 355 | GLN  |
| 2   | C     | 64  | ASN  |
| 2   | C     | 173 | GLN  |
| 2   | C     | 260 | GLN  |
| 2   | C     | 373 | GLN  |
| 2   | C     | 388 | HIS  |
| 2   | C     | 679 | GLN  |
| 2   | D     | 38  | GLN  |
| 2   | D     | 64  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 241 | GLN  |
| 2   | D     | 260 | GLN  |
| 2   | D     | 462 | HIS  |
| 2   | D     | 518 | HIS  |
| 1   | E     | 75  | ASN  |
| 1   | E     | 108 | ASN  |
| 1   | E     | 201 | GLN  |
| 1   | E     | 202 | GLN  |
| 1   | E     | 211 | GLN  |
| 1   | E     | 264 | HIS  |
| 1   | E     | 349 | GLN  |
| 1   | F     | 28  | GLN  |
| 1   | F     | 75  | ASN  |
| 1   | F     | 313 | GLN  |
| 2   | G     | 346 | ASN  |
| 2   | G     | 405 | GLN  |
| 2   | G     | 435 | HIS  |
| 2   | G     | 468 | GLN  |
| 2   | G     | 518 | HIS  |
| 2   | H     | 64  | ASN  |
| 2   | H     | 260 | GLN  |
| 2   | H     | 412 | GLN  |
| 2   | H     | 518 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

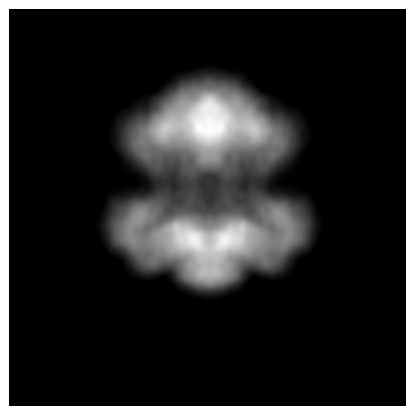
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16134. These allow visual inspection of the internal detail of the map and identification of artifacts.

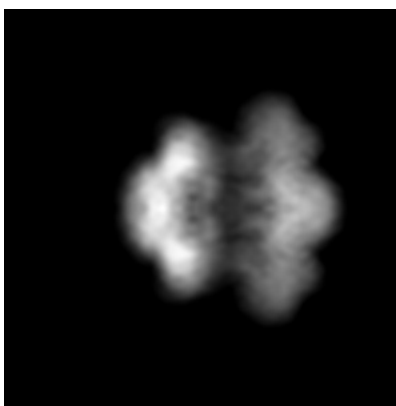
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



X

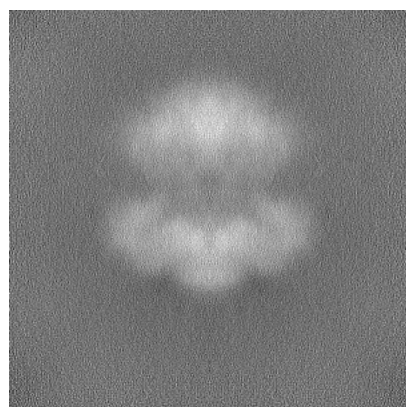


Y

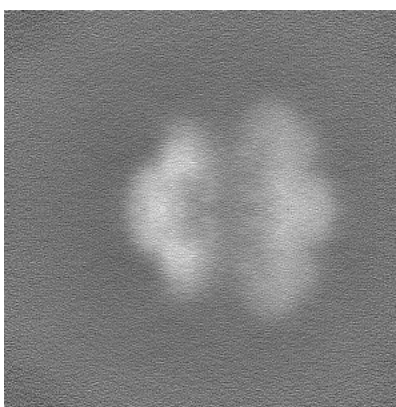


Z

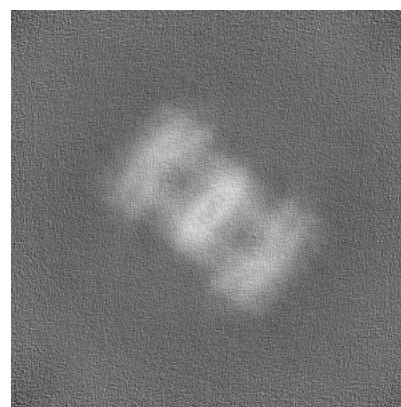
#### 6.1.2 Raw map



X



Y



Z

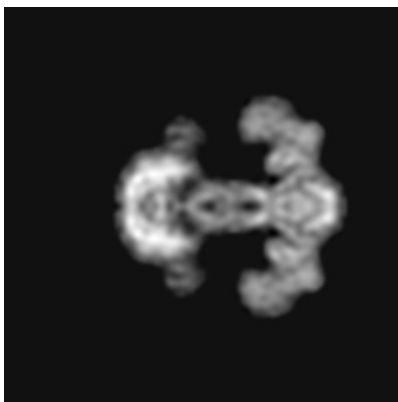
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 180

