



## Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 08:13 PM UTC

PDB ID : 9C0D / pdb\_00009c0d  
EMDB ID : EMD-45080  
Title : E.Faecium GroEL  
Authors : Watson, E.R.; Lander, G.C.  
Deposited on : 2024-05-25  
Resolution : 3.97 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:

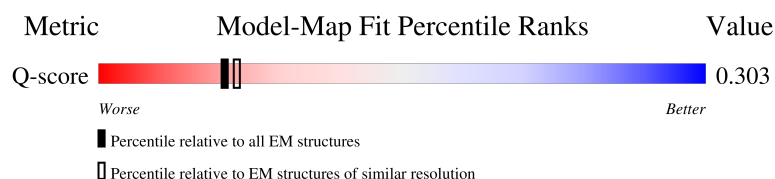
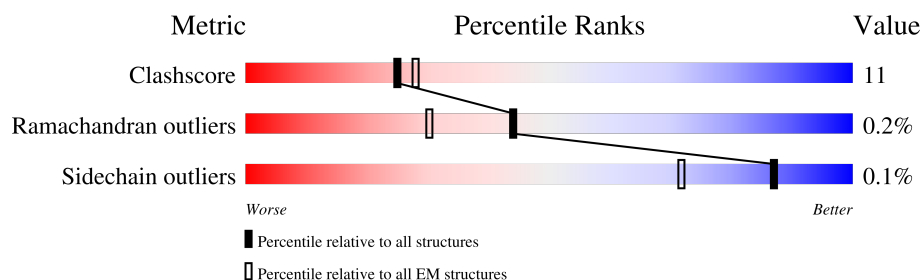
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 3.97 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.



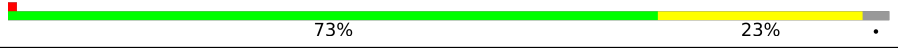
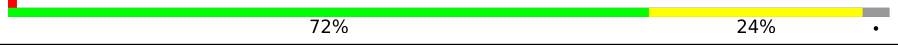
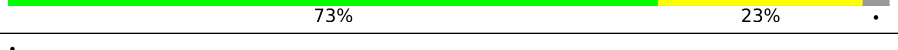
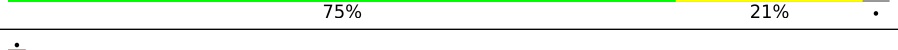
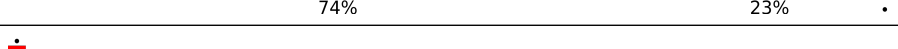
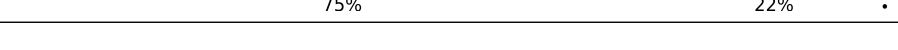
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 7578 ( 3.47 - 4.47 )                                     |

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     | 541    |                  |
| 1   | B     | 541    |                  |
| 1   | C     | 541    |                  |
| 1   | D     | 541    |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 1   | E     | 541    |  |
| 1   | F     | 541    |  |
| 1   | G     | 541    |  |
| 1   | H     | 541    |  |
| 1   | I     | 541    |  |
| 1   | J     | 541    |  |
| 1   | K     | 541    |  |
| 1   | L     | 541    |  |
| 1   | M     | 541    |  |
| 1   | N     | 541    |  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 54530 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.

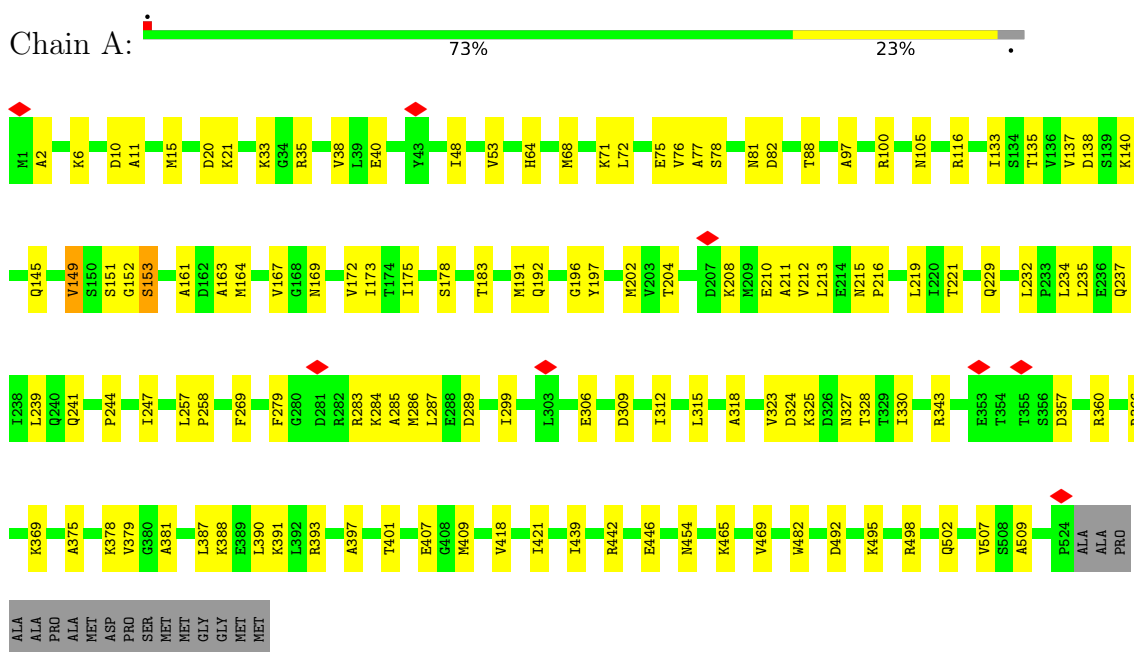
- Molecule 1 is a protein called Chaperonin GroEL.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3895  | 2428 | 662 | 795 | 10 |         |       |
| 1   | B     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3895  | 2428 | 662 | 795 | 10 |         |       |
| 1   | C     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3895  | 2428 | 662 | 795 | 10 |         |       |
| 1   | I     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3895  | 2428 | 662 | 795 | 10 |         |       |
| 1   | D     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3895  | 2428 | 662 | 795 | 10 |         |       |
| 1   | J     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3895  | 2428 | 662 | 795 | 10 |         |       |
| 1   | E     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3895  | 2428 | 662 | 795 | 10 |         |       |
| 1   | K     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3895  | 2428 | 662 | 795 | 10 |         |       |
| 1   | F     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3895  | 2428 | 662 | 795 | 10 |         |       |
| 1   | L     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3895  | 2428 | 662 | 795 | 10 |         |       |
| 1   | G     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3895  | 2428 | 662 | 795 | 10 |         |       |
| 1   | M     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3895  | 2428 | 662 | 795 | 10 |         |       |
| 1   | H     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3895  | 2428 | 662 | 795 | 10 |         |       |
| 1   | N     | 524      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3895  | 2428 | 662 | 795 | 10 |         |       |

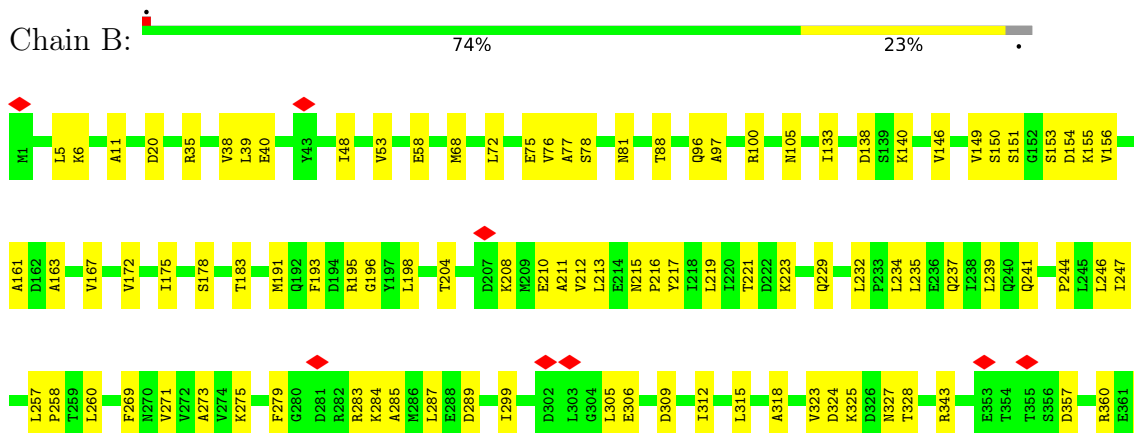
### 3 Residue-property plots

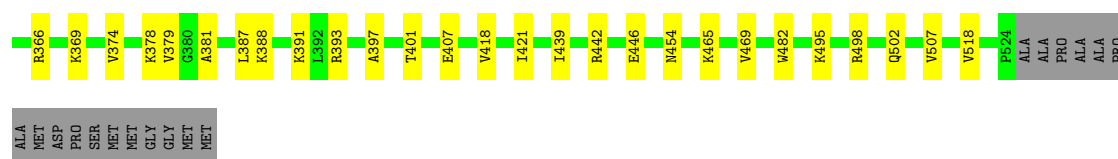
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