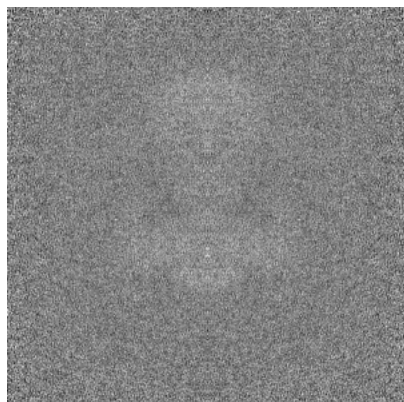


Y Index: 180

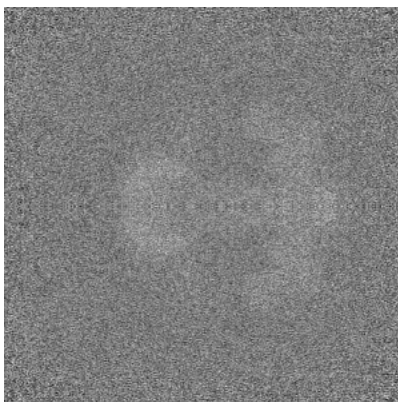


Z Index: 180

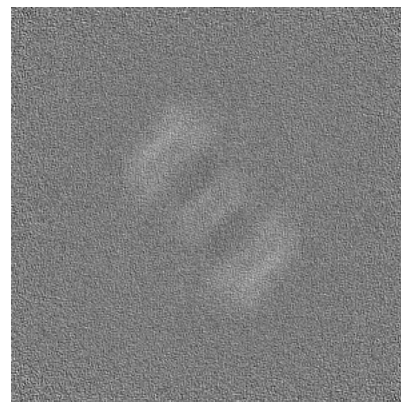
### 6.2.2 Raw map



X Index: 180



Y Index: 180

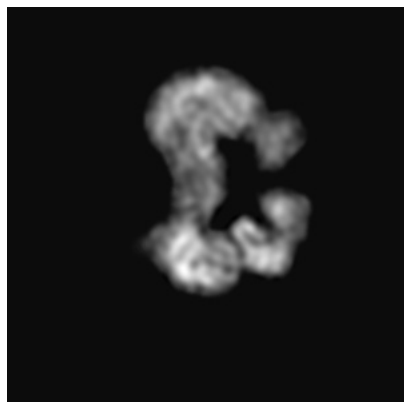


Z Index: 180

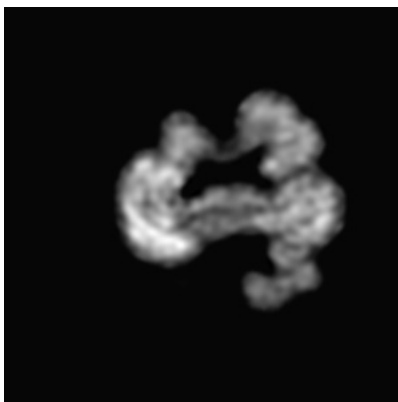
The images above show central slices of the map in three orthogonal directions.

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

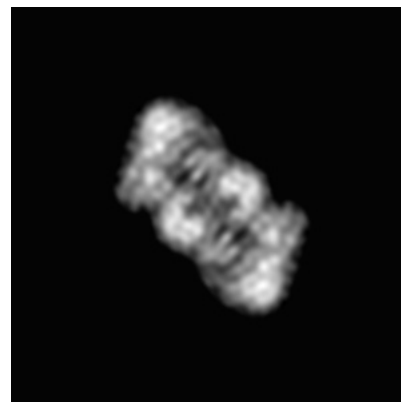
### 6.3.1 Primary map



X Index: 168

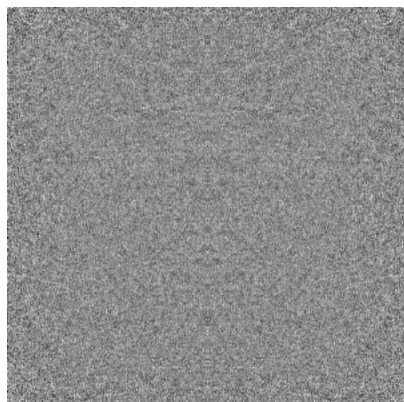


Y Index: 172

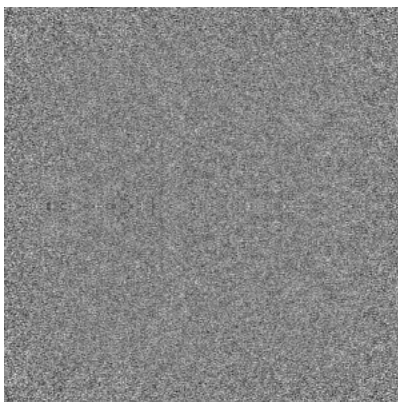


Z Index: 153

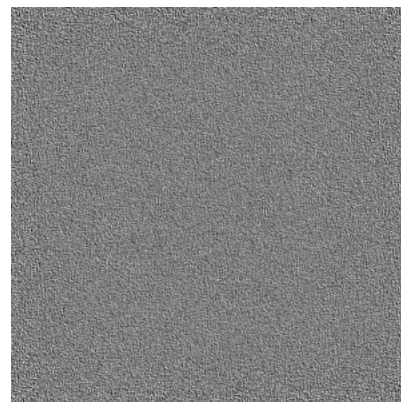
### 6.3.2 Raw map



X Index: 0



Y Index: 0

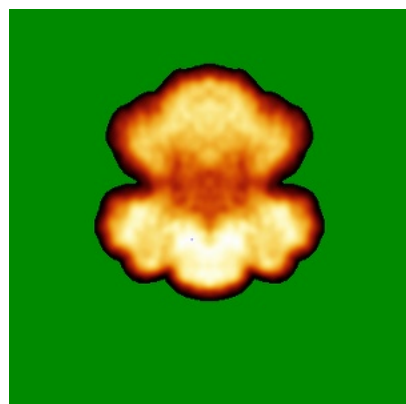


Z Index: 0

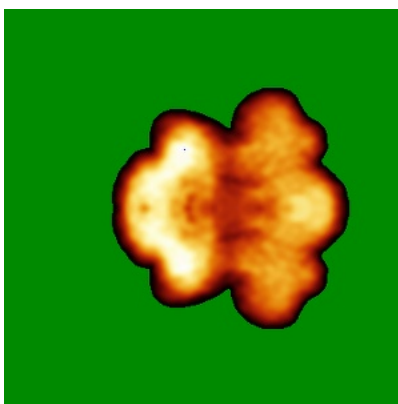
The images above show the largest variance slices of the map in three orthogonal directions.

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

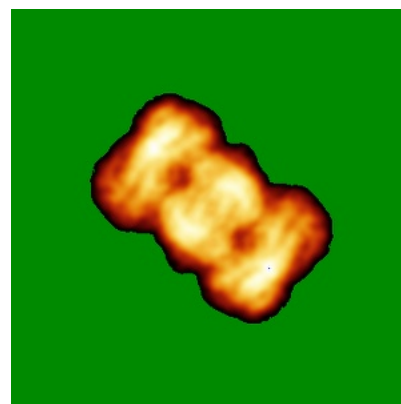
### 6.4.1 Primary map



X

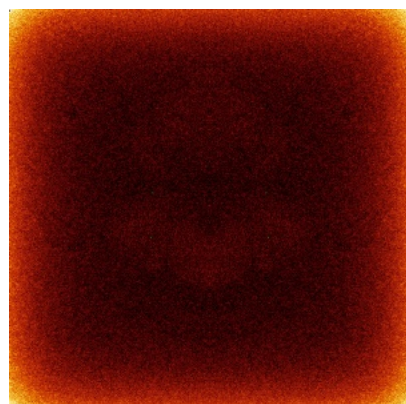


Y

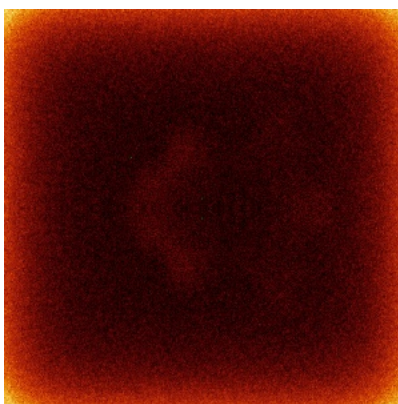


Z

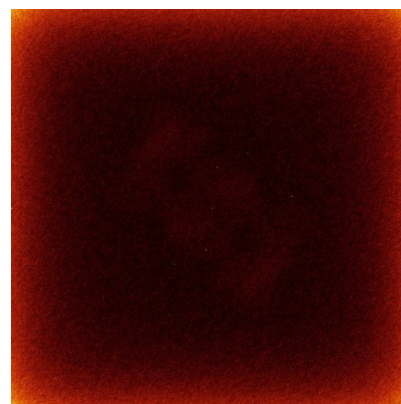
### 6.4.2 Raw map



X



Y

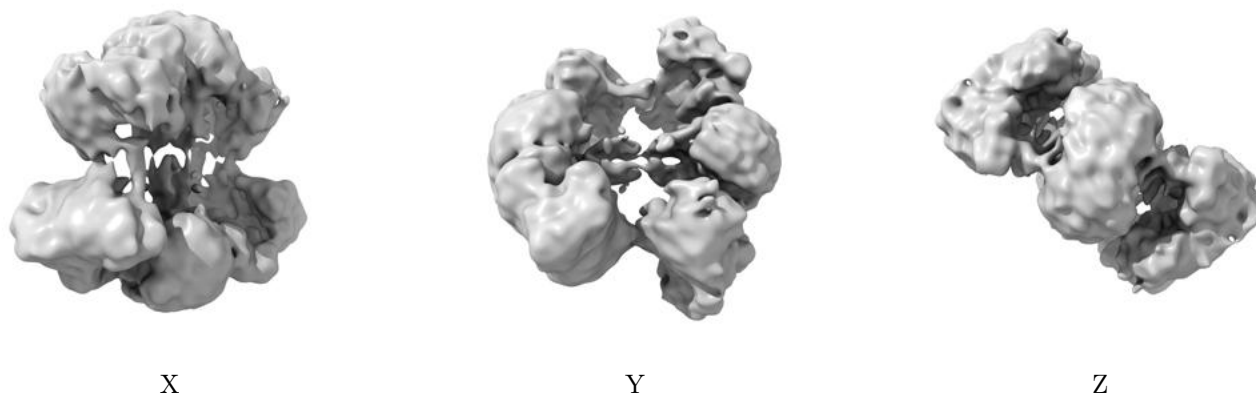


Z

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.