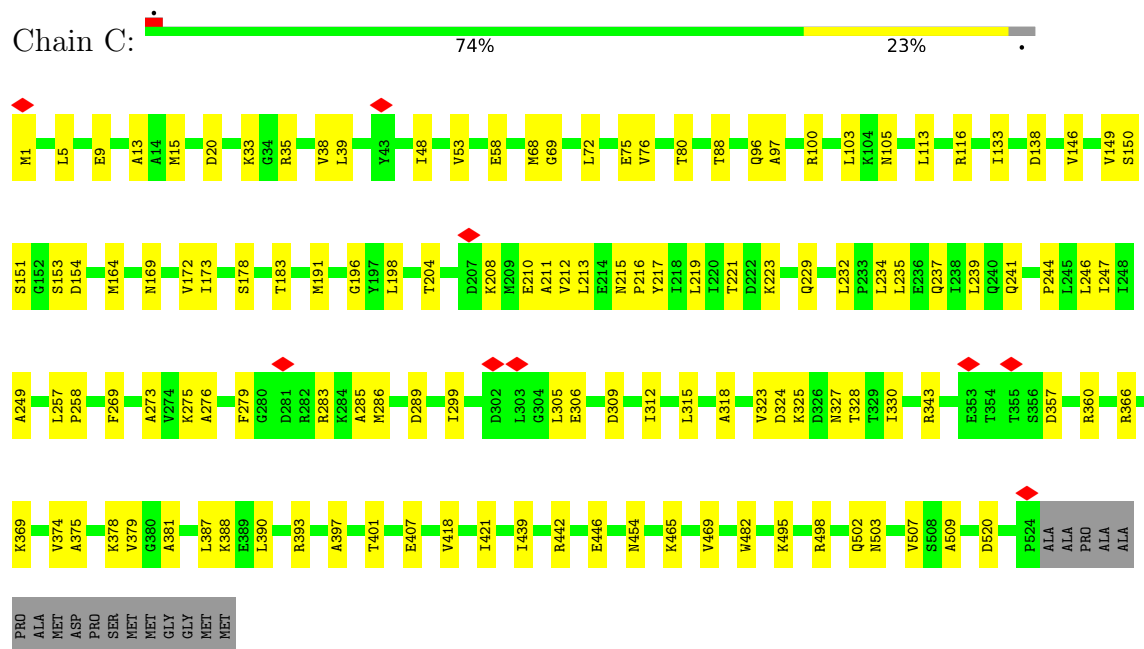


#### • Molecule 1: Chaperonin GroEL

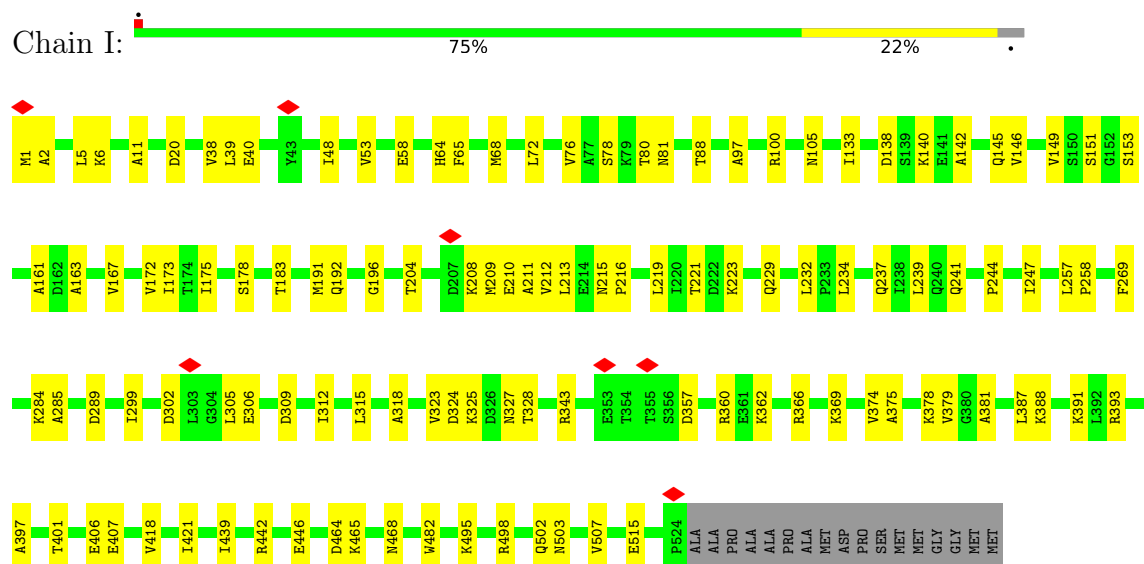




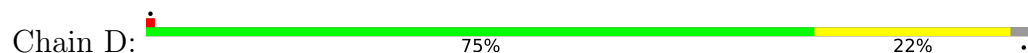
• Molecule 1: Chaperonin GroEL

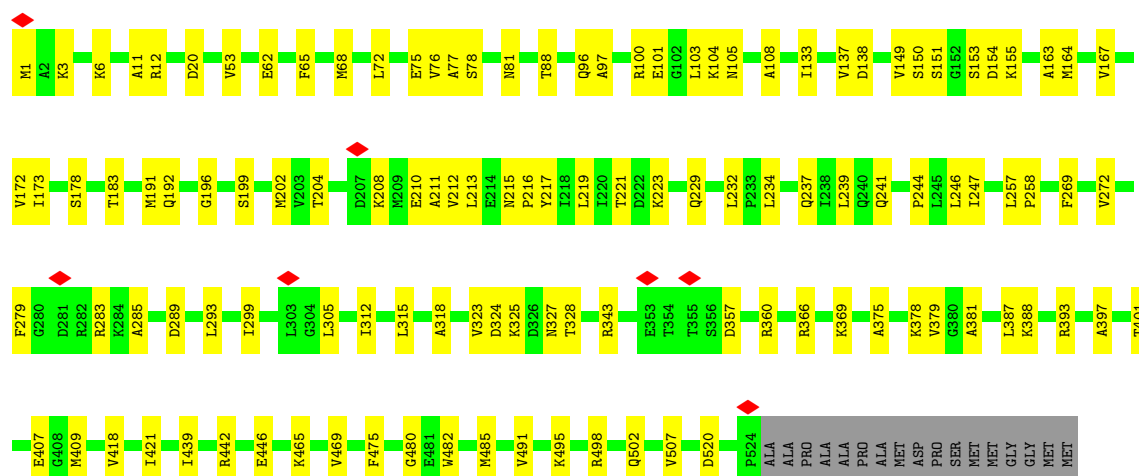


• Molecule 1: Chaperonin GroEL



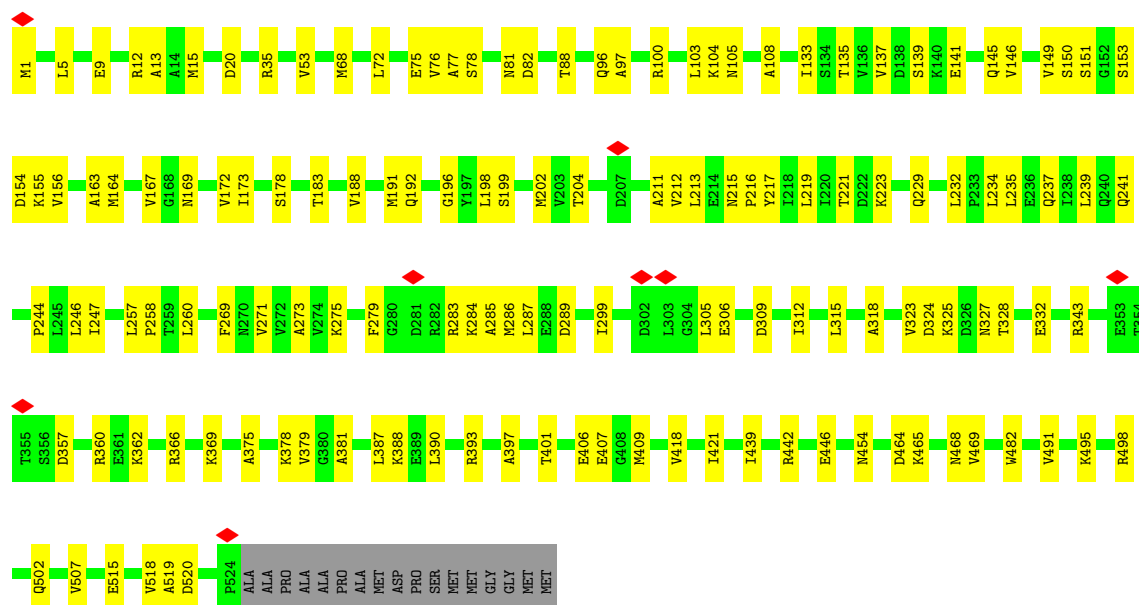
• Molecule 1: Chaperonin GroEL





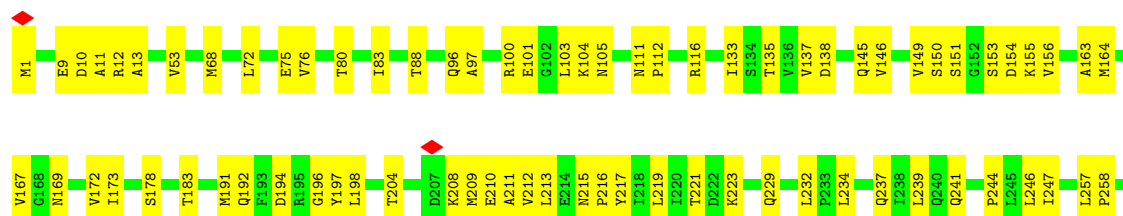
• Molecule 1: Chaperonin GroEL

Chain J: 71% 26%

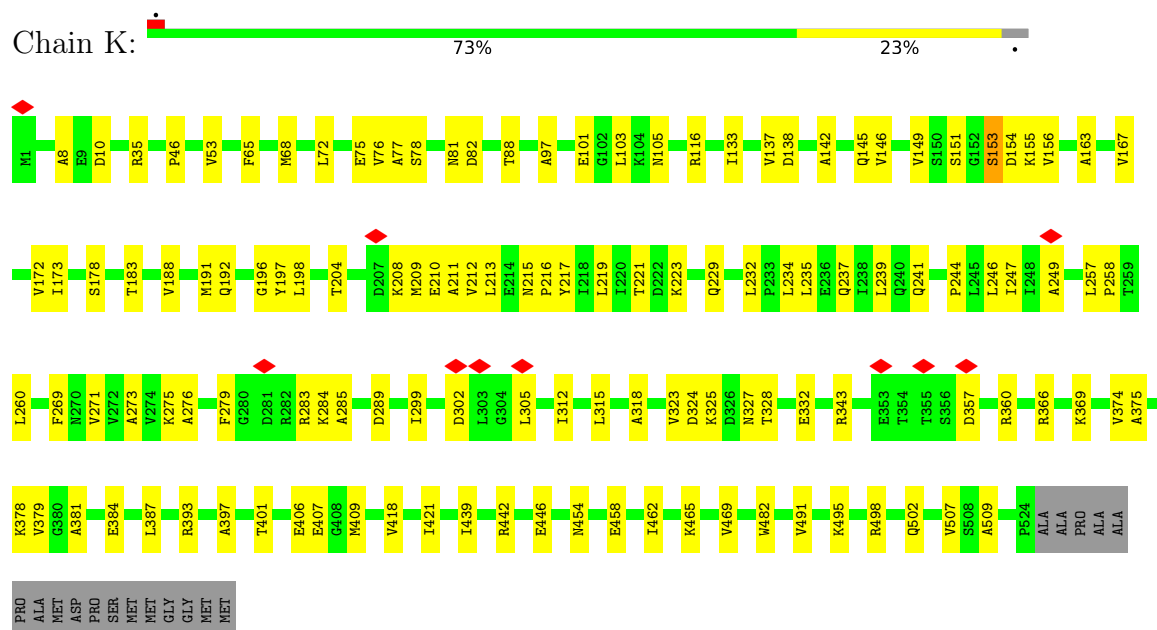


• Molecule 1: Chaperonin GroEL

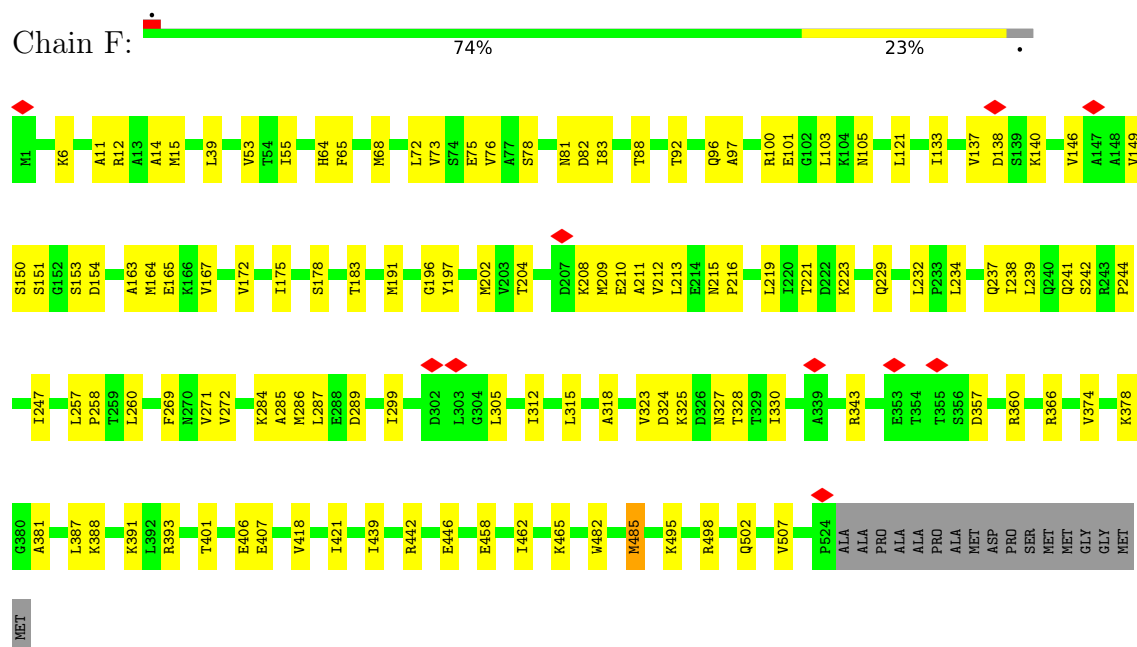
Chain E: 72% 25%



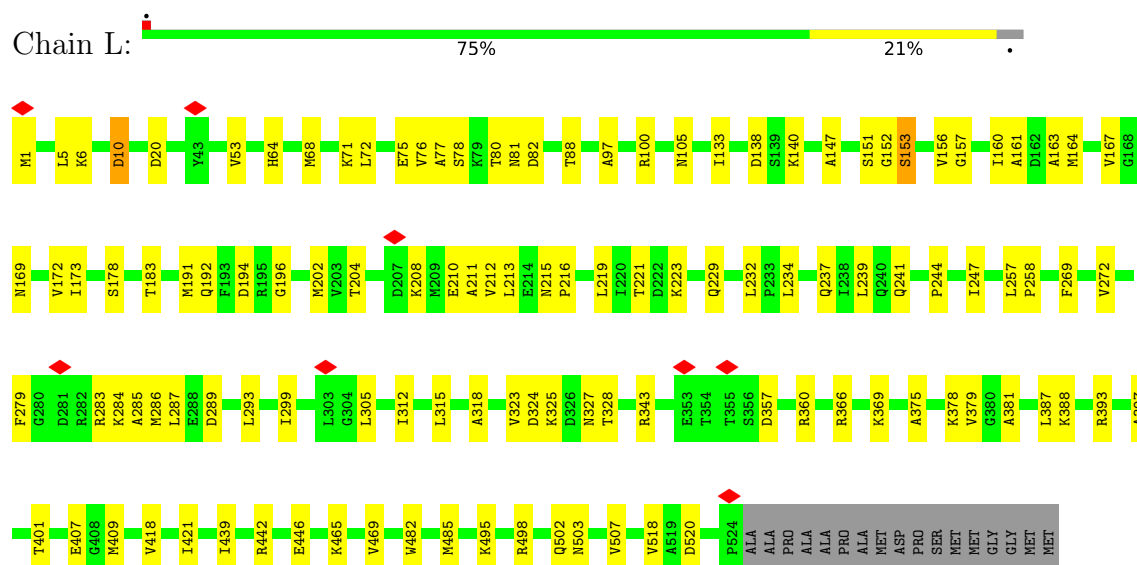
- Molecule 1: Chaperonin GroEL



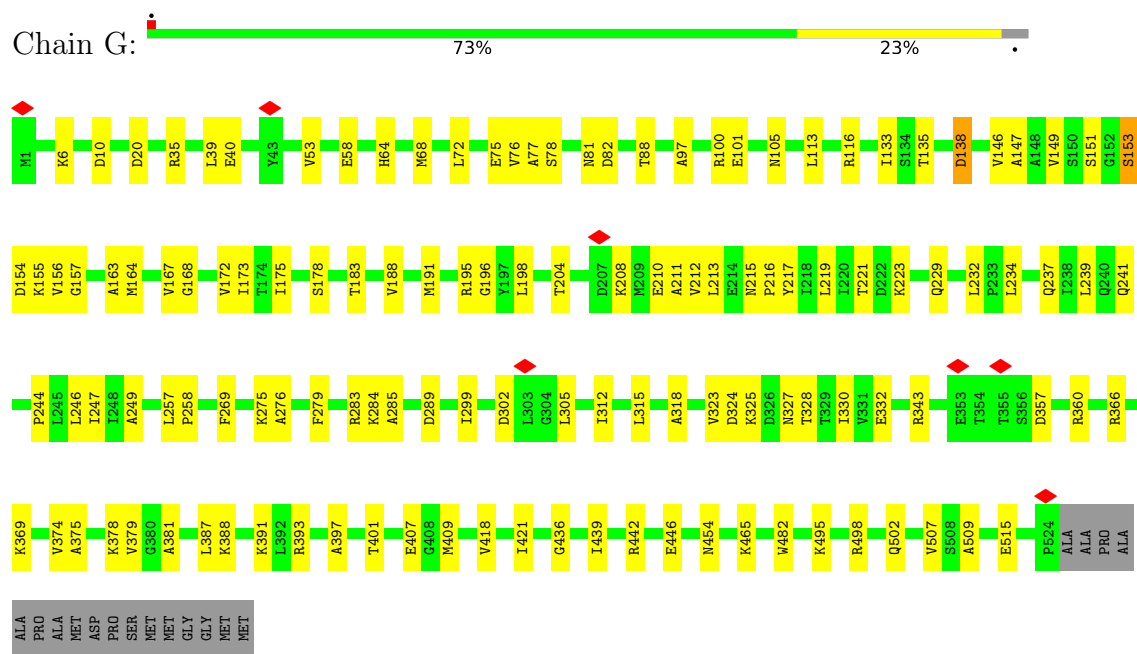
- Molecule 1: Chaperonin GroEL



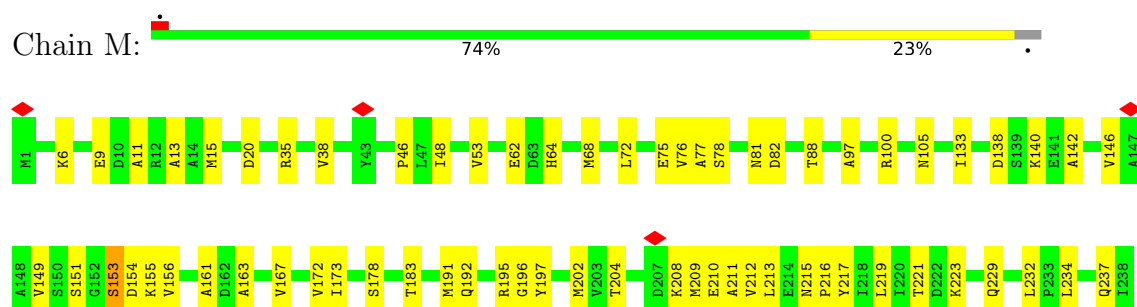
- Molecule 1: Chaperonin GroEL

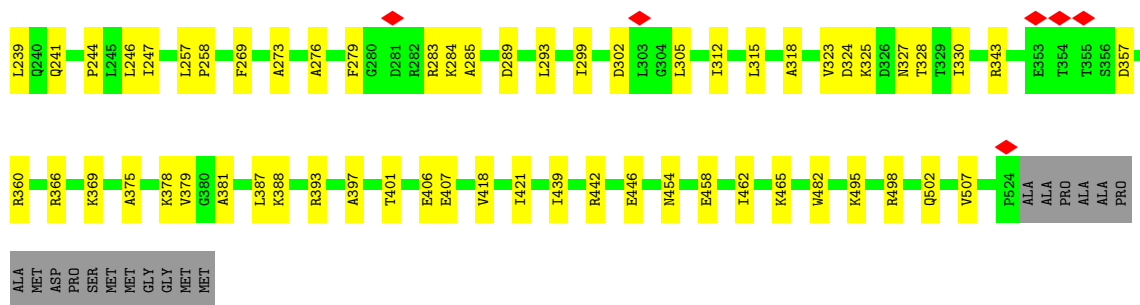


- Molecule 1: Chaperonin GroEL



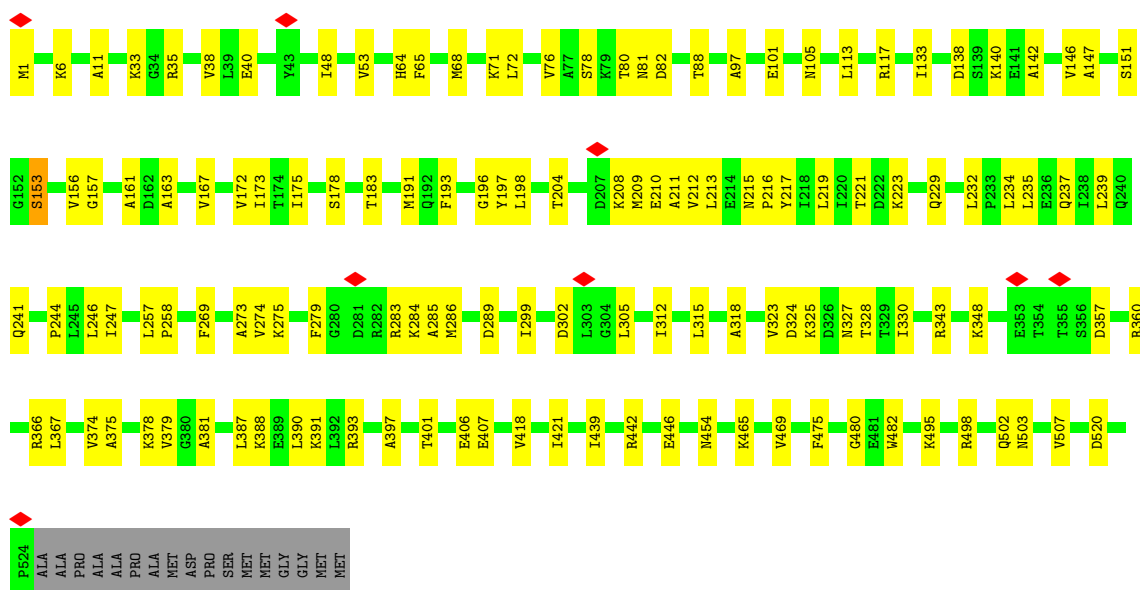
- Molecule 1: Chaperonin GroEL





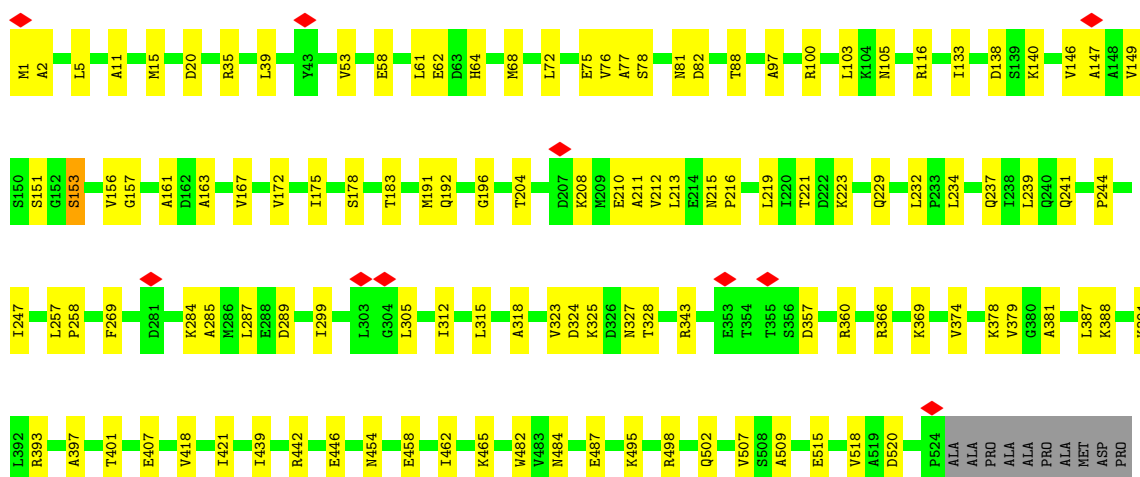
### • Molecule 1: Chaperonin GroEL

Chain H: 72% 24%



### • Molecule 1: Chaperonin GroEL

Chain N: 75% 22%



SER  
MET  
MET  
GLY  
GLY  
MET  
MET

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 10837                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TALOS ARCTICA                       | Depositor |
| Voltage (kV)                         | 200                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 62.5                                    | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 1500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.923                                   | Depositor |
| Minimum map value                    | -0.356                                  | Depositor |
| Average map value                    | 0.014                                   | Depositor |
| Map value standard deviation         | 0.053                                   | Depositor |
| Recommended contour level            | 0.175                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 294.4, 294.4, 294.4                     | wwPDB     |
| Map dimensions                       | 256, 256, 256                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.15, 1.15, 1.15                        | 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     | 0.14         | 0/3923  | 0.32        | 0/5312         |
| 1   | B     | 0.15         | 0/3923  | 0.32        | 0/5312         |
| 1   | C     | 0.15         | 0/3923  | 0.32        | 0/5312         |
| 1   | D     | 0.14         | 0/3923  | 0.32        | 0/5312         |
| 1   | E     | 0.14         | 0/3923  | 0.31        | 0/5312         |
| 1   | F     | 0.15         | 0/3923  | 0.33        | 0/5312         |
| 1   | G     | 0.14         | 0/3923  | 0.32        | 0/5312         |
| 1   | H     | 0.14         | 0/3923  | 0.33        | 0/5312         |
| 1   | I     | 0.14         | 0/3923  | 0.33        | 0/5312         |
| 1   | J     | 0.14         | 0/3923  | 0.32        | 0/5312         |
| 1   | K     | 0.15         | 0/3923  | 0.34        | 1/5312 (0.0%)  |
| 1   | L     | 0.15         | 0/3923  | 0.33        | 0/5312         |
| 1   | M     | 0.15         | 0/3923  | 0.32        | 0/5312         |
| 1   | N     | 0.14         | 0/3923  | 0.32        | 0/5312         |
| All | All   | 0.15         | 0/54922 | 0.32        | 1/74368 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | K     | 8   | ALA  | CB-CA-C | -5.82 | 109.88      | 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     | 3895  | 0        | 4014     | 87      | 0            |
| 1   | B     | 3895  | 0        | 4014     | 87      | 0            |
| 1   | C     | 3895  | 0        | 4014     | 84      | 0            |
| 1   | D     | 3895  | 0        | 4014     | 80      | 0            |
| 1   | E     | 3895  | 0        | 4014     | 90      | 0            |
| 1   | F     | 3895  | 0        | 4014     | 82      | 0            |
| 1   | G     | 3895  | 0        | 4014     | 85      | 0            |
| 1   | H     | 3895  | 0        | 4014     | 89      | 0            |
| 1   | I     | 3895  | 0        | 4014     | 79      | 0            |
| 1   | J     | 3895  | 0        | 4014     | 96      | 0            |
| 1   | K     | 3895  | 0        | 4014     | 85      | 0            |
| 1   | L     | 3895  | 0        | 4014     | 80      | 0            |
| 1   | M     | 3895  | 0        | 4014     | 82      | 0            |
| 1   | N     | 3895  | 0        | 4014     | 82      | 0            |
| All | All   | 54530 | 0        | 56196    | 1167    | 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 11.