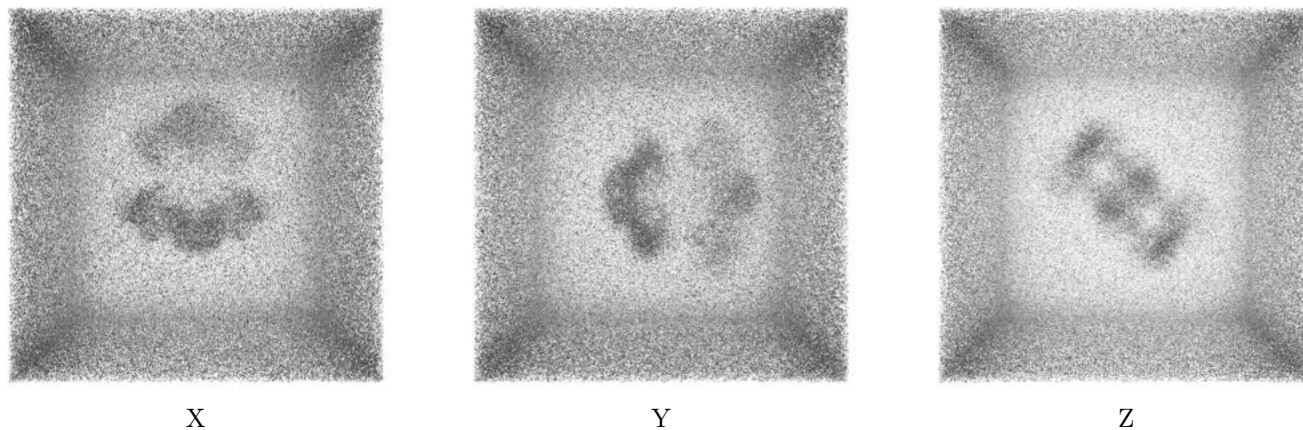
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

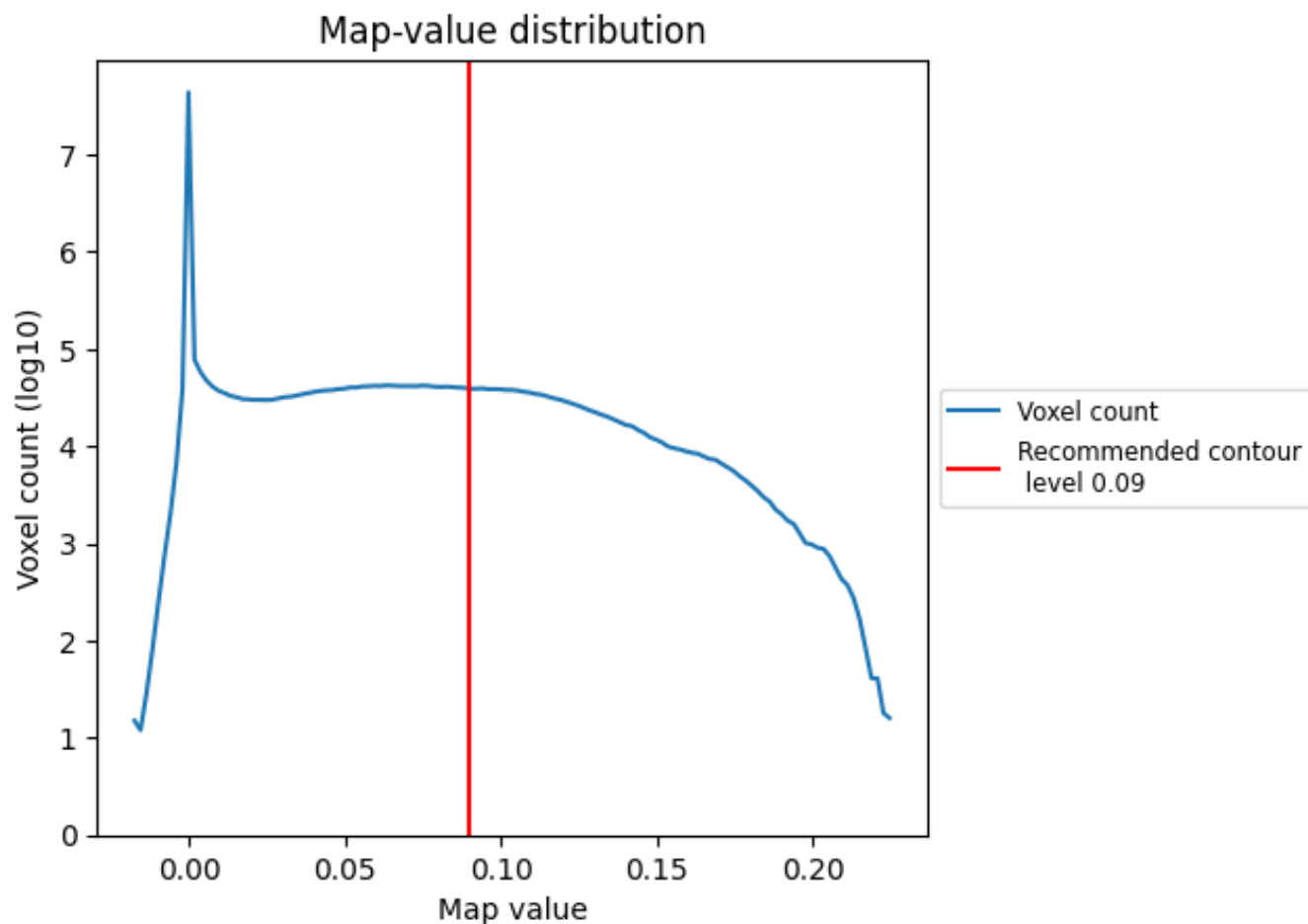
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

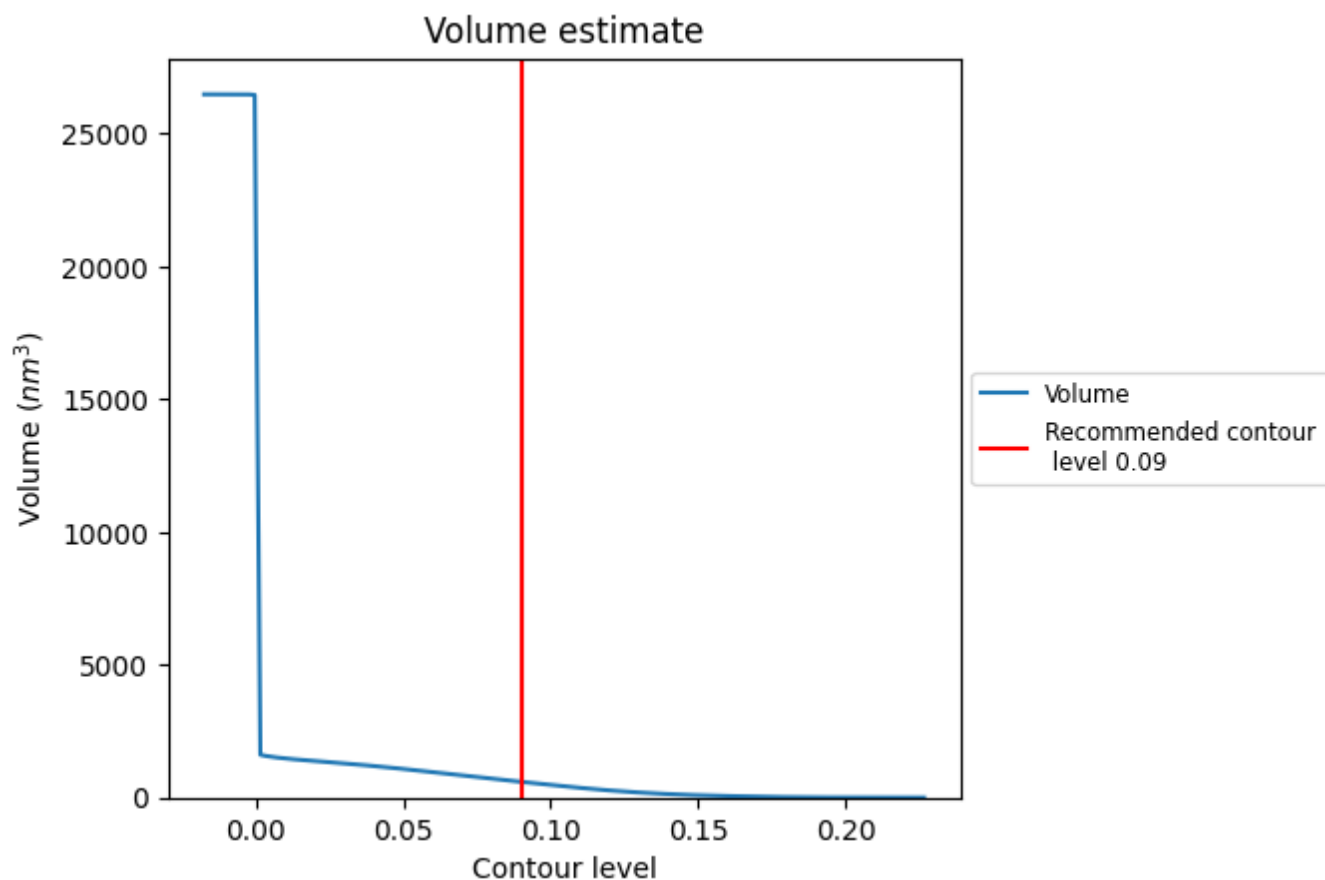
This section contains the results of statistical analysis of the map.