All (1167) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:K:151:SER:HB2 | 1:K:393:ARG:HE   | 1.49                     | 0.78              |
| 1:M:151:SER:HB2 | 1:M:393:ARG:HE   | 1.50                     | 0.77              |
| 1:J:76:VAL:HG22 | 1:J:507:VAL:HG21 | 1.67                     | 0.76              |
| 1:N:151:SER:HB2 | 1:N:393:ARG:HE   | 1.52                     | 0.75              |
| 1:F:381:ALA:HB3 | 1:F:387:LEU:HG   | 1.68                     | 0.74              |
| 1:N:381:ALA:HB3 | 1:N:387:LEU:HG   | 1.69                     | 0.74              |
| 1:M:381:ALA:HB3 | 1:M:387:LEU:HG   | 1.69                     | 0.74              |
| 1:H:151:SER:HB2 | 1:H:393:ARG:HE   | 1.53                     | 0.74              |
| 1:I:151:SER:HB2 | 1:I:393:ARG:HE   | 1.52                     | 0.74              |
| 1:G:76:VAL:HG22 | 1:G:507:VAL:HG21 | 1.70                     | 0.73              |
| 1:G:151:SER:HB2 | 1:G:393:ARG:HE   | 1.54                     | 0.73              |
| 1:D:381:ALA:HB3 | 1:D:387:LEU:HG   | 1.70                     | 0.73              |
| 1:L:151:SER:HB2 | 1:L:393:ARG:HE   | 1.53                     | 0.73              |
| 1:A:381:ALA:HB3 | 1:A:387:LEU:HG   | 1.70                     | 0.73              |
| 1:I:381:ALA:HB3 | 1:I:387:LEU:HG   | 1.70                     | 0.73              |
| 1:G:381:ALA:HB3 | 1:G:387:LEU:HG   | 1.71                     | 0.72              |
| 1:E:381:ALA:HB3 | 1:E:387:LEU:HG   | 1.70                     | 0.72              |
| 1:K:381:ALA:HB3 | 1:K:387:LEU:HG   | 1.69                     | 0.72              |
| 1:H:381:ALA:HB3 | 1:H:387:LEU:HG   | 1.70                     | 0.72              |
| 1:E:72:LEU:O    | 1:E:76:VAL:HG23  | 1.90                     | 0.72              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:L:381:ALA:HB3 | 1:L:387:LEU:HG   | 1.70                     | 0.72              |
| 1:E:191:MET:HE1 | 1:E:369:LYS:HB3  | 1.71                     | 0.72              |
| 1:C:381:ALA:HB3 | 1:C:387:LEU:HG   | 1.70                     | 0.71              |
| 1:F:151:SER:HB2 | 1:F:393:ARG:HH21 | 1.54                     | 0.71              |
| 1:B:381:ALA:HB3 | 1:B:387:LEU:HG   | 1.70                     | 0.71              |
| 1:J:381:ALA:HB3 | 1:J:387:LEU:HG   | 1.71                     | 0.70              |
| 1:E:153:SER:OG  | 1:E:154:ASP:N    | 2.23                     | 0.70              |
| 1:M:191:MET:HG2 | 1:M:293:LEU:HD22 | 1.72                     | 0.70              |
| 1:F:76:VAL:HG22 | 1:F:507:VAL:HG21 | 1.74                     | 0.70              |
| 1:H:1:MET:HE3   | 1:H:520:ASP:HB3  | 1.72                     | 0.70              |
| 1:E:153:SER:H   | 1:E:393:ARG:HH11 | 1.37                     | 0.70              |
| 1:D:485:MET:N   | 1:D:485:MET:SD   | 2.65                     | 0.69              |
| 1:J:151:SER:HB2 | 1:J:393:ARG:HE   | 1.57                     | 0.69              |
| 1:G:191:MET:HE1 | 1:G:369:LYS:HB3  | 1.75                     | 0.69              |
| 1:F:72:LEU:O    | 1:F:76:VAL:HG23  | 1.93                     | 0.68              |
| 1:B:68:MET:SD   | 1:I:40:GLU:HG2   | 2.33                     | 0.68              |
| 1:B:191:MET:HE1 | 1:B:369:LYS:HB3  | 1.76                     | 0.68              |
| 1:L:1:MET:HE3   | 1:L:520:ASP:HB3  | 1.76                     | 0.68              |
| 1:D:151:SER:HB2 | 1:D:393:ARG:HE   | 1.59                     | 0.67              |
| 1:J:1:MET:HE1   | 1:J:520:ASP:HB3  | 1.76                     | 0.67              |
| 1:D:72:LEU:O    | 1:D:76:VAL:HG23  | 1.92                     | 0.67              |
| 1:F:485:MET:SD  | 1:F:485:MET:N    | 2.67                     | 0.67              |
| 1:M:6:LYS:HG2   | 1:M:11:ALA:HB2   | 1.75                     | 0.67              |
| 1:A:76:VAL:HG22 | 1:A:507:VAL:HG21 | 1.77                     | 0.67              |
| 1:A:72:LEU:O    | 1:A:76:VAL:HG23  | 1.94                     | 0.67              |
| 1:M:191:MET:HE1 | 1:M:369:LYS:HB3  | 1.77                     | 0.66              |
| 1:E:191:MET:HG2 | 1:E:293:LEU:HD22 | 1.77                     | 0.66              |
| 1:K:191:MET:HE1 | 1:K:369:LYS:HB3  | 1.76                     | 0.66              |
| 1:B:72:LEU:O    | 1:B:76:VAL:HG23  | 1.95                     | 0.66              |
| 1:L:72:LEU:O    | 1:L:76:VAL:HG23  | 1.95                     | 0.66              |
| 1:C:72:LEU:O    | 1:C:76:VAL:HG23  | 1.95                     | 0.66              |
| 1:K:76:VAL:HG22 | 1:K:507:VAL:HG21 | 1.78                     | 0.66              |
| 1:F:324:ASP:OD1 | 1:F:327:ASN:N    | 2.28                     | 0.65              |
| 1:L:76:VAL:HG22 | 1:L:507:VAL:HG21 | 1.78                     | 0.65              |
| 1:J:191:MET:HE1 | 1:J:369:LYS:HB3  | 1.78                     | 0.65              |
| 1:J:153:SER:OG  | 1:J:154:ASP:N    | 2.25                     | 0.65              |
| 1:G:498:ARG:NH1 | 1:G:502:GLN:OE1  | 2.30                     | 0.65              |
| 1:G:324:ASP:OD1 | 1:G:327:ASN:N    | 2.28                     | 0.65              |
| 1:M:324:ASP:OD1 | 1:M:327:ASN:N    | 2.28                     | 0.65              |
| 1:D:6:LYS:HG2   | 1:D:11:ALA:HB2   | 1.78                     | 0.65              |
| 1:D:78:SER:HA   | 1:D:81:ASN:HD21  | 1.60                     | 0.65              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:498:ARG:NH1 | 1:D:502:GLN:OE1  | 2.30                     | 0.65              |
| 1:M:72:LEU:O    | 1:M:76:VAL:HG23  | 1.96                     | 0.65              |
| 1:I:80:THR:OG1  | 1:I:503:ASN:ND2  | 2.30                     | 0.65              |
| 1:J:72:LEU:O    | 1:J:76:VAL:HG23  | 1.96                     | 0.65              |
| 1:J:324:ASP:OD1 | 1:J:327:ASN:N    | 2.28                     | 0.64              |
| 1:H:324:ASP:OD1 | 1:H:327:ASN:N    | 2.28                     | 0.64              |
| 1:L:324:ASP:OD1 | 1:L:327:ASN:N    | 2.28                     | 0.64              |
| 1:G:289:ASP:OD1 | 1:G:343:ARG:NE   | 2.29                     | 0.64              |
| 1:N:324:ASP:OD1 | 1:N:327:ASN:N    | 2.28                     | 0.64              |
| 1:N:76:VAL:HG22 | 1:N:507:VAL:HG21 | 1.78                     | 0.64              |
| 1:D:191:MET:HE1 | 1:D:369:LYS:HB3  | 1.80                     | 0.64              |
| 1:N:72:LEU:O    | 1:N:76:VAL:HG23  | 1.96                     | 0.64              |
| 1:B:76:VAL:HG22 | 1:B:507:VAL:HG21 | 1.79                     | 0.64              |
| 1:I:81:ASN:HB3  | 1:I:88:THR:HB    | 1.80                     | 0.64              |
| 1:M:289:ASP:OD1 | 1:M:343:ARG:NE   | 2.31                     | 0.64              |
| 1:M:76:VAL:HG22 | 1:M:507:VAL:HG21 | 1.79                     | 0.63              |
| 1:E:407:GLU:HG3 | 1:E:495:LYS:HB2  | 1.80                     | 0.63              |
| 1:B:324:ASP:OD1 | 1:B:327:ASN:N    | 2.28                     | 0.63              |
| 1:H:72:LEU:O    | 1:H:76:VAL:HG23  | 1.98                     | 0.63              |
| 1:D:324:ASP:OD1 | 1:D:327:ASN:N    | 2.28                     | 0.63              |
| 1:B:6:LYS:HG2   | 1:B:11:ALA:HB2   | 1.80                     | 0.63              |
| 1:A:6:LYS:HG2   | 1:A:11:ALA:HB2   | 1.80                     | 0.63              |
| 1:A:324:ASP:OD1 | 1:A:327:ASN:N    | 2.28                     | 0.63              |
| 1:C:76:VAL:HG22 | 1:C:507:VAL:HG21 | 1.81                     | 0.62              |
| 1:E:324:ASP:OD1 | 1:E:327:ASN:N    | 2.28                     | 0.62              |
| 1:N:289:ASP:OD1 | 1:N:343:ARG:NE   | 2.28                     | 0.62              |
| 1:I:324:ASP:OD1 | 1:I:327:ASN:N    | 2.28                     | 0.62              |
| 1:K:211:ALA:HB3 | 1:K:323:VAL:HB   | 1.82                     | 0.62              |
| 1:C:80:THR:OG1  | 1:C:503:ASN:ND2  | 2.33                     | 0.62              |
| 1:N:11:ALA:O    | 1:N:15:MET:HG2   | 1.99                     | 0.62              |
| 1:C:498:ARG:NH1 | 1:C:502:GLN:OE1  | 2.33                     | 0.62              |
| 1:I:498:ARG:NH1 | 1:I:502:GLN:OE1  | 2.32                     | 0.62              |
| 1:K:324:ASP:OD1 | 1:K:327:ASN:N    | 2.28                     | 0.62              |
| 1:G:442:ARG:O   | 1:G:442:ARG:NH1  | 2.31                     | 0.62              |
| 1:J:77:ALA:O    | 1:J:81:ASN:ND2   | 2.33                     | 0.62              |
| 1:L:442:ARG:O   | 1:L:442:ARG:NH1  | 2.32                     | 0.62              |
| 1:C:442:ARG:O   | 1:C:442:ARG:NH1  | 2.31                     | 0.62              |
| 1:D:1:MET:HE3   | 1:D:520:ASP:HB3  | 1.82                     | 0.62              |
| 1:L:68:MET:HA   | 1:L:68:MET:HE3   | 1.81                     | 0.62              |
| 1:H:442:ARG:O   | 1:H:442:ARG:NH1  | 2.31                     | 0.62              |
| 1:F:211:ALA:HB3 | 1:F:323:VAL:HB   | 1.82                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:77:ALA:O     | 1:N:81:ASN:ND2   | 2.33                     | 0.62              |
| 1:H:323:VAL:HG22 | 1:H:328:THR:HG23 | 1.81                     | 0.62              |
| 1:N:498:ARG:NH1  | 1:N:502:GLN:OE1  | 2.33                     | 0.62              |
| 1:A:64:HIS:O     | 1:A:68:MET:HG2   | 1.99                     | 0.61              |
| 1:I:442:ARG:O    | 1:I:442:ARG:NH1  | 2.32                     | 0.61              |
| 1:E:76:VAL:HG22  | 1:E:507:VAL:HG21 | 1.82                     | 0.61              |
| 1:E:211:ALA:HB3  | 1:E:323:VAL:HB   | 1.82                     | 0.61              |
| 1:G:77:ALA:O     | 1:G:81:ASN:ND2   | 2.33                     | 0.61              |
| 1:E:498:ARG:NH1  | 1:E:502:GLN:OE1  | 2.34                     | 0.61              |
| 1:K:216:PRO:HB3  | 1:K:244:PRO:HB2  | 1.82                     | 0.61              |
| 1:L:289:ASP:OD1  | 1:L:343:ARG:NE   | 2.33                     | 0.61              |
| 1:M:498:ARG:NH1  | 1:M:502:GLN:OE1  | 2.33                     | 0.61              |
| 1:A:289:ASP:OD1  | 1:A:343:ARG:NE   | 2.33                     | 0.61              |
| 1:I:72:LEU:O     | 1:I:76:VAL:HG23  | 1.99                     | 0.61              |
| 1:L:191:MET:HE1  | 1:L:369:LYS:HB3  | 1.83                     | 0.61              |
| 1:E:442:ARG:O    | 1:E:442:ARG:NH1  | 2.30                     | 0.61              |
| 1:L:211:ALA:HB3  | 1:L:323:VAL:HB   | 1.82                     | 0.61              |
| 1:G:515:GLU:N    | 1:G:515:GLU:OE1  | 2.34                     | 0.61              |
| 1:C:164:MET:HE1  | 1:C:169:ASN:HA   | 1.83                     | 0.61              |
| 1:C:323:VAL:HG22 | 1:C:328:THR:HG23 | 1.82                     | 0.61              |
| 1:D:76:VAL:HG22  | 1:D:507:VAL:HG21 | 1.83                     | 0.61              |
| 1:D:442:ARG:O    | 1:D:442:ARG:NH1  | 2.31                     | 0.61              |
| 1:J:216:PRO:HB3  | 1:J:244:PRO:HB2  | 1.83                     | 0.61              |
| 1:A:211:ALA:HB3  | 1:A:323:VAL:HB   | 1.84                     | 0.60              |
| 1:C:211:ALA:HB3  | 1:C:323:VAL:HB   | 1.83                     | 0.60              |
| 1:D:211:ALA:HB3  | 1:D:323:VAL:HB   | 1.83                     | 0.60              |
| 1:J:323:VAL:HG22 | 1:J:328:THR:HG23 | 1.83                     | 0.60              |
| 1:F:465:LYS:HZ3  | 1:F:482:TRP:CD1  | 2.19                     | 0.60              |
| 1:B:442:ARG:O    | 1:B:442:ARG:NH1  | 2.33                     | 0.60              |
| 1:I:289:ASP:OD1  | 1:I:343:ARG:NE   | 2.31                     | 0.60              |
| 1:H:76:VAL:HG22  | 1:H:507:VAL:HG21 | 1.83                     | 0.60              |
| 1:L:498:ARG:NH1  | 1:L:502:GLN:OE1  | 2.34                     | 0.60              |
| 1:H:407:GLU:HG3  | 1:H:495:LYS:HB2  | 1.83                     | 0.60              |
| 1:A:323:VAL:HG22 | 1:A:328:THR:HG23 | 1.82                     | 0.60              |
| 1:K:442:ARG:O    | 1:K:442:ARG:NH1  | 2.33                     | 0.60              |
| 1:F:498:ARG:NH1  | 1:F:502:GLN:OE1  | 2.34                     | 0.60              |
| 1:G:211:ALA:HB3  | 1:G:323:VAL:HB   | 1.83                     | 0.60              |
| 1:N:241:GLN:HE21 | 1:N:312:ILE:HD13 | 1.66                     | 0.60              |
| 1:B:216:PRO:HB3  | 1:B:244:PRO:HB2  | 1.83                     | 0.60              |
| 1:C:216:PRO:HB3  | 1:C:244:PRO:HB2  | 1.84                     | 0.60              |
| 1:E:401:THR:O    | 1:E:405:VAL:HG23 | 2.01                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:77:ALA:O     | 1:M:81:ASN:ND2   | 2.35                     | 0.60              |
| 1:N:323:VAL:HG22 | 1:N:328:THR:HG23 | 1.83                     | 0.60              |
| 1:I:241:GLN:HE21 | 1:I:312:ILE:HD13 | 1.67                     | 0.60              |
| 1:I:323:VAL:HG22 | 1:I:328:THR:HG23 | 1.82                     | 0.60              |
| 1:B:323:VAL:HG22 | 1:B:328:THR:HG23 | 1.82                     | 0.60              |
| 1:C:324:ASP:OD1  | 1:C:327:ASN:N    | 2.28                     | 0.60              |
| 1:E:1:MET:HE3    | 1:E:520:ASP:HB3  | 1.84                     | 0.60              |
| 1:H:498:ARG:NH1  | 1:H:502:GLN:OE1  | 2.34                     | 0.60              |
| 1:K:323:VAL:HG22 | 1:K:328:THR:HG23 | 1.83                     | 0.60              |
| 1:A:442:ARG:O    | 1:A:442:ARG:NH1  | 2.31                     | 0.60              |
| 1:K:72:LEU:O     | 1:K:76:VAL:HG23  | 2.02                     | 0.60              |
| 1:A:498:ARG:NH1  | 1:A:502:GLN:OE1  | 2.35                     | 0.60              |
| 1:J:442:ARG:O    | 1:J:442:ARG:NH1  | 2.31                     | 0.60              |
| 1:M:357:ASP:OD1  | 1:M:360:ARG:NH1  | 2.34                     | 0.60              |
| 1:I:76:VAL:HG22  | 1:I:507:VAL:HG21 | 1.84                     | 0.59              |
| 1:F:53:VAL:HB    | 1:F:88:THR:HG21  | 1.84                     | 0.59              |
| 1:L:5:LEU:HD22   | 1:L:518:VAL:HG22 | 1.83                     | 0.59              |
| 1:N:465:LYS:HZ3  | 1:N:482:TRP:CD1  | 2.20                     | 0.59              |
| 1:B:498:ARG:NH1  | 1:B:502:GLN:OE1  | 2.35                     | 0.59              |
| 1:F:323:VAL:HG22 | 1:F:328:THR:HG23 | 1.82                     | 0.59              |
| 1:M:465:LYS:HZ3  | 1:M:482:TRP:CD1  | 2.20                     | 0.59              |
| 1:B:211:ALA:HB3  | 1:B:323:VAL:HB   | 1.85                     | 0.59              |
| 1:C:151:SER:O    | 1:C:393:ARG:NE   | 2.34                     | 0.59              |
| 1:L:323:VAL:HG22 | 1:L:328:THR:HG23 | 1.83                     | 0.59              |
| 1:G:323:VAL:HG22 | 1:G:328:THR:HG23 | 1.82                     | 0.59              |
| 1:I:465:LYS:HZ3  | 1:I:482:TRP:CD1  | 2.21                     | 0.59              |
| 1:E:53:VAL:HB    | 1:E:88:THR:HG21  | 1.84                     | 0.59              |
| 1:F:149:VAL:HG12 | 1:F:150:SER:H    | 1.68                     | 0.59              |
| 1:G:465:LYS:HZ3  | 1:G:482:TRP:CD1  | 2.21                     | 0.59              |
| 1:H:211:ALA:HB3  | 1:H:323:VAL:HB   | 1.84                     | 0.59              |
| 1:H:216:PRO:HB3  | 1:H:244:PRO:HB2  | 1.85                     | 0.59              |
| 1:H:241:GLN:HE21 | 1:H:312:ILE:HD13 | 1.68                     | 0.59              |
| 1:A:216:PRO:HB3  | 1:A:244:PRO:HB2  | 1.85                     | 0.59              |
| 1:C:20:ASP:OD1   | 1:C:100:ARG:NH1  | 2.35                     | 0.59              |
| 1:K:241:GLN:HE21 | 1:K:312:ILE:HD13 | 1.68                     | 0.59              |
| 1:M:20:ASP:OD1   | 1:M:100:ARG:NH1  | 2.36                     | 0.59              |
| 1:K:77:ALA:O     | 1:K:81:ASN:ND2   | 2.36                     | 0.59              |
| 1:I:515:GLU:N    | 1:I:515:GLU:OE1  | 2.35                     | 0.59              |
| 1:J:498:ARG:NH1  | 1:J:502:GLN:OE1  | 2.36                     | 0.59              |
| 1:F:241:GLN:HE21 | 1:F:312:ILE:HD13 | 1.66                     | 0.59              |
| 1:G:241:GLN:HE21 | 1:G:312:ILE:HD13 | 1.68                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:211:ALA:HB3  | 1:I:323:VAL:HB   | 1.85                     | 0.59              |
| 1:J:149:VAL:HG12 | 1:J:150:SER:H    | 1.66                     | 0.59              |
| 1:M:211:ALA:HB3  | 1:M:323:VAL:HB   | 1.85                     | 0.59              |
| 1:M:241:GLN:HE21 | 1:M:312:ILE:HD13 | 1.67                     | 0.59              |
| 1:D:289:ASP:OD1  | 1:D:343:ARG:NE   | 2.34                     | 0.58              |
| 1:E:323:VAL:HG22 | 1:E:328:THR:HG23 | 1.84                     | 0.58              |
| 1:L:241:GLN:HE21 | 1:L:312:ILE:HD13 | 1.68                     | 0.58              |
| 1:C:241:GLN:HE21 | 1:C:312:ILE:HD13 | 1.68                     | 0.58              |
| 1:D:323:VAL:HG22 | 1:D:328:THR:HG23 | 1.84                     | 0.58              |
| 1:F:289:ASP:OD1  | 1:F:343:ARG:NE   | 2.33                     | 0.58              |
| 1:F:442:ARG:NH1  | 1:F:442:ARG:O    | 2.33                     | 0.58              |
| 1:N:211:ALA:HB3  | 1:N:323:VAL:HB   | 1.85                     | 0.58              |
| 1:A:241:GLN:HE21 | 1:A:312:ILE:HD13 | 1.68                     | 0.58              |
| 1:J:211:ALA:HB3  | 1:J:323:VAL:HB   | 1.86                     | 0.58              |
| 1:E:149:VAL:HG12 | 1:E:150:SER:H    | 1.69                     | 0.58              |
| 1:E:465:LYS:HZ3  | 1:E:482:TRP:CD1  | 2.22                     | 0.58              |
| 1:L:216:PRO:HB3  | 1:L:244:PRO:HB2  | 1.85                     | 0.58              |
| 1:J:53:VAL:HB    | 1:J:88:THR:HG21  | 1.85                     | 0.58              |
| 1:K:65:PHE:O     | 1:K:68:MET:HB2   | 2.03                     | 0.58              |
| 1:M:442:ARG:O    | 1:M:442:ARG:NH1  | 2.34                     | 0.58              |
| 1:F:6:LYS:HG2    | 1:F:11:ALA:HB2   | 1.85                     | 0.58              |
| 1:F:153:SER:OG   | 1:F:154:ASP:N    | 2.31                     | 0.58              |
| 1:N:20:ASP:OD1   | 1:N:100:ARG:NH1  | 2.36                     | 0.58              |
| 1:A:20:ASP:OD1   | 1:A:100:ARG:NH1  | 2.37                     | 0.58              |
| 1:B:20:ASP:OD1   | 1:B:100:ARG:NH1  | 2.37                     | 0.58              |
| 1:C:289:ASP:OD1  | 1:C:343:ARG:NE   | 2.36                     | 0.58              |
| 1:K:498:ARG:NH1  | 1:K:502:GLN:OE1  | 2.37                     | 0.58              |
| 1:G:6:LYS:HD3    | 1:G:10:ASP:OD2   | 2.03                     | 0.58              |
| 1:E:241:GLN:HE21 | 1:E:312:ILE:HD13 | 1.69                     | 0.58              |
| 1:M:323:VAL:HG22 | 1:M:328:THR:HG23 | 1.84                     | 0.58              |
| 1:N:78:SER:HA    | 1:N:81:ASN:HD21  | 1.69                     | 0.58              |
| 1:N:442:ARG:O    | 1:N:442:ARG:NH1  | 2.33                     | 0.58              |
| 1:A:191:MET:HE2  | 1:A:191:MET:HA   | 1.85                     | 0.58              |
| 1:D:241:GLN:HE21 | 1:D:312:ILE:HD13 | 1.68                     | 0.58              |
| 1:J:465:LYS:HZ3  | 1:J:482:TRP:CD1  | 2.21                     | 0.58              |
| 1:G:20:ASP:OD1   | 1:G:100:ARG:NH1  | 2.37                     | 0.58              |
| 1:N:515:GLU:N    | 1:N:515:GLU:OE1  | 2.36                     | 0.58              |
| 1:J:15:MET:HA    | 1:J:15:MET:HE3   | 1.85                     | 0.57              |
| 1:J:78:SER:HA    | 1:J:81:ASN:HD21  | 1.68                     | 0.57              |
| 1:E:216:PRO:HB3  | 1:E:244:PRO:HB2  | 1.85                     | 0.57              |
| 1:H:289:ASP:OD1  | 1:H:343:ARG:NE   | 2.35                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:178:SER:N    | 1:K:379:VAL:O    | 2.36                     | 0.57              |
| 1:E:164:MET:SD   | 1:E:169:ASN:HA   | 2.44                     | 0.57              |
| 1:M:64:HIS:O     | 1:M:68:MET:HG2   | 2.04                     | 0.57              |
| 1:A:191:MET:O    | 1:A:330:ILE:N    | 2.29                     | 0.57              |
| 1:E:178:SER:N    | 1:E:379:VAL:O    | 2.37                     | 0.57              |
| 1:F:216:PRO:HB3  | 1:F:244:PRO:HB2  | 1.86                     | 0.57              |
| 1:L:80:THR:OG1   | 1:L:503:ASN:ND2  | 2.37                     | 0.57              |
| 1:A:191:MET:HB3  | 1:A:330:ILE:HB   | 1.87                     | 0.57              |
| 1:I:78:SER:HA    | 1:I:81:ASN:HD21  | 1.70                     | 0.57              |
| 1:J:515:GLU:OE1  | 1:J:515:GLU:N    | 2.38                     | 0.57              |
| 1:K:78:SER:HA    | 1:K:81:ASN:HD21  | 1.68                     | 0.57              |
| 1:G:216:PRO:HB3  | 1:G:244:PRO:HB2  | 1.86                     | 0.57              |
| 1:J:178:SER:N    | 1:J:379:VAL:O    | 2.37                     | 0.57              |
| 1:B:178:SER:N    | 1:B:379:VAL:O    | 2.37                     | 0.57              |
| 1:I:65:PHE:O     | 1:I:68:MET:HB2   | 2.04                     | 0.57              |
| 1:D:216:PRO:HB3  | 1:D:244:PRO:HB2  | 1.86                     | 0.57              |
| 1:F:357:ASP:OD1  | 1:F:360:ARG:NH1  | 2.37                     | 0.57              |
| 1:J:289:ASP:OD1  | 1:J:343:ARG:NE   | 2.37                     | 0.57              |
| 1:F:72:LEU:O     | 1:F:75:GLU:HG3   | 2.04                     | 0.57              |
| 1:E:150:SER:OG   | 1:E:151:SER:N    | 2.37                     | 0.57              |
| 1:L:178:SER:HB2  | 1:L:378:LYS:HB3  | 1.86                     | 0.57              |
| 1:K:465:LYS:HZ3  | 1:K:482:TRP:CD1  | 2.22                     | 0.56              |
| 1:G:72:LEU:O     | 1:G:76:VAL:HG23  | 2.05                     | 0.56              |
| 1:M:178:SER:HB2  | 1:M:378:LYS:HB3  | 1.86                     | 0.56              |
| 1:B:241:GLN:HE21 | 1:B:312:ILE:HD13 | 1.69                     | 0.56              |
| 1:B:465:LYS:HZ3  | 1:B:482:TRP:CD1  | 2.23                     | 0.56              |
| 1:I:407:GLU:HG3  | 1:I:495:LYS:HB2  | 1.88                     | 0.56              |
| 1:J:150:SER:OG   | 1:J:151:SER:N    | 2.38                     | 0.56              |
| 1:L:465:LYS:HZ3  | 1:L:482:TRP:CD1  | 2.24                     | 0.56              |
| 1:H:465:LYS:HZ3  | 1:H:482:TRP:CD1  | 2.23                     | 0.56              |
| 1:M:216:PRO:HB3  | 1:M:244:PRO:HB2  | 1.86                     | 0.56              |
| 1:J:241:GLN:HE21 | 1:J:312:ILE:HD13 | 1.70                     | 0.56              |
| 1:F:68:MET:SD    | 1:G:40:GLU:HG2   | 2.45                     | 0.56              |
| 1:L:160:ILE:O    | 1:L:164:MET:HB2  | 2.06                     | 0.56              |
| 1:M:407:GLU:HG3  | 1:M:495:LYS:HB2  | 1.86                     | 0.56              |
| 1:I:216:PRO:HB3  | 1:I:244:PRO:HB2  | 1.87                     | 0.56              |
| 1:D:407:GLU:HG3  | 1:D:495:LYS:HB2  | 1.87                     | 0.56              |
| 1:J:407:GLU:HG3  | 1:J:495:LYS:HB2  | 1.87                     | 0.56              |
| 1:K:137:VAL:HG21 | 1:K:409:MET:HG2  | 1.88                     | 0.56              |
| 1:A:407:GLU:HG3  | 1:A:495:LYS:HB2  | 1.87                     | 0.56              |
| 1:H:65:PHE:O     | 1:H:68:MET:HB2   | 2.06                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:357:ASP:OD1  | 1:H:360:ARG:NH1  | 2.38                     | 0.56              |
| 1:B:407:GLU:HG3  | 1:B:495:LYS:HB2  | 1.88                     | 0.56              |
| 1:C:465:LYS:HZ3  | 1:C:482:TRP:CD1  | 2.23                     | 0.56              |
| 1:D:465:LYS:HZ3  | 1:D:482:TRP:CD1  | 2.24                     | 0.56              |
| 1:L:178:SER:N    | 1:L:379:VAL:O    | 2.39                     | 0.56              |
| 1:E:135:THR:OG1  | 1:E:409:MET:O    | 2.22                     | 0.56              |
| 1:K:219:LEU:HD23 | 1:K:247:ILE:HG23 | 1.88                     | 0.56              |
| 1:N:178:SER:HB2  | 1:N:378:LYS:HB3  | 1.88                     | 0.56              |
| 1:B:234:LEU:HD11 | 1:B:315:LEU:HD11 | 1.88                     | 0.55              |
| 1:D:53:VAL:HB    | 1:D:88:THR:HG21  | 1.88                     | 0.55              |
| 1:D:202:MET:HG3  | 1:D:272:VAL:HG22 | 1.88                     | 0.55              |
| 1:G:357:ASP:OD1  | 1:G:360:ARG:NH1  | 2.35                     | 0.55              |
| 1:G:407:GLU:HG3  | 1:G:495:LYS:HB2  | 1.86                     | 0.55              |
| 1:M:178:SER:N    | 1:M:379:VAL:O    | 2.38                     | 0.55              |
| 1:N:216:PRO:HB3  | 1:N:244:PRO:HB2  | 1.87                     | 0.55              |
| 1:A:78:SER:HA    | 1:A:81:ASN:HD21  | 1.72                     | 0.55              |
| 1:B:78:SER:HA    | 1:B:81:ASN:HD21  | 1.72                     | 0.55              |
| 1:J:219:LEU:HD23 | 1:J:247:ILE:HG23 | 1.88                     | 0.55              |
| 1:F:418:VAL:HG13 | 1:F:421:ILE:HD12 | 1.88                     | 0.55              |
| 1:L:219:LEU:HD23 | 1:L:247:ILE:HG23 | 1.89                     | 0.55              |
| 1:G:191:MET:HE2  | 1:G:191:MET:HA   | 1.89                     | 0.55              |
| 1:N:204:THR:OG1  | 1:N:212:VAL:N    | 2.34                     | 0.55              |
| 1:A:465:LYS:HZ3  | 1:A:482:TRP:CD1  | 2.25                     | 0.55              |
| 1:H:178:SER:HB2  | 1:H:378:LYS:HB3  | 1.87                     | 0.55              |
| 1:N:35:ARG:HH12  | 1:N:454:ASN:HA   | 1.70                     | 0.55              |
| 1:N:5:LEU:HD22   | 1:N:518:VAL:HG22 | 1.88                     | 0.55              |
| 1:A:234:LEU:HD11 | 1:A:315:LEU:HD11 | 1.89                     | 0.55              |
| 1:L:234:LEU:HD11 | 1:L:315:LEU:HD11 | 1.89                     | 0.55              |
| 1:A:178:SER:N    | 1:A:379:VAL:O    | 2.39                     | 0.55              |
| 1:C:1:MET:HE1    | 1:C:520:ASP:HB3  | 1.89                     | 0.55              |
| 1:C:407:GLU:HG3  | 1:C:495:LYS:HB2  | 1.88                     | 0.55              |
| 1:L:223:LYS:NZ   | 1:L:305:LEU:O    | 2.33                     | 0.55              |
| 1:L:357:ASP:OD1  | 1:L:360:ARG:NH1  | 2.37                     | 0.55              |
| 1:G:178:SER:N    | 1:G:379:VAL:O    | 2.40                     | 0.55              |
| 1:B:153:SER:OG   | 1:B:154:ASP:N    | 2.40                     | 0.55              |
| 1:B:219:LEU:HD23 | 1:B:247:ILE:HG23 | 1.88                     | 0.55              |
| 1:F:178:SER:N    | 1:F:379:VAL:O    | 2.38                     | 0.55              |
| 1:L:78:SER:HA    | 1:L:81:ASN:HD21  | 1.71                     | 0.55              |
| 1:M:35:ARG:HH12  | 1:M:454:ASN:HA   | 1.72                     | 0.55              |
| 1:D:105:ASN:ND2  | 1:D:439:ILE:HD11 | 2.22                     | 0.55              |
| 1:E:97:ALA:HB2   | 1:E:446:GLU:HG3  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:219:LEU:HD23 | 1:F:247:ILE:HG23 | 1.88                     | 0.55              |
| 1:I:178:SER:HB2  | 1:I:378:LYS:HB3  | 1.89                     | 0.54              |
| 1:E:105:ASN:ND2  | 1:E:439:ILE:HD11 | 2.23                     | 0.54              |
| 1:F:78:SER:HA    | 1:F:81:ASN:ND2   | 2.22                     | 0.54              |
| 1:L:407:GLU:HG3  | 1:L:495:LYS:HB2  | 1.88                     | 0.54              |
| 1:M:78:SER:HA    | 1:M:81:ASN:HD21  | 1.72                     | 0.54              |
| 1:C:234:LEU:HD11 | 1:C:315:LEU:HD11 | 1.89                     | 0.54              |
| 1:I:80:THR:HG1   | 1:I:503:ASN:HD22 | 1.56                     | 0.54              |
| 1:G:78:SER:HA    | 1:G:81:ASN:HD21  | 1.72                     | 0.54              |
| 1:H:234:LEU:HD11 | 1:H:315:LEU:HD11 | 1.88                     | 0.54              |
| 1:I:219:LEU:HD23 | 1:I:247:ILE:HG23 | 1.88                     | 0.54              |
| 1:D:178:SER:N    | 1:D:379:VAL:O    | 2.39                     | 0.54              |
| 1:J:191:MET:HA   | 1:J:191:MET:HE2  | 1.90                     | 0.54              |
| 1:E:178:SER:HB2  | 1:E:378:LYS:HB3  | 1.88                     | 0.54              |
| 1:E:219:LEU:HD23 | 1:E:247:ILE:HG23 | 1.88                     | 0.54              |
| 1:E:289:ASP:OD1  | 1:E:343:ARG:NE   | 2.34                     | 0.54              |
| 1:K:183:THR:HG23 | 1:K:379:VAL:HA   | 1.89                     | 0.54              |
| 1:M:81:ASN:HB3   | 1:M:88:THR:HB    | 1.89                     | 0.54              |
| 1:M:219:LEU:HD23 | 1:M:247:ILE:HG23 | 1.89                     | 0.54              |
| 1:C:76:VAL:HG21  | 1:C:507:VAL:HG11 | 1.88                     | 0.54              |
| 1:C:178:SER:N    | 1:C:379:VAL:O    | 2.39                     | 0.54              |
| 1:F:178:SER:HB2  | 1:F:378:LYS:HB3  | 1.90                     | 0.54              |
| 1:F:234:LEU:HD11 | 1:F:315:LEU:HD11 | 1.88                     | 0.54              |
| 1:N:105:ASN:ND2  | 1:N:439:ILE:HD11 | 2.22                     | 0.54              |
| 1:B:150:SER:OG   | 1:B:151:SER:N    | 2.39                     | 0.54              |
| 1:D:234:LEU:HD11 | 1:D:315:LEU:HD11 | 1.90                     | 0.54              |
| 1:L:6:LYS:HD3    | 1:L:10:ASP:OD2   | 2.08                     | 0.54              |
| 1:L:64:HIS:O     | 1:L:68:MET:HG2   | 2.08                     | 0.54              |
| 1:L:202:MET:HG3  | 1:L:272:VAL:HG22 | 1.90                     | 0.54              |
| 1:I:178:SER:N    | 1:I:379:VAL:O    | 2.39                     | 0.54              |
| 1:I:234:LEU:HD11 | 1:I:315:LEU:HD11 | 1.89                     | 0.54              |
| 1:G:178:SER:HB2  | 1:G:378:LYS:HB3  | 1.89                     | 0.54              |
| 1:A:81:ASN:HB3   | 1:A:88:THR:HB    | 1.90                     | 0.54              |
| 1:H:213:LEU:HD22 | 1:H:244:PRO:HB3  | 1.89                     | 0.54              |
| 1:C:219:LEU:HD23 | 1:C:247:ILE:HG23 | 1.88                     | 0.54              |
| 1:H:191:MET:O    | 1:H:330:ILE:N    | 2.35                     | 0.54              |
| 1:B:97:ALA:HB2   | 1:B:446:GLU:HG3  | 1.90                     | 0.54              |
| 1:I:213:LEU:HD22 | 1:I:244:PRO:HB3  | 1.89                     | 0.54              |
| 1:G:219:LEU:HD23 | 1:G:247:ILE:HG23 | 1.88                     | 0.54              |
| 1:M:105:ASN:ND2  | 1:M:439:ILE:HD11 | 2.23                     | 0.54              |
| 1:H:105:ASN:ND2  | 1:H:439:ILE:HD11 | 2.23                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:64:HIS:O     | 1:N:68:MET:HG2   | 2.07                     | 0.54              |
| 1:N:213:LEU:HD22 | 1:N:244:PRO:HB3  | 1.89                     | 0.54              |
| 1:B:5:LEU:HD22   | 1:B:518:VAL:HG22 | 1.89                     | 0.54              |
| 1:I:105:ASN:ND2  | 1:I:439:ILE:HD11 | 2.22                     | 0.54              |
| 1:K:407:GLU:HG3  | 1:K:495:LYS:HB2  | 1.88                     | 0.53              |
| 1:M:97:ALA:HB2   | 1:M:446:GLU:HG3  | 1.90                     | 0.53              |
| 1:I:97:ALA:HB2   | 1:I:446:GLU:HG3  | 1.90                     | 0.53              |
| 1:D:219:LEU:HD23 | 1:D:247:ILE:HG23 | 1.89                     | 0.53              |
| 1:E:76:VAL:HG21  | 1:E:507:VAL:HG11 | 1.90                     | 0.53              |
| 1:F:105:ASN:ND2  | 1:F:439:ILE:HD11 | 2.23                     | 0.53              |
| 1:E:12:ARG:HD2   | 1:E:103:LEU:HD21 | 1.90                     | 0.53              |
| 1:K:234:LEU:HD11 | 1:K:315:LEU:HD11 | 1.90                     | 0.53              |
| 1:N:97:ALA:HB2   | 1:N:446:GLU:HG3  | 1.91                     | 0.53              |
| 1:A:219:LEU:HD23 | 1:A:247:ILE:HG23 | 1.89                     | 0.53              |
| 1:A:213:LEU:HD22 | 1:A:244:PRO:HB3  | 1.90                     | 0.53              |
| 1:J:105:ASN:ND2  | 1:J:439:ILE:HD11 | 2.23                     | 0.53              |
| 1:J:183:THR:HG23 | 1:J:379:VAL:HA   | 1.90                     | 0.53              |
| 1:F:191:MET:O    | 1:F:330:ILE:N    | 2.32                     | 0.53              |
| 1:B:289:ASP:OD1  | 1:B:343:ARG:NE   | 2.34                     | 0.53              |
| 1:D:72:LEU:O     | 1:D:75:GLU:HG3   | 2.08                     | 0.53              |
| 1:K:105:ASN:ND2  | 1:K:439:ILE:HD11 | 2.24                     | 0.53              |
| 1:M:234:LEU:HD21 | 1:M:315:LEU:HD21 | 1.91                     | 0.53              |
| 1:N:219:LEU:HD23 | 1:N:247:ILE:HG23 | 1.89                     | 0.53              |
| 1:D:178:SER:HB2  | 1:D:378:LYS:HB3  | 1.89                     | 0.53              |
| 1:E:72:LEU:O     | 1:E:75:GLU:HG3   | 2.09                     | 0.53              |
| 1:F:285:ALA:HB1  | 1:F:366:ARG:CZ   | 2.39                     | 0.53              |
| 1:H:219:LEU:HD23 | 1:H:247:ILE:HG23 | 1.89                     | 0.53              |
| 1:N:407:GLU:HG3  | 1:N:495:LYS:HB2  | 1.91                     | 0.53              |
| 1:C:150:SER:OG   | 1:C:151:SER:N    | 2.42                     | 0.53              |
| 1:K:191:MET:HE2  | 1:K:191:MET:HA   | 1.91                     | 0.53              |
| 1:L:81:ASN:HB3   | 1:L:88:THR:HB    | 1.90                     | 0.53              |
| 1:M:213:LEU:HD22 | 1:M:244:PRO:HB3  | 1.90                     | 0.53              |
| 1:A:105:ASN:ND2  | 1:A:439:ILE:HD11 | 2.23                     | 0.53              |
| 1:J:234:LEU:HD11 | 1:J:315:LEU:HD11 | 1.89                     | 0.53              |
| 1:K:10:ASP:N     | 1:K:10:ASP:OD1   | 2.39                     | 0.53              |
| 1:L:97:ALA:HB2   | 1:L:446:GLU:HG3  | 1.91                     | 0.53              |
| 1:L:213:LEU:HD22 | 1:L:244:PRO:HB3  | 1.91                     | 0.53              |
| 1:C:183:THR:HG23 | 1:C:379:VAL:HA   | 1.91                     | 0.52              |
| 1:I:191:MET:HE1  | 1:I:369:LYS:HD3  | 1.91                     | 0.52              |
| 1:N:178:SER:N    | 1:N:379:VAL:O    | 2.39                     | 0.52              |
| 1:A:97:ALA:HB2   | 1:A:446:GLU:HG3  | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:5:LEU:HD22   | 1:N:61:LEU:HD21  | 1.89                     | 0.52              |
| 1:I:357:ASP:OD1  | 1:I:360:ARG:NH1  | 2.36                     | 0.52              |
| 1:E:234:LEU:HD11 | 1:E:315:LEU:HD11 | 1.90                     | 0.52              |
| 1:F:137:VAL:HG11 | 1:F:146:VAL:HG21 | 1.90                     | 0.52              |
| 1:N:357:ASP:OD1  | 1:N:360:ARG:NH1  | 2.33                     | 0.52              |
| 1:K:409:MET:HE2  | 1:K:491:VAL:HB   | 1.91                     | 0.52              |
| 1:F:213:LEU:HD22 | 1:F:244:PRO:HB3  | 1.90                     | 0.52              |
| 1:H:78:SER:HA    | 1:H:81:ASN:HD21  | 1.74                     | 0.52              |
| 1:N:53:VAL:HB    | 1:N:88:THR:HG21  | 1.91                     | 0.52              |
| 1:M:223:LYS:NZ   | 1:M:305:LEU:O    | 2.30                     | 0.52              |
| 1:N:191:MET:HE1  | 1:N:369:LYS:HD3  | 1.92                     | 0.52              |
| 1:C:105:ASN:ND2  | 1:C:439:ILE:HD11 | 2.24                     | 0.52              |
| 1:L:183:THR:HG23 | 1:L:379:VAL:HA   | 1.91                     | 0.52              |
| 1:N:1:MET:HE1    | 1:N:520:ASP:HB3  | 1.92                     | 0.52              |
| 1:N:234:LEU:HD11 | 1:N:315:LEU:HD11 | 1.90                     | 0.52              |
| 1:B:105:ASN:ND2  | 1:B:439:ILE:HD11 | 2.23                     | 0.52              |
| 1:C:213:LEU:HD22 | 1:C:244:PRO:HB3  | 1.91                     | 0.52              |
| 1:I:397:ALA:O    | 1:I:401:THR:OG1  | 2.27                     | 0.52              |
| 1:E:183:THR:HG23 | 1:E:379:VAL:HA   | 1.91                     | 0.52              |
| 1:L:105:ASN:ND2  | 1:L:439:ILE:HD11 | 2.24                     | 0.52              |
| 1:A:178:SER:HB2  | 1:A:378:LYS:HB3  | 1.90                     | 0.52              |
| 1:I:234:LEU:HD21 | 1:I:315:LEU:HD21 | 1.92                     | 0.52              |
| 1:J:164:MET:SD   | 1:J:169:ASN:HA   | 2.49                     | 0.52              |
| 1:F:234:LEU:HD21 | 1:F:315:LEU:HD21 | 1.92                     | 0.52              |
| 1:G:223:LYS:NZ   | 1:G:305:LEU:O    | 2.30                     | 0.52              |
| 1:C:97:ALA:HB2   | 1:C:446:GLU:HG3  | 1.91                     | 0.52              |
| 1:J:5:LEU:HG     | 1:J:518:VAL:HG22 | 1.92                     | 0.52              |
| 1:G:68:MET:SD    | 1:H:40:GLU:HG2   | 2.50                     | 0.52              |
| 1:G:234:LEU:HD11 | 1:G:315:LEU:HD11 | 1.90                     | 0.52              |
| 1:A:418:VAL:HG13 | 1:A:421:ILE:HD12 | 1.92                     | 0.52              |
| 1:D:357:ASP:OD1  | 1:D:360:ARG:NH1  | 2.37                     | 0.52              |
| 1:L:191:MET:HG2  | 1:L:293:LEU:HD22 | 1.92                     | 0.52              |
| 1:H:82:ASP:OD1   | 1:H:82:ASP:N     | 2.43                     | 0.52              |
| 1:A:197:TYR:HB2  | 1:A:202:MET:HE3  | 1.91                     | 0.52              |
| 1:B:191:MET:HE2  | 1:B:191:MET:HA   | 1.92                     | 0.52              |
| 1:B:183:THR:HG23 | 1:B:379:VAL:HA   | 1.90                     | 0.51              |
| 1:C:178:SER:HB2  | 1:C:378:LYS:HB3  | 1.91                     | 0.51              |
| 1:C:191:MET:HE1  | 1:C:369:LYS:HB3  | 1.92                     | 0.51              |
| 1:M:234:LEU:HD11 | 1:M:315:LEU:HD11 | 1.91                     | 0.51              |
| 1:N:140:LYS:HE3  | 1:N:161:ALA:HB1  | 1.92                     | 0.51              |
| 1:C:191:MET:HA   | 1:C:191:MET:HE2  | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:97:ALA:HB2   | 1:D:446:GLU:HG3  | 1.93                     | 0.51              |
| 1:D:213:LEU:HD22 | 1:D:244:PRO:HB3  | 1.91                     | 0.51              |
| 1:H:97:ALA:HB2   | 1:H:446:GLU:HG3  | 1.92                     | 0.51              |
| 1:H:183:THR:HG23 | 1:H:379:VAL:HA   | 1.92                     | 0.51              |
| 1:C:72:LEU:O     | 1:C:75:GLU:HG3   | 2.10                     | 0.51              |
| 1:N:1:MET:SD     | 1:N:2:ALA:N      | 2.83                     | 0.51              |
| 1:A:183:THR:HG23 | 1:A:379:VAL:HA   | 1.92                     | 0.51              |
| 1:D:183:THR:HG23 | 1:D:379:VAL:HA   | 1.92                     | 0.51              |
| 1:E:204:THR:OG1  | 1:E:212:VAL:N    | 2.35                     | 0.51              |
| 1:F:15:MET:HE3   | 1:F:15:MET:HA    | 1.91                     | 0.51              |
| 1:F:204:THR:OG1  | 1:F:212:VAL:N    | 2.35                     | 0.51              |
| 1:G:76:VAL:CG2   | 1:G:507:VAL:HG21 | 2.40                     | 0.51              |
| 1:G:97:ALA:HB2   | 1:G:446:GLU:HG3  | 1.91                     | 0.51              |
| 1:J:221:THR:HB   | 1:J:299:ILE:HB   | 1.92                     | 0.51              |
| 1:K:260:LEU:HD22 | 1:K:271:VAL:HG11 | 1.93                     | 0.51              |
| 1:G:213:LEU:HD22 | 1:G:244:PRO:HB3  | 1.91                     | 0.51              |
| 1:H:279:PHE:HD1  | 1:H:283:ARG:HH21 | 1.59                     | 0.51              |
| 1:N:223:LYS:NZ   | 1:N:305:LEU:O    | 2.30                     | 0.51              |
| 1:I:204:THR:OG1  | 1:I:212:VAL:N    | 2.36                     | 0.51              |
| 1:F:183:THR:HG23 | 1:F:379:VAL:HA   | 1.92                     | 0.51              |
| 1:F:407:GLU:HG3  | 1:F:495:LYS:HB2  | 1.93                     | 0.51              |
| 1:G:436:GLY:O    | 1:G:439:ILE:HG22 | 2.11                     | 0.51              |
| 1:N:72:LEU:O     | 1:N:75:GLU:HG3   | 2.11                     | 0.51              |
| 1:N:234:LEU:HD21 | 1:N:315:LEU:HD21 | 1.93                     | 0.51              |
| 1:A:279:PHE:HD1  | 1:A:283:ARG:HH21 | 1.59                     | 0.51              |
| 1:D:221:THR:HB   | 1:D:299:ILE:HB   | 1.92                     | 0.51              |
| 1:E:83:ILE:HD13  | 1:E:495:LYS:HG2  | 1.92                     | 0.51              |
| 1:L:485:MET:SD   | 1:L:485:MET:N    | 2.84                     | 0.51              |
| 1:G:53:VAL:HB    | 1:G:88:THR:HG21  | 1.93                     | 0.51              |
| 1:M:62:GLU:HB2   | 1:N:2:ALA:HB1    | 1.91                     | 0.51              |
| 1:B:357:ASP:OD1  | 1:B:360:ARG:NH1  | 2.37                     | 0.51              |
| 1:C:279:PHE:HD1  | 1:C:283:ARG:HH21 | 1.59                     | 0.51              |
| 1:L:76:VAL:HG21  | 1:L:507:VAL:HG11 | 1.93                     | 0.51              |
| 1:A:10:ASP:OD1   | 1:A:11:ALA:N     | 2.44                     | 0.51              |
| 1:L:72:LEU:O     | 1:L:75:GLU:HG3   | 2.11                     | 0.51              |
| 1:H:178:SER:N    | 1:H:379:VAL:O    | 2.40                     | 0.51              |
| 1:I:53:VAL:HB    | 1:I:88:THR:HG21  | 1.91                     | 0.50              |
| 1:L:397:ALA:O    | 1:L:401:THR:OG1  | 2.25                     | 0.50              |
| 1:G:183:THR:HG23 | 1:G:379:VAL:HA   | 1.92                     | 0.50              |
| 1:M:53:VAL:HB    | 1:M:88:THR:HG21  | 1.93                     | 0.50              |
| 1:M:285:ALA:HB1  | 1:M:366:ARG:CZ   | 2.42                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:81:ASN:HB3   | 1:N:88:THR:HB    | 1.92                     | 0.50              |