### 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.

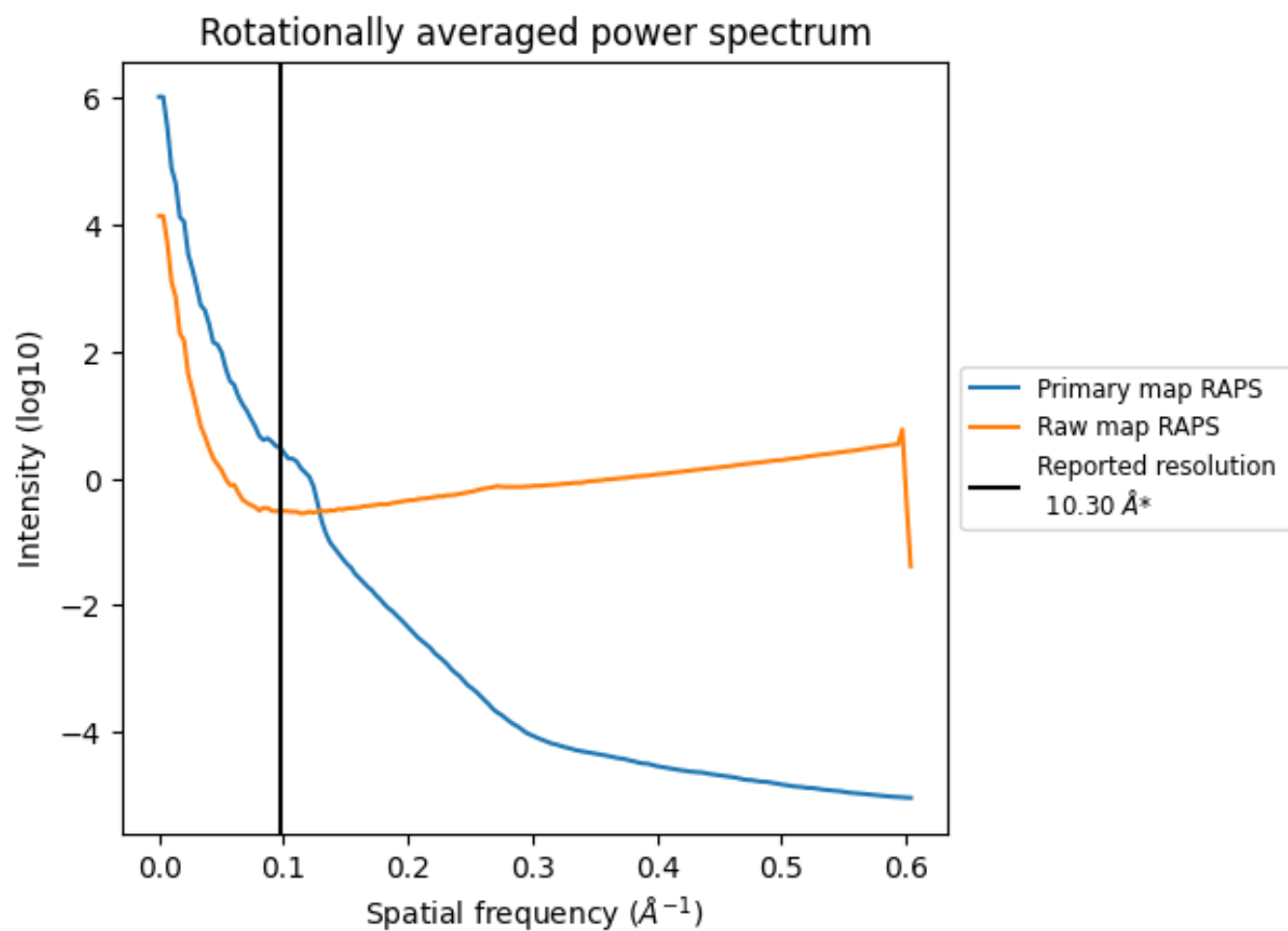
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 592 nm<sup>3</sup>; this corresponds to an approximate mass of 534 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 ⓘ