| 1:A:137:VAL:HG21 | 1:A:409:MET:HG2  | 1.94                     | 0.50              |
| 1:K:178:SER:HB2  | 1:K:378:LYS:HB3  | 1.93                     | 0.50              |
| 1:K:221:THR:HB   | 1:K:299:ILE:HB   | 1.91                     | 0.50              |
| 1:K:234:LEU:HD21 | 1:K:315:LEU:HD21 | 1.93                     | 0.50              |
| 1:L:77:ALA:O     | 1:L:81:ASN:ND2   | 2.45                     | 0.50              |
| 1:B:153:SER:HB3  | 1:B:393:ARG:HD3  | 1.92                     | 0.50              |
| 1:B:178:SER:HB2  | 1:B:378:LYS:HB3  | 1.92                     | 0.50              |
| 1:B:221:THR:HB   | 1:B:299:ILE:HB   | 1.94                     | 0.50              |
| 1:D:104:LYS:HE3  | 1:J:108:ALA:HA   | 1.94                     | 0.50              |
| 1:D:191:MET:HG2  | 1:D:293:LEU:HD22 | 1.92                     | 0.50              |
| 1:M:72:LEU:O     | 1:M:75:GLU:HG3   | 2.11                     | 0.50              |
| 1:I:418:VAL:HG13 | 1:I:421:ILE:HD12 | 1.94                     | 0.50              |
| 1:D:285:ALA:HB1  | 1:D:366:ARG:CZ   | 2.41                     | 0.50              |
| 1:J:213:LEU:HD22 | 1:J:244:PRO:HB3  | 1.93                     | 0.50              |
| 1:J:279:PHE:HD1  | 1:J:283:ARG:HH21 | 1.58                     | 0.50              |
| 1:F:83:ILE:HD13  | 1:F:495:LYS:HG2  | 1.92                     | 0.50              |
| 1:G:72:LEU:O     | 1:G:75:GLU:HG3   | 2.11                     | 0.50              |
| 1:C:285:ALA:HB1  | 1:C:366:ARG:CZ   | 2.42                     | 0.50              |
| 1:E:221:THR:HB   | 1:E:299:ILE:HB   | 1.92                     | 0.50              |
| 1:E:357:ASP:OD1  | 1:E:360:ARG:NH1  | 2.38                     | 0.50              |
| 1:K:213:LEU:HD22 | 1:K:244:PRO:HB3  | 1.94                     | 0.50              |
| 1:A:77:ALA:O     | 1:A:81:ASN:ND2   | 2.45                     | 0.50              |
| 1:A:357:ASP:OD1  | 1:A:360:ARG:NH1  | 2.37                     | 0.50              |
| 1:G:234:LEU:HD21 | 1:G:315:LEU:HD21 | 1.93                     | 0.50              |
| 1:H:418:VAL:HG13 | 1:H:421:ILE:HD12 | 1.93                     | 0.50              |
| 1:B:77:ALA:O     | 1:B:81:ASN:ND2   | 2.45                     | 0.50              |
| 1:A:221:THR:HB   | 1:A:299:ILE:HB   | 1.93                     | 0.50              |
| 1:B:81:ASN:HB3   | 1:B:88:THR:HB    | 1.93                     | 0.50              |
| 1:B:146:VAL:HA   | 1:B:149:VAL:HG22 | 1.92                     | 0.50              |
| 1:B:418:VAL:HG13 | 1:B:421:ILE:HD12 | 1.94                     | 0.50              |
| 1:C:221:THR:HB   | 1:C:299:ILE:HB   | 1.93                     | 0.50              |
| 1:D:234:LEU:HD21 | 1:D:315:LEU:HD21 | 1.93                     | 0.50              |
| 1:D:279:PHE:HD1  | 1:D:283:ARG:HH21 | 1.59                     | 0.50              |
| 1:L:221:THR:HB   | 1:L:299:ILE:HB   | 1.92                     | 0.50              |
| 1:M:221:THR:HB   | 1:M:299:ILE:HB   | 1.93                     | 0.50              |
| 1:N:183:THR:HG23 | 1:N:379:VAL:HA   | 1.94                     | 0.50              |
| 1:G:279:PHE:HD1  | 1:G:283:ARG:HH21 | 1.58                     | 0.50              |
| 1:M:284:LYS:NZ   | 1:M:302:ASP:OD2  | 2.45                     | 0.50              |
| 1:B:213:LEU:HD22 | 1:B:244:PRO:HB3  | 1.92                     | 0.49              |
| 1:I:183:THR:HG23 | 1:I:379:VAL:HA   | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:76:VAL:HG21  | 1:D:507:VAL:HG11 | 1.94                     | 0.49              |
| 1:H:285:ALA:HB1  | 1:H:366:ARG:CZ   | 2.42                     | 0.49              |
| 1:A:38:VAL:HG13  | 1:A:48:ILE:HG12  | 1.94                     | 0.49              |
| 1:F:97:ALA:HB2   | 1:F:446:GLU:HG3  | 1.94                     | 0.49              |
| 1:H:191:MET:HE2  | 1:H:191:MET:HA   | 1.94                     | 0.49              |
| 1:I:191:MET:SD   | 1:I:369:LYS:HB3  | 2.52                     | 0.49              |
| 1:M:183:THR:HG23 | 1:M:379:VAL:HA   | 1.93                     | 0.49              |
| 1:M:204:THR:OG1  | 1:M:212:VAL:N    | 2.33                     | 0.49              |
| 1:N:221:THR:HB   | 1:N:299:ILE:HB   | 1.93                     | 0.49              |
| 1:A:40:GLU:HG2   | 1:C:68:MET:SD    | 2.52                     | 0.49              |
| 1:C:418:VAL:HG13 | 1:C:421:ILE:HD12 | 1.94                     | 0.49              |
| 1:E:213:LEU:HD22 | 1:E:244:PRO:HB3  | 1.93                     | 0.49              |
| 1:K:285:ALA:HB1  | 1:K:366:ARG:CZ   | 2.43                     | 0.49              |
| 1:G:113:LEU:HD13 | 1:H:33:LYS:HD2   | 1.93                     | 0.49              |
| 1:G:221:THR:HB   | 1:G:299:ILE:HB   | 1.92                     | 0.49              |
| 1:H:221:THR:HB   | 1:H:299:ILE:HB   | 1.93                     | 0.49              |
| 1:B:72:LEU:O     | 1:B:75:GLU:HG3   | 2.12                     | 0.49              |
| 1:K:53:VAL:HB    | 1:K:88:THR:HG21  | 1.94                     | 0.49              |
| 1:E:464:ASP:O    | 1:E:468:ASN:ND2  | 2.45                     | 0.49              |
| 1:K:198:LEU:HD21 | 1:K:275:LYS:HG3  | 1.95                     | 0.49              |
| 1:M:9:GLU:O      | 1:M:13:ALA:N     | 2.43                     | 0.49              |
| 1:N:418:VAL:HG13 | 1:N:421:ILE:HD12 | 1.94                     | 0.49              |
| 1:A:76:VAL:HG21  | 1:A:507:VAL:HG11 | 1.95                     | 0.49              |
| 1:A:135:THR:OG1  | 1:A:409:MET:O    | 2.28                     | 0.49              |
| 1:B:40:GLU:HG2   | 1:J:68:MET:SD    | 2.52                     | 0.49              |
| 1:C:204:THR:OG1  | 1:C:212:VAL:N    | 2.35                     | 0.49              |
| 1:C:397:ALA:O    | 1:C:401:THR:OG1  | 2.24                     | 0.49              |
| 1:I:285:ALA:HB1  | 1:I:366:ARG:CZ   | 2.42                     | 0.49              |
| 1:J:145:GLN:O    | 1:J:149:VAL:HG23 | 2.13                     | 0.49              |
| 1:J:234:LEU:HD21 | 1:J:315:LEU:HD21 | 1.95                     | 0.49              |
| 1:E:145:GLN:O    | 1:E:149:VAL:HG23 | 2.12                     | 0.49              |
| 1:K:397:ALA:O    | 1:K:401:THR:OG1  | 2.25                     | 0.49              |
| 1:L:164:MET:CE   | 1:L:169:ASN:HA   | 2.43                     | 0.49              |
| 1:G:285:ALA:HB1  | 1:G:366:ARG:CZ   | 2.43                     | 0.49              |
| 1:N:76:VAL:HG21  | 1:N:507:VAL:HG11 | 1.94                     | 0.49              |
| 1:E:80:THR:OG1   | 1:E:503:ASN:OD1  | 2.30                     | 0.49              |
| 1:K:289:ASP:OD1  | 1:K:343:ARG:NE   | 2.40                     | 0.49              |
| 1:K:357:ASP:OD1  | 1:K:360:ARG:NH1  | 2.40                     | 0.49              |
| 1:L:53:VAL:HB    | 1:L:88:THR:HG21  | 1.95                     | 0.49              |
| 1:M:15:MET:HE3   | 1:M:15:MET:HA    | 1.93                     | 0.49              |
| 1:H:76:VAL:HG21  | 1:H:507:VAL:HG11 | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:234:LEU:HD21 | 1:A:315:LEU:HD21 | 1.93                     | 0.49              |
| 1:I:221:THR:HB   | 1:I:299:ILE:HB   | 1.94                     | 0.49              |
| 1:M:418:VAL:HG13 | 1:M:421:ILE:HD12 | 1.94                     | 0.49              |
| 1:N:191:MET:SD   | 1:N:369:LYS:HB3  | 2.52                     | 0.49              |
| 1:A:15:MET:HE3   | 1:A:15:MET:HA    | 1.94                     | 0.48              |
| 1:A:72:LEU:O     | 1:A:75:GLU:HG3   | 2.12                     | 0.48              |
| 1:C:357:ASP:OD1  | 1:C:360:ARG:NH1  | 2.38                     | 0.48              |
| 1:G:172:VAL:HB   | 1:G:374:VAL:HG22 | 1.95                     | 0.48              |
| 1:A:172:VAL:HG21 | 1:A:192:GLN:HB3  | 1.95                     | 0.48              |
| 1:J:97:ALA:HB2   | 1:J:446:GLU:HG3  | 1.94                     | 0.48              |
| 1:J:178:SER:HB2  | 1:J:378:LYS:HB3  | 1.94                     | 0.48              |
| 1:J:285:ALA:HB1  | 1:J:366:ARG:CZ   | 2.43                     | 0.48              |
| 1:K:97:ALA:HB2   | 1:K:446:GLU:HG3  | 1.96                     | 0.48              |
| 1:G:81:ASN:HB3   | 1:G:88:THR:HB    | 1.94                     | 0.48              |
| 1:G:138:ASP:OD1  | 1:G:138:ASP:N    | 2.45                     | 0.48              |
| 1:I:76:VAL:HG21  | 1:I:507:VAL:HG11 | 1.94                     | 0.48              |
| 1:D:65:PHE:O     | 1:D:68:MET:HB2   | 2.14                     | 0.48              |
| 1:F:12:ARG:HD2   | 1:F:103:LEU:HD21 | 1.96                     | 0.48              |
| 1:N:138:ASP:OD1  | 1:N:138:ASP:N    | 2.45                     | 0.48              |
| 1:K:197:TYR:OH   | 1:K:209:MET:SD   | 2.71                     | 0.48              |
| 1:M:76:VAL:HG21  | 1:M:507:VAL:HG11 | 1.96                     | 0.48              |
| 1:H:81:ASN:HB3   | 1:H:88:THR:HB    | 1.94                     | 0.48              |
| 1:H:234:LEU:HD21 | 1:H:315:LEU:HD21 | 1.94                     | 0.48              |
| 1:C:53:VAL:HB    | 1:C:88:THR:HG21  | 1.95                     | 0.48              |
| 1:J:82:ASP:N     | 1:J:82:ASP:OD1   | 2.46                     | 0.48              |
| 1:H:53:VAL:HB    | 1:H:88:THR:HG21  | 1.95                     | 0.48              |
| 1:B:149:VAL:O    | 1:B:150:SER:HB3  | 2.14                     | 0.48              |
| 1:B:234:LEU:HD21 | 1:B:315:LEU:HD21 | 1.94                     | 0.48              |
| 1:C:234:LEU:HD21 | 1:C:315:LEU:HD21 | 1.95                     | 0.48              |
| 1:E:76:VAL:CG2   | 1:E:507:VAL:HG21 | 2.44                     | 0.48              |
| 1:E:173:ILE:HA   | 1:E:375:ALA:HB3  | 1.96                     | 0.48              |
| 1:E:234:LEU:HD21 | 1:E:315:LEU:HD21 | 1.94                     | 0.48              |
| 1:A:33:LYS:HD2   | 1:C:113:LEU:HD13 | 1.95                     | 0.48              |
| 1:B:237:GLN:HB3  | 1:B:312:ILE:HD11 | 1.95                     | 0.48              |
| 1:F:202:MET:SD   | 1:F:272:VAL:HA   | 2.53                     | 0.48              |
| 1:L:204:THR:OG1  | 1:L:212:VAL:N    | 2.36                     | 0.48              |
| 1:G:418:VAL:HG13 | 1:G:421:ILE:HD12 | 1.95                     | 0.48              |
| 1:J:418:VAL:HG13 | 1:J:421:ILE:HD12 | 1.96                     | 0.48              |
| 1:L:234:LEU:HD21 | 1:L:315:LEU:HD21 | 1.94                     | 0.48              |
| 1:M:397:ALA:O    | 1:M:401:THR:OG1  | 2.25                     | 0.48              |
| 1:H:140:LYS:HE3  | 1:H:161:ALA:HB1  | 1.94                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:198:LEU:HD21 | 1:H:275:LYS:HG3  | 1.95                     | 0.48              |
| 1:C:76:VAL:CG2   | 1:C:507:VAL:HG21 | 2.44                     | 0.48              |
| 1:D:138:ASP:OD1  | 1:D:138:ASP:N    | 2.45                     | 0.48              |
| 1:E:138:ASP:OD1  | 1:E:138:ASP:N    | 2.45                     | 0.48              |
| 1:G:204:THR:OG1  | 1:G:212:VAL:N    | 2.34                     | 0.48              |
| 1:G:229:GLN:HA   | 1:G:232:LEU:HG   | 1.96                     | 0.48              |
| 1:C:80:THR:HG1   | 1:C:503:ASN:HD22 | 1.62                     | 0.48              |
| 1:J:357:ASP:OD1  | 1:J:360:ARG:NH1  | 2.39                     | 0.48              |
| 1:E:279:PHE:HD1  | 1:E:283:ARG:HH21 | 1.60                     | 0.48              |
| 1:G:195:ARG:NH2  | 1:G:276:ALA:O    | 2.41                     | 0.48              |
| 1:M:163:ALA:O    | 1:M:167:VAL:HG22 | 2.14                     | 0.48              |
| 1:A:53:VAL:HB    | 1:A:88:THR:HG21  | 1.96                     | 0.47              |
| 1:A:397:ALA:O    | 1:A:401:THR:OG1  | 2.25                     | 0.47              |
| 1:I:6:LYS:HG2    | 1:I:11:ALA:HB2   | 1.94                     | 0.47              |
| 1:E:163:ALA:O    | 1:E:167:VAL:HG22 | 2.14                     | 0.47              |
| 1:M:46:PRO:HB3   | 1:N:68:MET:HE1   | 1.95                     | 0.47              |
| 1:H:204:THR:OG1  | 1:H:212:VAL:N    | 2.37                     | 0.47              |
| 1:A:21:LYS:HB3   | 1:C:5:LEU:HD11   | 1.97                     | 0.47              |
| 1:I:1:MET:SD     | 1:I:2:ALA:N      | 2.87                     | 0.47              |
| 1:J:237:GLN:HB3  | 1:J:312:ILE:HD11 | 1.96                     | 0.47              |
| 1:F:164:MET:HA   | 1:F:167:VAL:HG22 | 1.95                     | 0.47              |
| 1:M:229:GLN:HA   | 1:M:232:LEU:HG   | 1.96                     | 0.47              |
| 1:H:397:ALA:O    | 1:H:401:THR:OG1  | 2.26                     | 0.47              |
| 1:A:237:GLN:HB3  | 1:A:312:ILE:HD11 | 1.96                     | 0.47              |
| 1:E:149:VAL:HG12 | 1:E:150:SER:N    | 2.28                     | 0.47              |
| 1:F:140:LYS:NZ   | 1:F:165:GLU:HB2  | 2.30                     | 0.47              |
| 1:F:146:VAL:HG12 | 1:F:401:THR:HG23 | 1.96                     | 0.47              |
| 1:G:64:HIS:O     | 1:G:68:MET:HG2   | 2.14                     | 0.47              |
| 1:N:285:ALA:HB1  | 1:N:366:ARG:CZ   | 2.44                     | 0.47              |
| 1:C:39:LEU:HD13  | 1:C:58:GLU:HG3   | 1.97                     | 0.47              |
| 1:J:149:VAL:HG12 | 1:J:150:SER:N    | 2.29                     | 0.47              |
| 1:E:146:VAL:HG11 | 1:E:404:ALA:HB3  | 1.95                     | 0.47              |
| 1:K:35:ARG:HH12  | 1:K:454:ASN:HA   | 1.79                     | 0.47              |
| 1:G:163:ALA:O    | 1:G:167:VAL:HG22 | 2.15                     | 0.47              |
| 1:I:138:ASP:OD1  | 1:I:138:ASP:N    | 2.44                     | 0.47              |
| 1:D:418:VAL:HG13 | 1:D:421:ILE:HD12 | 1.97                     | 0.47              |
| 1:J:204:THR:OG1  | 1:J:212:VAL:N    | 2.36                     | 0.47              |
| 1:E:285:ALA:HB1  | 1:E:366:ARG:CZ   | 2.45                     | 0.47              |
| 1:M:279:PHE:HD1  | 1:M:283:ARG:HH21 | 1.61                     | 0.47              |
| 1:H:6:LYS:HG2    | 1:H:11:ALA:HB2   | 1.97                     | 0.47              |
| 1:I:223:LYS:NZ   | 1:I:305:LEU:O    | 2.31                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:151:SER:HB2  | 1:E:393:ARG:NH1  | 2.30                     | 0.47              |
| 1:K:204:THR:OG1  | 1:K:212:VAL:N    | 2.37                     | 0.47              |
| 1:N:229:GLN:HA   | 1:N:232:LEU:HG   | 1.96                     | 0.47              |
| 1:A:153:SER:H    | 1:A:393:ARG:CZ   | 2.28                     | 0.47              |
| 1:C:237:GLN:HB3  | 1:C:312:ILE:HD11 | 1.96                     | 0.47              |
| 1:I:38:VAL:HG22  | 1:I:48:ILE:HG12  | 1.96                     | 0.47              |
| 1:J:72:LEU:O     | 1:J:75:GLU:HG3   | 2.14                     | 0.47              |
| 1:G:35:ARG:HH12  | 1:G:454:ASN:HA   | 1.78                     | 0.47              |
| 1:J:397:ALA:O    | 1:J:401:THR:OG1  | 2.26                     | 0.47              |
| 1:E:146:VAL:HA   | 1:E:149:VAL:HG23 | 1.97                     | 0.47              |
| 1:K:163:ALA:O    | 1:K:167:VAL:HG22 | 2.15                     | 0.47              |
| 1:H:223:LYS:NZ   | 1:H:305:LEU:O    | 2.34                     | 0.47              |
| 1:C:198:LEU:HD21 | 1:C:275:LYS:HG3  | 1.97                     | 0.47              |
| 1:C:223:LYS:NZ   | 1:C:305:LEU:O    | 2.34                     | 0.47              |
| 1:D:229:GLN:HA   | 1:D:232:LEU:HG   | 1.96                     | 0.47              |
| 1:F:219:LEU:HB3  | 1:F:247:ILE:HA   | 1.97                     | 0.47              |
| 1:E:101:GLU:O    | 1:E:104:LYS:HG2  | 2.14                     | 0.46              |
| 1:F:82:ASP:OD1   | 1:F:82:ASP:N     | 2.48                     | 0.46              |
| 1:L:172:VAL:HG21 | 1:L:192:GLN:HB3  | 1.97                     | 0.46              |
| 1:H:217:TYR:O    | 1:H:246:LEU:N    | 2.33                     | 0.46              |
| 1:B:388:LYS:HB2  | 1:B:388:LYS:HE2  | 1.73                     | 0.46              |
| 1:J:173:ILE:HA   | 1:J:375:ALA:HB3  | 1.97                     | 0.46              |
| 1:K:46:PRO:HB3   | 1:L:68:MET:HE1   | 1.97                     | 0.46              |
| 1:M:191:MET:O    | 1:M:330:ILE:N    | 2.36                     | 0.46              |
| 1:B:39:LEU:HD13  | 1:B:58:GLU:HG3   | 1.98                     | 0.46              |
| 1:B:198:LEU:HD21 | 1:B:275:LYS:HG3  | 1.97                     | 0.46              |
| 1:B:217:TYR:O    | 1:B:246:LEU:N    | 2.32                     | 0.46              |
| 1:C:172:VAL:HB   | 1:C:374:VAL:HG22 | 1.97                     | 0.46              |
| 1:E:237:GLN:HB3  | 1:E:312:ILE:HD11 | 1.97                     | 0.46              |
| 1:H:229:GLN:HA   | 1:H:232:LEU:HG   | 1.97                     | 0.46              |
| 1:B:163:ALA:O    | 1:B:167:VAL:HG22 | 2.16                     | 0.46              |
| 1:D:108:ALA:HA   | 1:J:104:LYS:HE3  | 1.98                     | 0.46              |
| 1:D:137:VAL:HG21 | 1:D:409:MET:HG2  | 1.98                     | 0.46              |
| 1:J:217:TYR:O    | 1:J:246:LEU:N    | 2.32                     | 0.46              |
| 1:L:237:GLN:HB3  | 1:L:312:ILE:HD11 | 1.97                     | 0.46              |
| 1:I:39:LEU:HD13  | 1:I:58:GLU:HG3   | 1.97                     | 0.46              |
| 1:E:418:VAL:HG13 | 1:E:421:ILE:HD12 | 1.97                     | 0.46              |
| 1:F:164:MET:C    | 1:F:164:MET:HE2  | 2.40                     | 0.46              |
| 1:L:229:GLN:HA   | 1:L:232:LEU:HG   | 1.98                     | 0.46              |
| 1:M:237:GLN:HB3  | 1:M:312:ILE:HD11 | 1.98                     | 0.46              |
| 1:M:388:LYS:HB2  | 1:M:388:LYS:HE2  | 1.71                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:237:GLN:HB3  | 1:H:312:ILE:HD11 | 1.96                     | 0.46              |
| 1:B:35:ARG:HH12  | 1:B:454:ASN:HA   | 1.81                     | 0.46              |
| 1:B:53:VAL:HB    | 1:B:88:THR:HG21  | 1.97                     | 0.46              |
| 1:C:33:LYS:HD2   | 1:H:113:LEU:HD13 | 1.96                     | 0.46              |
| 1:K:232:LEU:HD23 | 1:K:235:LEU:HD12 | 1.98                     | 0.46              |
| 1:L:279:PHE:HD1  | 1:L:283:ARG:HH21 | 1.64                     | 0.46              |
| 1:L:285:ALA:HB1  | 1:L:366:ARG:CZ   | 2.46                     | 0.46              |
| 1:K:151:SER:HB2  | 1:K:393:ARG:NE   | 2.26                     | 0.46              |
| 1:F:237:GLN:HB3  | 1:F:312:ILE:HD11 | 1.98                     | 0.46              |
| 1:N:215:ASN:HA   | 1:N:318:ALA:O    | 2.16                     | 0.46              |
| 1:B:38:VAL:HG22  | 1:B:48:ILE:HG12  | 1.96                     | 0.46              |
| 1:J:163:ALA:O    | 1:J:167:VAL:HG22 | 2.16                     | 0.46              |
| 1:F:221:THR:HB   | 1:F:299:ILE:HB   | 1.96                     | 0.46              |
| 1:A:151:SER:HB2  | 1:A:393:ARG:HE   | 1.81                     | 0.46              |
| 1:B:223:LYS:NZ   | 1:B:305:LEU:O    | 2.35                     | 0.46              |
| 1:D:409:MET:HE2  | 1:D:491:VAL:HB   | 1.97                     | 0.46              |
| 1:E:390:LEU:HD12 | 1:E:393:ARG:HD2  | 1.97                     | 0.46              |
| 1:H:388:LYS:HB2  | 1:H:388:LYS:HE2  | 1.72                     | 0.46              |
| 1:A:229:GLN:HA   | 1:A:232:LEU:HG   | 1.98                     | 0.45              |
| 1:B:140:LYS:HE3  | 1:B:161:ALA:HB1  | 1.98                     | 0.45              |
| 1:B:172:VAL:HB   | 1:B:374:VAL:HG22 | 1.98                     | 0.45              |
| 1:L:140:LYS:HE3  | 1:L:161:ALA:HB1  | 1.98                     | 0.45              |
| 1:H:286:MET:SD   | 1:H:286:MET:N    | 2.89                     | 0.45              |
| 1:K:72:LEU:O     | 1:K:75:GLU:HG3   | 2.16                     | 0.45              |
| 1:L:418:VAL:HG13 | 1:L:421:ILE:HD12 | 1.97                     | 0.45              |
| 1:A:76:VAL:CG2   | 1:A:507:VAL:HG21 | 2.45                     | 0.45              |
| 1:B:204:THR:OG1  | 1:B:212:VAL:N    | 2.35                     | 0.45              |
| 1:B:285:ALA:HB1  | 1:B:366:ARG:CZ   | 2.46                     | 0.45              |
| 1:I:215:ASN:HA   | 1:I:318:ALA:O    | 2.17                     | 0.45              |
| 1:I:237:GLN:HB3  | 1:I:312:ILE:HD11 | 1.98                     | 0.45              |
| 1:K:82:ASP:OD1   | 1:K:82:ASP:N     | 2.50                     | 0.45              |
| 1:M:68:MET:HE3   | 1:M:68:MET:HB3   | 1.70                     | 0.45              |
| 1:M:195:ARG:NH2  | 1:M:276:ALA:O    | 2.42                     | 0.45              |
| 1:A:204:THR:OG1  | 1:A:212:VAL:N    | 2.36                     | 0.45              |
| 1:C:35:ARG:HH12  | 1:C:454:ASN:HA   | 1.81                     | 0.45              |
| 1:C:138:ASP:N    | 1:C:138:ASP:OD1  | 2.48                     | 0.45              |
| 1:I:229:GLN:HA   | 1:I:232:LEU:HG   | 1.98                     | 0.45              |
| 1:D:77:ALA:O     | 1:D:81:ASN:ND2   | 2.49                     | 0.45              |
| 1:D:388:LYS:HE2  | 1:D:388:LYS:HB2  | 1.75                     | 0.45              |
| 1:K:237:GLN:HB3  | 1:K:312:ILE:HD11 | 1.97                     | 0.45              |
| 1:D:76:VAL:CG2   | 1:D:507:VAL:HG21 | 2.46                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:237:GLN:HB3  | 1:D:312:ILE:HD11 | 1.97                     | 0.45              |
| 1:F:388:LYS:HB2  | 1:F:388:LYS:HE2  | 1.73                     | 0.45              |
| 1:L:388:LYS:HB2  | 1:L:388:LYS:HE2  | 1.72                     | 0.45              |
| 1:B:219:LEU:HB3  | 1:B:247:ILE:HA   | 1.98                     | 0.45              |
| 1:I:140:LYS:HE3  | 1:I:161:ALA:HB1  | 1.98                     | 0.45              |
| 1:J:20:ASP:OD1   | 1:J:100:ARG:NH1  | 2.50                     | 0.45              |
| 1:G:237:GLN:HB3  | 1:G:312:ILE:HD11 | 1.99                     | 0.45              |
| 1:M:215:ASN:HA   | 1:M:318:ALA:O    | 2.17                     | 0.45              |
| 1:H:78:SER:HA    | 1:H:81:ASN:ND2   | 2.31                     | 0.45              |
| 1:D:149:VAL:O    | 1:D:150:SER:HB3  | 2.16                     | 0.45              |
| 1:D:204:THR:OG1  | 1:D:212:VAL:N    | 2.34                     | 0.45              |
| 1:J:198:LEU:HD21 | 1:J:275:LYS:HG3  | 1.98                     | 0.45              |
| 1:I:142:ALA:O    | 1:I:146:VAL:HG23 | 2.17                     | 0.45              |
| 1:I:191:MET:HE3  | 1:I:192:GLN:N    | 2.32                     | 0.45              |
| 1:E:229:GLN:HA   | 1:E:232:LEU:HG   | 1.98                     | 0.45              |
| 1:F:138:ASP:OD1  | 1:F:138:ASP:N    | 2.47                     | 0.45              |
| 1:F:196:GLY:HA3  | 1:F:325:LYS:O    | 2.17                     | 0.45              |
| 1:G:215:ASN:HA   | 1:G:318:ALA:O    | 2.16                     | 0.45              |
| 1:H:219:LEU:HB3  | 1:H:247:ILE:HA   | 1.99                     | 0.45              |
| 1:C:229:GLN:HA   | 1:C:232:LEU:HG   | 1.97                     | 0.45              |
| 1:J:139:SER:OG   | 1:J:141:GLU:OE1  | 2.35                     | 0.45              |
| 1:K:172:VAL:HB   | 1:K:374:VAL:HG22 | 1.99                     | 0.45              |
| 1:H:173:ILE:HA   | 1:H:375:ALA:HB3  | 1.98                     | 0.45              |
| 1:B:279:PHE:HD1  | 1:B:283:ARG:HH21 | 1.63                     | 0.45              |
| 1:D:163:ALA:O    | 1:D:167:VAL:HG22 | 2.17                     | 0.45              |
| 1:L:173:ILE:HA   | 1:L:375:ALA:HB3  | 1.98                     | 0.45              |
| 1:G:101:GLU:C    | 1:G:439:ILE:HD11 | 2.42                     | 0.45              |
| 1:M:142:ALA:O    | 1:M:146:VAL:HG23 | 2.17                     | 0.45              |
| 1:H:38:VAL:HG13  | 1:H:48:ILE:HG12  | 1.99                     | 0.45              |
| 1:N:388:LYS:HB2  | 1:N:388:LYS:HE2  | 1.73                     | 0.45              |
| 1:I:219:LEU:HB3  | 1:I:247:ILE:HA   | 1.98                     | 0.44              |
| 1:D:397:ALA:O    | 1:D:401:THR:OG1  | 2.26                     | 0.44              |
| 1:E:9:GLU:O      | 1:E:13:ALA:N     | 2.47                     | 0.44              |
| 1:E:191:MET:O    | 1:E:330:ILE:N    | 2.38                     | 0.44              |
| 1:M:196:GLY:HA3  | 1:M:325:LYS:O    | 2.17                     | 0.44              |
| 1:B:284:LYS:HA   | 1:B:287:LEU:HB2  | 1.98                     | 0.44              |
| 1:J:196:GLY:HA3  | 1:J:325:LYS:O    | 2.17                     | 0.44              |
| 1:K:219:LEU:HB3  | 1:K:247:ILE:HA   | 1.99                     | 0.44              |
| 1:F:229:GLN:HA   | 1:F:232:LEU:HG   | 1.99                     | 0.44              |
| 1:L:286:MET:SD   | 1:L:286:MET:N    | 2.89                     | 0.44              |
| 1:I:196:GLY:HA3  | 1:I:325:LYS:O    | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:78:SER:HA    | 1:D:81:ASN:ND2   | 2.30                     | 0.44              |
| 1:E:196:GLY:HA3  | 1:E:325:LYS:O    | 2.17                     | 0.44              |
| 1:E:215:ASN:HA   | 1:E:318:ALA:O    | 2.17                     | 0.44              |
| 1:K:153:SER:OG   | 1:K:156:VAL:HG23 | 2.17                     | 0.44              |
| 1:M:289:ASP:CG   | 1:M:366:ARG:HH21 | 2.26                     | 0.44              |
| 1:N:191:MET:HE3  | 1:N:192:GLN:N    | 2.32                     | 0.44              |
| 1:N:237:GLN:HB3  | 1:N:312:ILE:HD11 | 2.00                     | 0.44              |
| 1:A:285:ALA:HB1  | 1:A:366:ARG:CZ   | 2.47                     | 0.44              |
| 1:C:173:ILE:HA   | 1:C:375:ALA:HB3  | 1.99                     | 0.44              |
| 1:J:12:ARG:HD2   | 1:J:103:LEU:HD21 | 2.00                     | 0.44              |
| 1:K:223:LYS:NZ   | 1:K:305:LEU:O    | 2.35                     | 0.44              |
| 1:L:20:ASP:OD1   | 1:L:100:ARG:NH1  | 2.50                     | 0.44              |
| 1:G:39:LEU:HD13  | 1:G:58:GLU:HG3   | 1.99                     | 0.44              |
| 1:G:388:LYS:HB2  | 1:G:388:LYS:HE2  | 1.73                     | 0.44              |
| 1:M:153:SER:OG   | 1:M:156:VAL:HG23 | 2.18                     | 0.44              |
| 1:A:163:ALA:O    | 1:A:167:VAL:HG22 | 2.17                     | 0.44              |
| 1:A:173:ILE:HA   | 1:A:375:ALA:HB3  | 1.99                     | 0.44              |
| 1:C:153:SER:OG   | 1:C:154:ASP:N    | 2.51                     | 0.44              |
| 1:C:286:MET:SD   | 1:C:286:MET:N    | 2.89                     | 0.44              |
| 1:D:223:LYS:NZ   | 1:D:305:LEU:O    | 2.32                     | 0.44              |
| 1:J:464:ASP:O    | 1:J:468:ASN:ND2  | 2.51                     | 0.44              |
| 1:K:142:ALA:O    | 1:K:146:VAL:HG23 | 2.17                     | 0.44              |
| 1:H:208:LYS:C    | 1:H:210:GLU:H    | 2.25                     | 0.44              |
| 1:N:219:LEU:HB3  | 1:N:247:ILE:HA   | 1.99                     | 0.44              |
| 1:N:397:ALA:O    | 1:N:401:THR:OG1  | 2.26                     | 0.44              |
| 1:B:232:LEU:HD23 | 1:B:235:LEU:HD12 | 2.00                     | 0.44              |
| 1:D:3:LYS:HA     | 1:D:3:LYS:HD3    | 1.78                     | 0.44              |
| 1:D:215:ASN:HA   | 1:D:318:ALA:O    | 2.17                     | 0.44              |
| 1:K:196:GLY:HA3  | 1:K:325:LYS:O    | 2.17                     | 0.44              |
| 1:B:151:SER:O    | 1:B:153:SER:N    | 2.50                     | 0.44              |
| 1:C:196:GLY:HA3  | 1:C:325:LYS:O    | 2.18                     | 0.44              |
| 1:C:219:LEU:HB3  | 1:C:247:ILE:HA   | 2.00                     | 0.44              |
| 1:I:146:VAL:O    | 1:I:149:VAL:HG22 | 2.17                     | 0.44              |
| 1:I:284:LYS:NZ   | 1:I:302:ASP:OD2  | 2.50                     | 0.44              |
| 1:D:20:ASP:OD1   | 1:D:100:ARG:NH1  | 2.50                     | 0.44              |
| 1:J:133:ILE:HG13 | 1:J:133:ILE:O    | 2.18                     | 0.44              |
| 1:L:153:SER:OG   | 1:L:156:VAL:HG23 | 2.17                     | 0.44              |
| 1:M:46:PRO:CB    | 1:N:68:MET:HE1   | 2.48                     | 0.44              |
| 1:H:196:GLY:HA3  | 1:H:325:LYS:O    | 2.17                     | 0.44              |
| 1:B:196:GLY:HA3  | 1:B:325:LYS:O    | 2.17                     | 0.44              |
| 1:J:76:VAL:CG2   | 1:J:507:VAL:HG21 | 2.45                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:409:MET:HE2  | 1:J:491:VAL:HB   | 1.98                     | 0.44              |
| 1:E:172:VAL:HG21 | 1:E:192:GLN:HB3  | 2.00                     | 0.44              |
| 1:G:164:MET:O    | 1:G:168:GLY:N    | 2.49                     | 0.44              |
| 1:G:219:LEU:HB3  | 1:G:247:ILE:HA   | 2.00                     | 0.44              |
| 1:G:397:ALA:O    | 1:G:401:THR:OG1  | 2.25                     | 0.44              |
| 1:A:208:LYS:C    | 1:A:210:GLU:H    | 2.26                     | 0.44              |
| 1:A:219:LEU:HB3  | 1:A:247:ILE:HA   | 2.00                     | 0.44              |
| 1:B:191:MET:CE   | 1:B:369:LYS:HB3  | 2.45                     | 0.44              |
| 1:C:164:MET:SD   | 1:C:169:ASN:HA   | 2.58                     | 0.44              |
| 1:M:38:VAL:HG22  | 1:M:48:ILE:HG12  | 1.98                     | 0.44              |
| 1:M:208:LYS:C    | 1:M:210:GLU:H    | 2.26                     | 0.44              |
| 1:H:172:VAL:HB   | 1:H:374:VAL:HG22 | 2.00                     | 0.44              |
| 1:H:191:MET:SD   | 1:H:193:PHE:HD1  | 2.41                     | 0.44              |
| 1:A:138:ASP:OD1  | 1:A:138:ASP:N    | 2.49                     | 0.43              |
| 1:B:40:GLU:HB2   | 1:J:519:ALA:HA   | 2.00                     | 0.43              |
| 1:B:151:SER:OG   | 1:B:393:ARG:NE   | 2.25                     | 0.43              |
| 1:D:208:LYS:C    | 1:D:210:GLU:H    | 2.26                     | 0.43              |
| 1:F:101:GLU:O    | 1:F:105:ASN:ND2  | 2.43                     | 0.43              |
| 1:G:196:GLY:HA3  | 1:G:325:LYS:O    | 2.18                     | 0.43              |
| 1:H:163:ALA:O    | 1:H:167:VAL:HG22 | 2.18                     | 0.43              |
| 1:H:284:LYS:NZ   | 1:H:302:ASP:OD2  | 2.51                     | 0.43              |
| 1:N:103:LEU:HD23 | 1:N:103:LEU:HA   | 1.81                     | 0.43              |
| 1:N:196:GLY:HA3  | 1:N:325:LYS:O    | 2.18                     | 0.43              |
| 1:B:76:VAL:HG21  | 1:B:507:VAL:HG11 | 1.98                     | 0.43              |
| 1:C:217:TYR:O    | 1:C:246:LEU:N    | 2.33                     | 0.43              |
| 1:I:163:ALA:O    | 1:I:167:VAL:HG22 | 2.18                     | 0.43              |
| 1:I:289:ASP:CG   | 1:I:366:ARG:HH21 | 2.27                     | 0.43              |
| 1:D:217:TYR:O    | 1:D:246:LEU:N    | 2.34                     | 0.43              |
| 1:J:219:LEU:HB3  | 1:J:247:ILE:HA   | 2.00                     | 0.43              |
| 1:E:133:ILE:O    | 1:E:133:ILE:HG13 | 2.18                     | 0.43              |
| 1:K:116:ARG:HG3  | 1:K:509:ALA:HB1  | 2.00                     | 0.43              |
| 1:D:289:ASP:CG   | 1:D:366:ARG:HH21 | 2.27                     | 0.43              |
| 1:J:260:LEU:HD22 | 1:J:271:VAL:HG11 | 1.99                     | 0.43              |
| 1:E:97:ALA:CB    | 1:E:446:GLU:HG3  | 2.48                     | 0.43              |
| 1:G:289:ASP:CG   | 1:G:366:ARG:HH21 | 2.26                     | 0.43              |
| 1:M:138:ASP:OD1  | 1:M:138:ASP:N    | 2.50                     | 0.43              |
| 1:H:80:THR:OG1   | 1:H:503:ASN:OD1  | 2.36                     | 0.43              |
| 1:H:215:ASN:HA   | 1:H:318:ALA:O    | 2.18                     | 0.43              |
| 1:J:153:SER:OG   | 1:J:156:VAL:HG23 | 2.18                     | 0.43              |
| 1:K:418:VAL:HG13 | 1:K:421:ILE:HD12 | 2.01                     | 0.43              |
| 1:F:223:LYS:NZ   | 1:F:305:LEU:O    | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:140:LYS:HE3  | 1:M:161:ALA:HB1  | 2.01                     | 0.43              |
| 1:H:289:ASP:CG   | 1:H:366:ARG:HH21 | 2.26                     | 0.43              |
| 1:A:2:ALA:HB1    | 1:D:62:GLU:HB2   | 2.00                     | 0.43              |
| 1:A:196:GLY:HA3  | 1:A:325:LYS:O    | 2.18                     | 0.43              |
| 1:C:15:MET:HE1   | 1:C:69:GLY:HA2   | 2.00                     | 0.43              |
| 1:I:208:LYS:C    | 1:I:210:GLU:H    | 2.26                     | 0.43              |
| 1:I:388:LYS:HB2  | 1:I:388:LYS:HE2  | 1.73                     | 0.43              |
| 1:J:191:MET:CE   | 1:J:369:LYS:HB3  | 2.47                     | 0.43              |
| 1:K:76:VAL:HG21  | 1:K:507:VAL:HG11 | 1.98                     | 0.43              |
| 1:L:76:VAL:CG2   | 1:L:507:VAL:HG21 | 2.47                     | 0.43              |
| 1:M:217:TYR:O    | 1:M:246:LEU:N    | 2.33                     | 0.43              |
| 1:H:76:VAL:CG2   | 1:H:507:VAL:HG21 | 2.48                     | 0.43              |
| 1:A:164:MET:HE1  | 1:A:169:ASN:HA   | 2.00                     | 0.43              |
| 1:K:138:ASP:OD1  | 1:K:138:ASP:N    | 2.49                     | 0.43              |
| 1:L:196:GLY:HA3  | 1:L:325:LYS:O    | 2.18                     | 0.43              |
| 1:G:198:LEU:HD21 | 1:G:275:LYS:HG3  | 2.01                     | 0.43              |
| 1:M:406:GLU:H    | 1:M:406:GLU:HG2  | 1.70                     | 0.43              |
| 1:A:116:ARG:HG3  | 1:A:509:ALA:HB1  | 2.01                     | 0.43              |
| 1:B:397:ALA:O    | 1:B:401:THR:OG1  | 2.27                     | 0.43              |
| 1:K:465:LYS:O    | 1:K:469:VAL:HG13 | 2.19                     | 0.43              |
| 1:B:68:MET:HE3   | 1:B:68:MET:HB3   | 1.94                     | 0.43              |
| 1:B:76:VAL:CG2   | 1:B:507:VAL:HG21 | 2.47                     | 0.43              |
| 1:C:215:ASN:HA   | 1:C:318:ALA:O    | 2.18                     | 0.43              |
| 1:D:103:LEU:HD12 | 1:D:103:LEU:HA   | 1.87                     | 0.43              |
| 1:K:101:GLU:O    | 1:K:105:ASN:ND2  | 2.44                     | 0.43              |
| 1:F:64:HIS:O     | 1:F:68:MET:HG2   | 2.19                     | 0.43              |
| 1:H:35:ARG:HH12  | 1:H:454:ASN:HA   | 1.84                     | 0.43              |
| 1:N:163:ALA:O    | 1:N:167:VAL:HG22 | 2.18                     | 0.43              |
| 1:A:286:MET:SD   | 1:A:286:MET:N    | 2.88                     | 0.43              |
| 1:I:78:SER:HA    | 1:I:81:ASN:ND2   | 2.32                     | 0.43              |
| 1:D:133:ILE:O    | 1:D:133:ILE:HG13 | 2.19                     | 0.43              |
| 1:D:172:VAL:HG21 | 1:D:192:GLN:HB3  | 2.00                     | 0.43              |
| 1:J:284:LYS:HA   | 1:J:287:LEU:HB2  | 2.00                     | 0.43              |
| 1:E:198:LEU:HD21 | 1:E:275:LYS:HG3  | 2.00                     | 0.43              |
| 1:E:217:TYR:O    | 1:E:246:LEU:N    | 2.33                     | 0.43              |
| 1:K:289:ASP:CG   | 1:K:366:ARG:HH21 | 2.27                     | 0.43              |
| 1:F:215:ASN:HA   | 1:F:318:ALA:O    | 2.19                     | 0.43              |
| 1:L:71:LYS:HD3   | 1:L:71:LYS:HA    | 1.83                     | 0.43              |
| 1:L:215:ASN:HA   | 1:L:318:ALA:O    | 2.18                     | 0.43              |
| 1:A:35:ARG:HH12  | 1:A:454:ASN:HA   | 1.84                     | 0.43              |
| 1:A:82:ASP:OD1   | 1:A:82:ASP:N     | 2.51                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:257:LEU:HB3  | 1:B:258:PRO:HD3  | 2.01                     | 0.43              |
| 1:E:96:GLN:CD    | 1:E:100:ARG:HH22 | 2.26                     | 0.43              |
| 1:E:208:LYS:C    | 1:E:210:GLU:H    | 2.27                     | 0.43              |
| 1:K:208:LYS:C    | 1:K:210:GLU:H    | 2.27                     | 0.43              |
| 1:F:458:GLU:O    | 1:F:462:ILE:HG12 | 2.19                     | 0.43              |
| 1:H:101:GLU:O    | 1:H:105:ASN:ND2  | 2.41                     | 0.43              |
| 1:A:145:GLN:O    | 1:A:149:VAL:HG23 | 2.19                     | 0.42              |
| 1:A:215:ASN:HA   | 1:A:318:ALA:O    | 2.18                     | 0.42              |
| 1:B:77:ALA:HB1   | 1:B:88:THR:OG1   | 2.19                     | 0.42              |
| 1:B:138:ASP:OD1  | 1:B:138:ASP:N    | 2.50                     | 0.42              |
| 1:B:229:GLN:HA   | 1:B:232:LEU:HG   | 2.01                     | 0.42              |
| 1:B:239:LEU:HB2  | 1:B:269:PHE:CE1  | 2.54                     | 0.42              |
| 1:J:199:SER:H    | 1:J:202:MET:HE3  | 1.83                     | 0.42              |
| 1:F:163:ALA:O    | 1:F:167:VAL:HG22 | 2.19                     | 0.42              |
| 1:F:197:TYR:OH   | 1:F:209:MET:SD   | 2.70                     | 0.42              |
| 1:G:208:LYS:C    | 1:G:210:GLU:H    | 2.27                     | 0.42              |
| 1:H:239:LEU:HB2  | 1:H:269:PHE:CE1  | 2.54                     | 0.42              |
| 1:N:208:LYS:C    | 1:N:210:GLU:H    | 2.27                     | 0.42              |
| 1:N:284:LYS:HA   | 1:N:287:LEU:HB2  | 2.01                     | 0.42              |
| 1:A:6:LYS:HB3    | 1:A:6:LYS:HE2    | 1.89                     | 0.42              |
| 1:A:140:LYS:HE3  | 1:A:161:ALA:HB1  | 2.00                     | 0.42              |
| 1:A:239:LEU:HB2  | 1:A:269:PHE:CE1  | 2.54                     | 0.42              |
| 1:C:289:ASP:CG   | 1:C:366:ARG:HH21 | 2.27                     | 0.42              |
| 1:I:76:VAL:CG2   | 1:I:507:VAL:HG21 | 2.48                     | 0.42              |
| 1:J:229:GLN:HA   | 1:J:232:LEU:HG   | 2.00                     | 0.42              |
| 1:J:232:LEU:HD23 | 1:J:235:LEU:HD12 | 2.01                     | 0.42              |
| 1:E:153:SER:OG   | 1:E:156:VAL:HG23 | 2.19                     | 0.42              |
| 1:K:406:GLU:H    | 1:K:406:GLU:HG2  | 1.69                     | 0.42              |
| 1:F:239:LEU:HB2  | 1:F:269:PHE:CE1  | 2.54                     | 0.42              |
| 1:L:219:LEU:HB3  | 1:L:247:ILE:HA   | 2.01                     | 0.42              |
| 1:G:191:MET:CE   | 1:G:369:LYS:HB3  | 2.47                     | 0.42              |
| 1:C:38:VAL:HG13  | 1:C:48:ILE:HG12  | 2.01                     | 0.42              |
| 1:C:257:LEU:HB3  | 1:C:258:PRO:HD3  | 2.02                     | 0.42              |
| 1:I:209:MET:SD   | 1:I:325:LYS:HB2  | 2.59                     | 0.42              |
| 1:F:39:LEU:HD21  | 1:F:55:ILE:HG23  | 2.01                     | 0.42              |
| 1:L:163:ALA:O    | 1:L:167:VAL:HG22 | 2.18                     | 0.42              |
| 1:M:173:ILE:HA   | 1:M:375:ALA:HB3  | 2.01                     | 0.42              |
| 1:A:77:ALA:HB1   | 1:A:88:THR:OG1   | 2.20                     | 0.42              |
| 1:B:260:LEU:HD22 | 1:B:271:VAL:HG11 | 2.00                     | 0.42              |
| 1:I:133:ILE:HG13 | 1:I:133:ILE:O    | 2.19                     | 0.42              |
| 1:F:76:VAL:HG21  | 1:F:507:VAL:HG11 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:97:ALA:CB    | 1:G:446:GLU:HG3  | 2.50                     | 0.42              |
| 1:G:147:ALA:HB3  | 1:G:157:GLY:HA2  | 2.00                     | 0.42              |
| 1:G:191:MET:O    | 1:G:330:ILE:N    | 2.44                     | 0.42              |
| 1:N:172:VAL:HB   | 1:N:374:VAL:HG22 | 2.02                     | 0.42              |
| 1:B:193:PHE:CE2  | 1:B:195:ARG:HB2  | 2.54                     | 0.42              |
| 1:C:164:MET:CE   | 1:C:169:ASN:HA   | 2.49                     | 0.42              |
| 1:I:64:HIS:O     | 1:I:68:MET:HG2   | 2.19                     | 0.42              |
| 1:E:103:LEU:HA   | 1:E:103:LEU:HD23 | 1.80                     | 0.42              |
| 1:L:80:THR:HG1   | 1:L:503:ASN:HD22 | 1.67                     | 0.42              |
| 1:L:257:LEU:HB3  | 1:L:258:PRO:HD3  | 2.02                     | 0.42              |
| 1:H:142:ALA:O    | 1:H:146:VAL:HG23 | 2.20                     | 0.42              |
| 1:H:257:LEU:HB3  | 1:H:258:PRO:HD3  | 2.02                     | 0.42              |
| 1:N:172:VAL:HG21 | 1:N:192:GLN:HB3  | 2.01                     | 0.42              |
| 1:C:116:ARG:HG3  | 1:C:509:ALA:HB1  | 2.02                     | 0.42              |
| 1:I:145:GLN:O    | 1:I:149:VAL:HG13 | 2.19                     | 0.42              |
| 1:J:135:THR:OG1  | 1:J:409:MET:O    | 2.31                     | 0.42              |
| 1:J:154:ASP:HB3  | 1:J:155:LYS:NZ   | 2.34                     | 0.42              |
| 1:J:239:LEU:HB2  | 1:J:269:PHE:CE1  | 2.54                     | 0.42              |
| 1:K:279:PHE:HD1  | 1:K:283:ARG:HH21 | 1.68                     | 0.42              |
| 1:K:458:GLU:O    | 1:K:462:ILE:HG12 | 2.20                     | 0.42              |
| 1:F:286:MET:SD   | 1:F:286:MET:N    | 2.82                     | 0.42              |
| 1:M:219:LEU:HB3  | 1:M:247:ILE:HA   | 2.01                     | 0.42              |
| 1:N:1:MET:CE     | 1:N:520:ASP:HB3  | 2.49                     | 0.42              |
| 1:N:39:LEU:HD13  | 1:N:58:GLU:HG3   | 2.01                     | 0.42              |