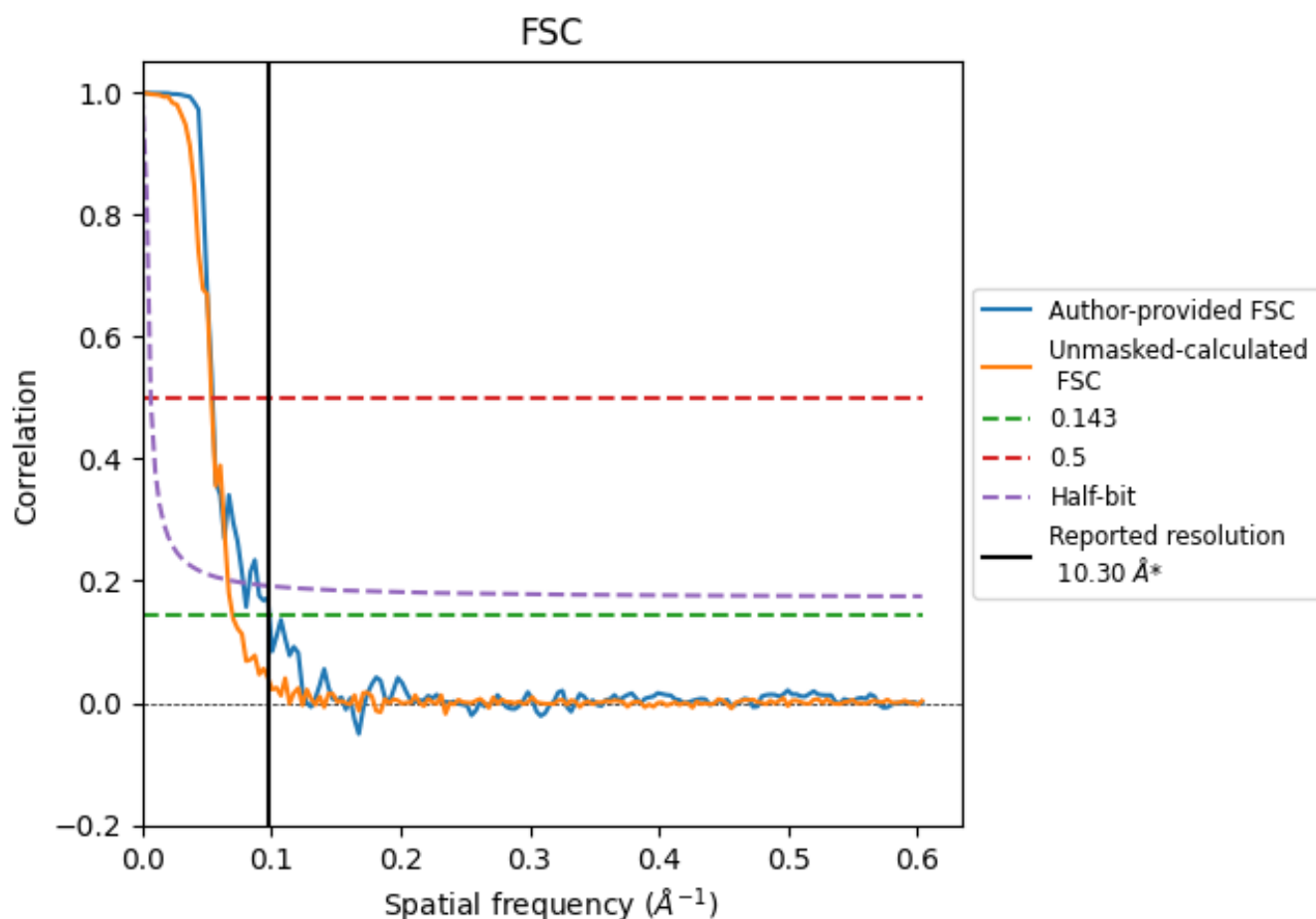


\*Reported resolution corresponds to spatial frequency of 0.097 Å⁻¹

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.097 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 10.30                              | -     | -        |
| Author-provided FSC curve | 10.16                              | 18.38 | 12.79    |
| Unmasked-calculated*      | 14.29                              | 18.66 | 15.06    |

\*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 14.29 differs from the reported value 10.3 by more than 10 %

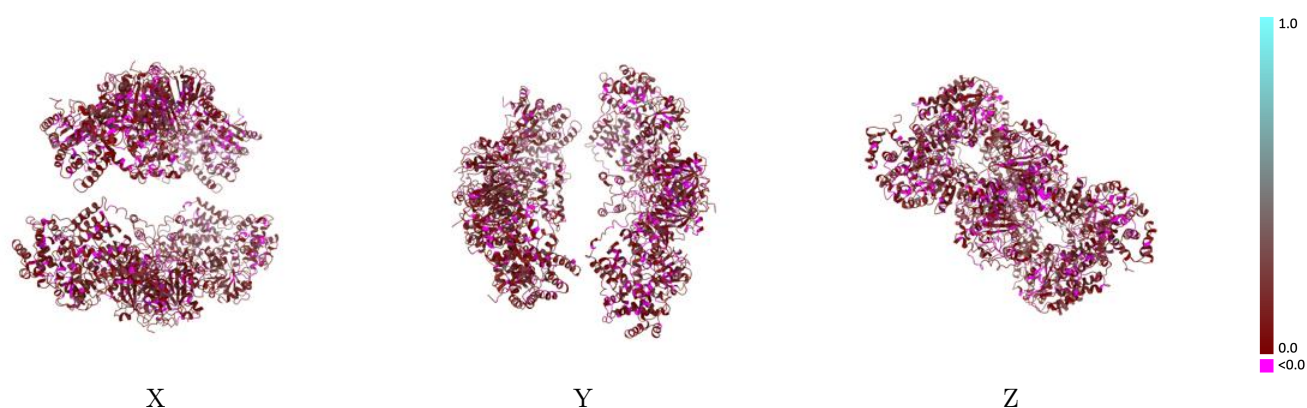
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16134 and PDB model 8BNR. Per-residue inclusion information can be found in section 3 on page 7.

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

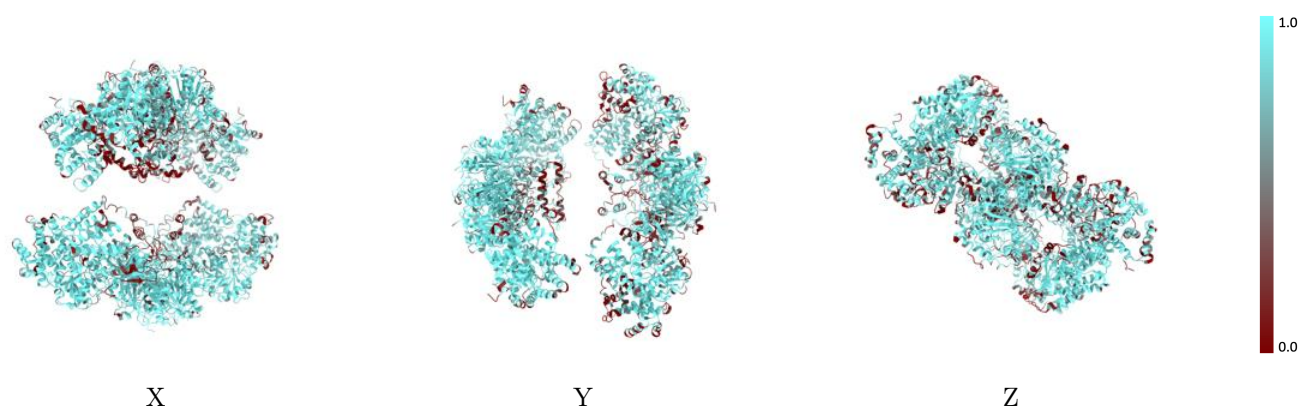
This section was not generated.