| 1:A:257:LEU:HB3  | 1:A:258:PRO:HD3  | 2.02                     | 0.42              |
| 1:A:390:LEU:HD12 | 1:A:390:LEU:HA   | 1.89                     | 0.42              |
| 1:C:208:LYS:C    | 1:C:210:GLU:H    | 2.28                     | 0.42              |
| 1:C:239:LEU:HB2  | 1:C:269:PHE:CE1  | 2.54                     | 0.42              |
| 1:D:239:LEU:HB2  | 1:D:269:PHE:CE1  | 2.55                     | 0.42              |
| 1:E:154:ASP:HB3  | 1:E:155:LYS:NZ   | 2.33                     | 0.42              |
| 1:E:219:LEU:HB3  | 1:E:247:ILE:HA   | 2.01                     | 0.42              |
| 1:F:208:LYS:C    | 1:F:210:GLU:H    | 2.27                     | 0.42              |
| 1:L:138:ASP:OD1  | 1:L:138:ASP:N    | 2.49                     | 0.42              |
| 1:G:82:ASP:OD1   | 1:G:82:ASP:N     | 2.52                     | 0.42              |
| 1:G:239:LEU:HB2  | 1:G:269:PHE:CE1  | 2.54                     | 0.42              |
| 1:H:147:ALA:HB3  | 1:H:157:GLY:HA2  | 2.00                     | 0.42              |
| 1:A:232:LEU:HD23 | 1:A:235:LEU:HD12 | 2.02                     | 0.42              |
| 1:B:154:ASP:HB3  | 1:B:155:LYS:NZ   | 2.34                     | 0.42              |
| 1:C:96:GLN:NE2   | 1:C:100:ARG:HH12 | 2.18                     | 0.42              |
| 1:I:239:LEU:HB2  | 1:I:269:PHE:CE1  | 2.55                     | 0.42              |
| 1:I:406:GLU:H    | 1:I:406:GLU:HG2  | 1.71                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:199:SER:O    | 1:D:202:MET:HE3  | 2.20                     | 0.42              |
| 1:J:306:GLU:HB2  | 1:J:309:ASP:OD2  | 2.20                     | 0.42              |
| 1:E:475:PHE:CZ   | 1:E:480:GLY:HA2  | 2.55                     | 0.42              |
| 1:L:191:MET:HE3  | 1:L:192:GLN:N    | 2.34                     | 0.42              |
| 1:L:239:LEU:HB2  | 1:L:269:PHE:CE1  | 2.55                     | 0.42              |
| 1:G:284:LYS:NZ   | 1:G:302:ASP:OD2  | 2.52                     | 0.42              |
| 1:M:239:LEU:HB2  | 1:M:269:PHE:CE1  | 2.55                     | 0.42              |
| 1:H:197:TYR:OH   | 1:H:209:MET:SD   | 2.74                     | 0.42              |
| 1:H:209:MET:SD   | 1:H:325:LYS:HB2  | 2.59                     | 0.42              |
| 1:N:153:SER:OG   | 1:N:156:VAL:HG23 | 2.20                     | 0.42              |
| 1:D:164:MET:HE2  | 1:D:164:MET:C    | 2.44                     | 0.42              |
| 1:J:406:GLU:H    | 1:J:406:GLU:HG2  | 1.71                     | 0.42              |
| 1:K:188:VAL:HG21 | 1:K:332:GLU:HG3  | 2.01                     | 0.42              |
| 1:L:82:ASP:OD1   | 1:L:82:ASP:N     | 2.51                     | 0.42              |
| 1:L:284:LYS:HA   | 1:L:287:LEU:HB2  | 2.02                     | 0.42              |
| 1:M:458:GLU:O    | 1:M:462:ILE:HG12 | 2.19                     | 0.42              |
| 1:H:71:LYS:HD3   | 1:H:71:LYS:HA    | 1.80                     | 0.42              |
| 1:H:151:SER:O    | 1:H:153:SER:N    | 2.53                     | 0.42              |
| 1:N:239:LEU:HB2  | 1:N:269:PHE:CE1  | 2.54                     | 0.42              |
| 1:N:458:GLU:O    | 1:N:462:ILE:HG12 | 2.20                     | 0.42              |
| 1:A:71:LYS:HD3   | 1:A:71:LYS:HA    | 1.83                     | 0.42              |
| 1:A:388:LYS:HB2  | 1:A:388:LYS:HE2  | 1.73                     | 0.42              |
| 1:A:409:MET:HE1  | 1:A:492:ASP:C    | 2.45                     | 0.42              |
| 1:B:215:ASN:HA   | 1:B:318:ALA:O    | 2.19                     | 0.42              |
| 1:C:103:LEU:HD23 | 1:C:103:LEU:HA   | 1.83                     | 0.42              |
| 1:D:196:GLY:HA3  | 1:D:325:LYS:O    | 2.20                     | 0.42              |
| 1:J:257:LEU:HB3  | 1:J:258:PRO:HD3  | 2.02                     | 0.42              |
| 1:K:173:ILE:HA   | 1:K:375:ALA:HB3  | 2.01                     | 0.42              |
| 1:F:406:GLU:H    | 1:F:406:GLU:HG2  | 1.73                     | 0.42              |
| 1:G:153:SER:OG   | 1:G:156:VAL:HG23 | 2.20                     | 0.42              |
| 1:H:153:SER:OG   | 1:H:156:VAL:HG23 | 2.20                     | 0.42              |
| 1:I:172:VAL:HB   | 1:I:374:VAL:HG22 | 2.02                     | 0.41              |
| 1:I:175:ILE:HG22 | 1:I:391:LYS:HD2  | 2.02                     | 0.41              |
| 1:D:191:MET:HE3  | 1:D:192:GLN:N    | 2.35                     | 0.41              |
| 1:J:68:MET:HE3   | 1:J:68:MET:HB3   | 1.95                     | 0.41              |
| 1:K:239:LEU:HB2  | 1:K:269:PHE:CE1  | 2.55                     | 0.41              |
| 1:K:249:ALA:O    | 1:K:276:ALA:N    | 2.52                     | 0.41              |
| 1:K:257:LEU:HB3  | 1:K:258:PRO:HD3  | 2.02                     | 0.41              |
| 1:G:249:ALA:O    | 1:G:276:ALA:N    | 2.53                     | 0.41              |
| 1:M:82:ASP:OD1   | 1:M:82:ASP:N     | 2.53                     | 0.41              |
| 1:H:406:GLU:H    | 1:H:406:GLU:HG2  | 1.71                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:146:VAL:HA   | 1:C:149:VAL:HG12 | 2.02                     | 0.41              |
| 1:D:96:GLN:CD    | 1:D:100:ARG:HH22 | 2.28                     | 0.41              |
| 1:D:219:LEU:HB3  | 1:D:247:ILE:HA   | 2.02                     | 0.41              |
| 1:E:10:ASP:OD1   | 1:E:11:ALA:N     | 2.53                     | 0.41              |
| 1:E:257:LEU:HB3  | 1:E:258:PRO:HD3  | 2.02                     | 0.41              |
| 1:K:217:TYR:O    | 1:K:246:LEU:N    | 2.32                     | 0.41              |
| 1:L:208:LYS:C    | 1:L:210:GLU:H    | 2.28                     | 0.41              |
| 1:B:208:LYS:C    | 1:B:210:GLU:H    | 2.27                     | 0.41              |
| 1:C:232:LEU:HD23 | 1:C:235:LEU:HD12 | 2.02                     | 0.41              |
| 1:D:101:GLU:O    | 1:D:105:ASN:ND2  | 2.45                     | 0.41              |
| 1:D:257:LEU:HB3  | 1:D:258:PRO:HD3  | 2.02                     | 0.41              |
| 1:J:35:ARG:HH12  | 1:J:454:ASN:HA   | 1.85                     | 0.41              |
| 1:K:145:GLN:O    | 1:K:149:VAL:HG13 | 2.20                     | 0.41              |
| 1:F:133:ILE:O    | 1:F:133:ILE:HG13 | 2.19                     | 0.41              |
| 1:M:146:VAL:O    | 1:M:149:VAL:HG22 | 2.21                     | 0.41              |
| 1:M:247:ILE:HB   | 1:M:273:ALA:HA   | 2.01                     | 0.41              |
| 1:A:465:LYS:O    | 1:A:469:VAL:HG13 | 2.21                     | 0.41              |
| 1:C:388:LYS:HE2  | 1:C:388:LYS:HB2  | 1.73                     | 0.41              |
| 1:D:154:ASP:HB3  | 1:D:155:LYS:NZ   | 2.34                     | 0.41              |
| 1:J:215:ASN:HA   | 1:J:318:ALA:O    | 2.19                     | 0.41              |
| 1:J:362:LYS:HA   | 1:J:362:LYS:HD3  | 1.88                     | 0.41              |
| 1:E:388:LYS:HB2  | 1:E:388:LYS:HE2  | 1.73                     | 0.41              |
| 1:K:103:LEU:HD23 | 1:K:103:LEU:HA   | 1.84                     | 0.41              |
| 1:F:96:GLN:CD    | 1:F:100:ARG:HH22 | 2.28                     | 0.41              |
| 1:G:173:ILE:HA   | 1:G:375:ALA:HB3  | 2.01                     | 0.41              |
| 1:G:175:ILE:HG22 | 1:G:391:LYS:HD2  | 2.02                     | 0.41              |
| 1:M:77:ALA:HB1   | 1:M:88:THR:OG1   | 2.20                     | 0.41              |
| 1:H:64:HIS:O     | 1:H:68:MET:HG2   | 2.20                     | 0.41              |
| 1:H:390:LEU:HD12 | 1:H:390:LEU:HA   | 1.89                     | 0.41              |
| 1:H:465:LYS:O    | 1:H:469:VAL:HG13 | 2.21                     | 0.41              |
| 1:N:147:ALA:HB3  | 1:N:157:GLY:HA2  | 2.02                     | 0.41              |
| 1:B:247:ILE:HB   | 1:B:273:ALA:HA   | 2.02                     | 0.41              |
| 1:D:465:LYS:O    | 1:D:469:VAL:HG13 | 2.21                     | 0.41              |
| 1:J:96:GLN:CD    | 1:J:100:ARG:HH22 | 2.28                     | 0.41              |
| 1:E:111:ASN:HA   | 1:E:112:PRO:HD3  | 1.94                     | 0.41              |
| 1:E:397:ALA:O    | 1:E:401:THR:OG1  | 2.27                     | 0.41              |
| 1:K:384:GLU:HG2  | 1:L:279:PHE:CZ   | 2.56                     | 0.41              |
| 1:F:175:ILE:HG22 | 1:F:391:LYS:HD2  | 2.02                     | 0.41              |
| 1:F:284:LYS:HA   | 1:F:287:LEU:HB2  | 2.03                     | 0.41              |
| 1:G:151:SER:O    | 1:G:153:SER:N    | 2.53                     | 0.41              |
| 1:A:284:LYS:HA   | 1:A:287:LEU:HB2  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:306:GLU:HB2  | 1:C:309:ASP:OD2  | 2.21                     | 0.41              |
| 1:D:475:PHE:CZ   | 1:D:480:GLY:HA2  | 2.56                     | 0.41              |
| 1:J:9:GLU:O      | 1:J:13:ALA:N     | 2.52                     | 0.41              |
| 1:J:286:MET:SD   | 1:J:286:MET:N    | 2.87                     | 0.41              |
| 1:J:388:LYS:HE2  | 1:J:388:LYS:HB2  | 1.74                     | 0.41              |
| 1:E:239:LEU:HB2  | 1:E:269:PHE:CE1  | 2.55                     | 0.41              |
| 1:E:306:GLU:HB2  | 1:E:309:ASP:OD2  | 2.21                     | 0.41              |
| 1:L:151:SER:O    | 1:L:153:SER:N    | 2.53                     | 0.41              |
| 1:L:164:MET:HE3  | 1:L:169:ASN:HA   | 2.01                     | 0.41              |
| 1:G:257:LEU:HB3  | 1:G:258:PRO:HD3  | 2.02                     | 0.41              |
| 1:H:247:ILE:HB   | 1:H:273:ALA:HA   | 2.03                     | 0.41              |
| 1:A:306:GLU:HB2  | 1:A:309:ASP:OD2  | 2.21                     | 0.41              |
| 1:C:9:GLU:O      | 1:C:13:ALA:N     | 2.51                     | 0.41              |
| 1:C:249:ALA:O    | 1:C:276:ALA:N    | 2.54                     | 0.41              |
| 1:I:257:LEU:HB3  | 1:I:258:PRO:HD3  | 2.02                     | 0.41              |
| 1:K:146:VAL:O    | 1:K:149:VAL:HG22 | 2.21                     | 0.41              |
| 1:G:154:ASP:HB3  | 1:G:155:LYS:NZ   | 2.36                     | 0.41              |
| 1:G:217:TYR:O    | 1:G:246:LEU:N    | 2.34                     | 0.41              |
| 1:A:152:GLY:O    | 1:A:153:SER:C    | 2.64                     | 0.41              |
| 1:C:33:LYS:HE3   | 1:H:117:ARG:HH21 | 1.85                     | 0.41              |
| 1:C:133:ILE:O    | 1:C:133:ILE:HG13 | 2.21                     | 0.41              |
| 1:I:173:ILE:HA   | 1:I:375:ALA:HB3  | 2.02                     | 0.41              |
| 1:I:464:ASP:O    | 1:I:468:ASN:ND2  | 2.54                     | 0.41              |
| 1:D:173:ILE:HA   | 1:D:375:ALA:HB3  | 2.02                     | 0.41              |
| 1:J:137:VAL:HG21 | 1:J:409:MET:HG2  | 2.03                     | 0.41              |
| 1:J:289:ASP:CG   | 1:J:366:ARG:HH21 | 2.28                     | 0.41              |
| 1:E:284:LYS:HA   | 1:E:287:LEU:HB2  | 2.02                     | 0.41              |
| 1:G:135:THR:OG1  | 1:G:409:MET:HB3  | 2.21                     | 0.41              |
| 1:M:172:VAL:HG21 | 1:M:192:GLN:HB3  | 2.02                     | 0.41              |
| 1:H:138:ASP:N    | 1:H:138:ASP:OD1  | 2.50                     | 0.41              |
| 1:N:116:ARG:HG3  | 1:N:509:ALA:HB1  | 2.02                     | 0.41              |
| 1:N:146:VAL:HA   | 1:N:149:VAL:HG22 | 2.02                     | 0.41              |
| 1:A:191:MET:HE1  | 1:A:369:LYS:HB3  | 2.03                     | 0.41              |
| 1:B:6:LYS:HB3    | 1:B:6:LYS:HE2    | 1.81                     | 0.41              |
| 1:B:153:SER:OG   | 1:B:156:VAL:HG23 | 2.21                     | 0.41              |
| 1:B:306:GLU:HB2  | 1:B:309:ASP:OD2  | 2.21                     | 0.41              |
| 1:C:191:MET:O    | 1:C:330:ILE:N    | 2.41                     | 0.41              |
| 1:C:465:LYS:O    | 1:C:469:VAL:HG13 | 2.21                     | 0.41              |
| 1:J:146:VAL:HA   | 1:J:149:VAL:HG23 | 2.02                     | 0.41              |
| 1:K:81:ASN:HB3   | 1:K:88:THR:HB    | 2.02                     | 0.41              |
| 1:K:284:LYS:NZ   | 1:K:302:ASP:OD2  | 2.52                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:146:VAL:O    | 1:F:149:VAL:HG23 | 2.21                     | 0.41              |
| 1:G:101:GLU:O    | 1:G:105:ASN:ND2  | 2.44                     | 0.41              |
| 1:G:133:ILE:HG13 | 1:G:133:ILE:O    | 2.21                     | 0.41              |
| 1:M:154:ASP:HB3  | 1:M:155:LYS:NZ   | 2.36                     | 0.41              |
| 1:M:257:LEU:HB3  | 1:M:258:PRO:HD3  | 2.02                     | 0.41              |
| 1:H:232:LEU:HD23 | 1:H:235:LEU:HD12 | 2.02                     | 0.41              |
| 1:N:175:ILE:HG22 | 1:N:391:LYS:HD2  | 2.03                     | 0.41              |
| 1:B:362:LYS:HD3  | 1:B:362:LYS:HA   | 1.88                     | 0.41              |
| 1:D:12:ARG:HD2   | 1:D:103:LEU:HD11 | 2.03                     | 0.41              |
| 1:J:76:VAL:HG21  | 1:J:507:VAL:HG11 | 2.02                     | 0.41              |
| 1:J:465:LYS:O    | 1:J:469:VAL:HG13 | 2.21                     | 0.41              |
| 1:E:68:MET:HE2   | 1:E:68:MET:HB2   | 1.88                     | 0.41              |
| 1:E:137:VAL:HG11 | 1:E:146:VAL:HG21 | 2.02                     | 0.41              |
| 1:K:77:ALA:HB1   | 1:K:88:THR:OG1   | 2.21                     | 0.41              |
| 1:K:172:VAL:HG21 | 1:K:192:GLN:HB3  | 2.03                     | 0.41              |
| 1:K:229:GLN:HA   | 1:K:232:LEU:HG   | 2.02                     | 0.41              |
| 1:K:247:ILE:HB   | 1:K:273:ALA:HA   | 2.03                     | 0.41              |
| 1:G:116:ARG:HG3  | 1:G:509:ALA:HB1  | 2.03                     | 0.41              |
| 1:G:146:VAL:HA   | 1:G:149:VAL:HG22 | 2.03                     | 0.41              |
| 1:A:175:ILE:HG22 | 1:A:391:LYS:HD2  | 2.04                     | 0.40              |
| 1:E:149:VAL:CG1  | 1:E:150:SER:H    | 2.33                     | 0.40              |
| 1:E:209:MET:SD   | 1:E:325:LYS:HB2  | 2.62                     | 0.40              |
| 1:K:154:ASP:HB3  | 1:K:155:LYS:NZ   | 2.36                     | 0.40              |
| 1:K:191:MET:CE   | 1:K:369:LYS:HB3  | 2.46                     | 0.40              |
| 1:N:82:ASP:OD1   | 1:N:82:ASP:N     | 2.53                     | 0.40              |
| 1:N:133:ILE:O    | 1:N:133:ILE:HG13 | 2.20                     | 0.40              |
| 1:N:151:SER:HB2  | 1:N:393:ARG:NE   | 2.30                     | 0.40              |
| 1:N:257:LEU:HB3  | 1:N:258:PRO:HD3  | 2.02                     | 0.40              |
| 1:B:133:ILE:O    | 1:B:133:ILE:HG13 | 2.20                     | 0.40              |
| 1:J:188:VAL:HG21 | 1:J:332:GLU:HG3  | 2.03                     | 0.40              |
| 1:J:247:ILE:HB   | 1:J:273:ALA:HA   | 2.03                     | 0.40              |
| 1:F:172:VAL:HB   | 1:F:374:VAL:HG22 | 2.02                     | 0.40              |
| 1:F:209:MET:SD   | 1:F:325:LYS:HB2  | 2.61                     | 0.40              |
| 1:F:260:LEU:HD22 | 1:F:271:VAL:HG11 | 2.04                     | 0.40              |
| 1:L:147:ALA:HB3  | 1:L:157:GLY:HA2  | 2.02                     | 0.40              |
| 1:L:465:LYS:O    | 1:L:469:VAL:HG13 | 2.22                     | 0.40              |
| 1:G:188:VAL:HG21 | 1:G:332:GLU:HG3  | 2.03                     | 0.40              |
| 1:M:197:TYR:HB2  | 1:M:202:MET:HE3  | 2.04                     | 0.40              |
| 1:H:475:PHE:CZ   | 1:H:480:GLY:HA2  | 2.56                     | 0.40              |
| 1:N:76:VAL:CG2   | 1:N:507:VAL:HG21 | 2.48                     | 0.40              |
| 1:N:151:SER:O    | 1:N:153:SER:N    | 2.54                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:390:LEU:HD12 | 1:C:390:LEU:HA   | 1.89                     | 0.40              |
| 1:I:2:ALA:HB1    | 1:N:62:GLU:HB2   | 2.03                     | 0.40              |
| 1:I:306:GLU:HB2  | 1:I:309:ASP:OD2  | 2.22                     | 0.40              |
| 1:J:223:LYS:NZ   | 1:J:305:LEU:O    | 2.35                     | 0.40              |
| 1:E:116:ARG:HG3  | 1:E:509:ALA:HB1  | 2.02                     | 0.40              |
| 1:E:223:LYS:NZ   | 1:E:305:LEU:O    | 2.34                     | 0.40              |
| 1:F:238:ILE:O    | 1:F:242:SER:N    | 2.54                     | 0.40              |
| 1:H:175:ILE:HG22 | 1:H:391:LYS:HD2  | 2.03                     | 0.40              |
| 1:N:484:ASN:HB3  | 1:N:487:GLU:HB2  | 2.04                     | 0.40              |
| 1:A:133:ILE:HG13 | 1:A:133:ILE:O    | 2.21                     | 0.40              |
| 1:B:96:GLN:NE2   | 1:B:100:ARG:HH12 | 2.19                     | 0.40              |
| 1:B:465:LYS:O    | 1:B:469:VAL:HG13 | 2.22                     | 0.40              |
| 1:C:247:ILE:HB   | 1:C:273:ALA:HA   | 2.03                     | 0.40              |
| 1:J:172:VAL:HG21 | 1:J:192:GLN:HB3  | 2.03                     | 0.40              |
| 1:J:390:LEU:HD12 | 1:J:390:LEU:HA   | 1.89                     | 0.40              |
| 1:E:465:LYS:O    | 1:E:469:VAL:HG13 | 2.22                     | 0.40              |
| 1:F:68:MET:HB3   | 1:F:68:MET:HE3   | 1.76                     | 0.40              |
| 1:F:97:ALA:CB    | 1:F:446:GLU:HG3  | 2.52                     | 0.40              |
| 1:F:121:LEU:HD23 | 1:F:121:LEU:HA   | 1.97                     | 0.40              |
| 1:F:289:ASP:CG   | 1:F:366:ARG:HH21 | 2.29                     | 0.40              |
| 1:L:409:MET:HA   | 1:L:409:MET:HE2  | 2.04                     | 0.40              |
| 1:G:76:VAL:HG21  | 1:G:507:VAL:HG11 | 2.03                     | 0.40              |
| 1:M:151:SER:HB2  | 1:M:393:ARG:NE   | 2.28                     | 0.40              |
| 1:M:209:MET:SD   | 1:M:325:LYS:HB2  | 2.61                     | 0.40              |
| 1:H:133:ILE:HG13 | 1:H:133:ILE:O    | 2.20                     | 0.40              |
| 1:B:175:ILE:HG22 | 1:B:391:LYS:HD2  | 2.04                     | 0.40              |
| 1:I:20:ASP:OD1   | 1:I:100:ARG:NH1  | 2.53                     | 0.40              |
| 1:I:209:MET:HE1  | 1:I:324:ASP:HB2  | 2.04                     | 0.40              |
| 1:I:362:LYS:HA   | 1:I:362:LYS:HD3  | 1.90                     | 0.40              |
| 1:D:97:ALA:CB    | 1:D:446:GLU:HG3  | 2.50                     | 0.40              |
| 1:E:197:TYR:HA   | 1:E:274:VAL:HG12 | 2.02                     | 0.40              |
| 1:K:133:ILE:O    | 1:K:133:ILE:HG13 | 2.21                     | 0.40              |
| 1:K:215:ASN:HA   | 1:K:318:ALA:O    | 2.21                     | 0.40              |
| 1:F:14:ALA:HB1   | 1:F:65:PHE:HB2   | 2.03                     | 0.40              |
| 1:F:73:VAL:HG11  | 1:F:92:THR:HG23  | 2.03                     | 0.40              |
| 1:F:257:LEU:HB3  | 1:F:258:PRO:HD3  | 2.02                     | 0.40              |
| 1:L:133:ILE:O    | 1:L:133:ILE:HG13 | 2.21                     | 0.40              |
| 1:M:133:ILE:HG13 | 1:M:133:ILE:O    | 2.21                     | 0.40              |
| 1:H:197:TYR:HA   | 1:H:274:VAL:HG12 | 2.04                     | 0.40              |
| 1:H:348:LYS:HE3  | 1:H:367:LEU:HD11 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 522/541 (96%)   | 502 (96%)  | 18 (3%)  | 2 (0%)   | 30          | 65  |
| 1   | B     | 522/541 (96%)   | 505 (97%)  | 17 (3%)  | 0        | 100         | 100 |
| 1   | C     | 522/541 (96%)   | 504 (97%)  | 18 (3%)  | 0        | 100         | 100 |
| 1   | D     | 522/541 (96%)   | 503 (96%)  | 18 (3%)  | 1 (0%)   | 43          | 75  |
| 1   | E     | 522/541 (96%)   | 504 (97%)  | 18 (3%)  | 0        | 100         | 100 |
| 1   | F     | 522/541 (96%)   | 504 (97%)  | 18 (3%)  | 0        | 100         | 100 |
| 1   | G     | 522/541 (96%)   | 504 (97%)  | 17 (3%)  | 1 (0%)   | 43          | 75  |
| 1   | H     | 522/541 (96%)   | 505 (97%)  | 16 (3%)  | 1 (0%)   | 43          | 75  |
| 1   | I     | 522/541 (96%)   | 503 (96%)  | 18 (3%)  | 1 (0%)   | 43          | 75  |
| 1   | J     | 522/541 (96%)   | 503 (96%)  | 19 (4%)  | 0        | 100         | 100 |
| 1   | K     | 522/541 (96%)   | 504 (97%)  | 17 (3%)  | 1 (0%)   | 43          | 75  |
| 1   | L     | 522/541 (96%)   | 504 (97%)  | 16 (3%)  | 2 (0%)   | 30          | 65  |
| 1   | M     | 522/541 (96%)   | 503 (96%)  | 18 (3%)  | 1 (0%)   | 43          | 75  |
| 1   | N     | 522/541 (96%)   | 505 (97%)  | 16 (3%)  | 1 (0%)   | 43          | 75  |
| All | All   | 7308/7574 (96%) | 7053 (96%) | 244 (3%) | 11 (0%)  | 44          | 75  |