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



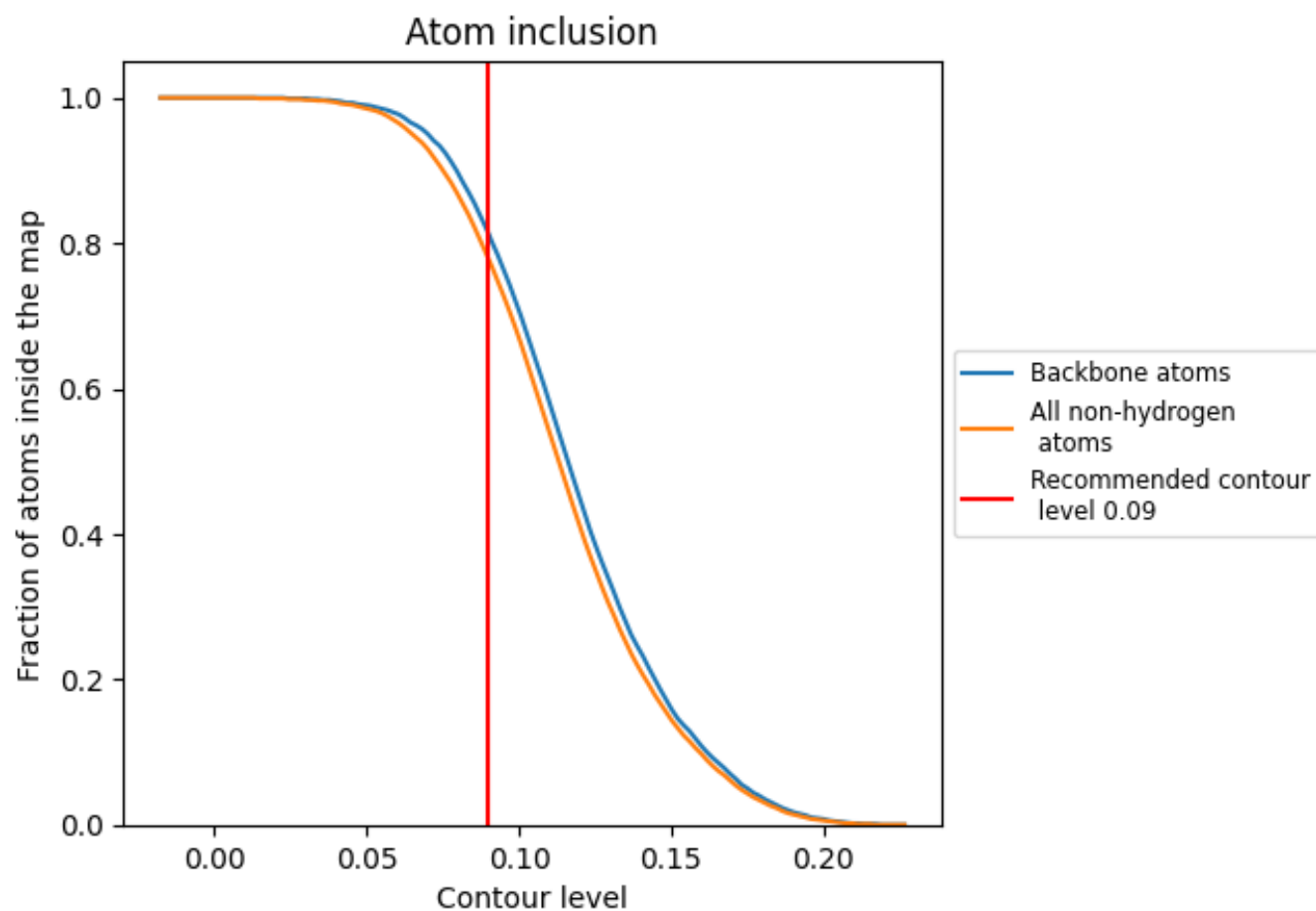
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 78% 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 (0.09) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion               | Q-score                      |
|-------|------------------------------|------------------------------|
| All   | <div><div></div>0.7790</div> | <div><div></div>0.1100</div> |
| A     | <div><div></div>0.8430</div> | <div><div></div>0.1230</div> |
| B     | <div><div></div>0.8440</div> | <div><div></div>0.1280</div> |
| C     | <div><div></div>0.8340</div> | <div><div></div>0.1220</div> |
| D     | <div><div></div>0.8300</div> | <div><div></div>0.1210</div> |
| E     | <div><div></div>0.7700</div> | <div><div></div>0.0910</div> |
| F     | <div><div></div>0.7770</div> | <div><div></div>0.0890</div> |
| G     | <div><div></div>0.6910</div> | <div><div></div>0.1020</div> |
| H     | <div><div></div>0.6910</div> | <div><div></div>0.0980</div> |

1.0

0.0

<0.0