All (11) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 149 | VAL  |
| 1   | A     | 153 | SER  |
| 1   | K     | 153 | SER  |
| 1   | L     | 153 | SER  |
| 1   | G     | 153 | SER  |
| 1   | H     | 153 | SER  |
| 1   | N     | 153 | SER  |
| 1   | I     | 153 | SER  |
| 1   | D     | 153 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 153 | SER  |
| 1   | L     | 152 | GLY  |

### 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     | 421/431 (98%)   | 421 (100%)  | 0        | 100         | 100 |
| 1   | B     | 421/431 (98%)   | 421 (100%)  | 0        | 100         | 100 |
| 1   | C     | 421/431 (98%)   | 421 (100%)  | 0        | 100         | 100 |
| 1   | D     | 421/431 (98%)   | 421 (100%)  | 0        | 100         | 100 |
| 1   | E     | 421/431 (98%)   | 420 (100%)  | 1 (0%)   | 87          | 87  |
| 1   | F     | 421/431 (98%)   | 420 (100%)  | 1 (0%)   | 87          | 87  |
| 1   | G     | 421/431 (98%)   | 420 (100%)  | 1 (0%)   | 87          | 87  |
| 1   | H     | 421/431 (98%)   | 421 (100%)  | 0        | 100         | 100 |
| 1   | I     | 421/431 (98%)   | 421 (100%)  | 0        | 100         | 100 |
| 1   | J     | 421/431 (98%)   | 421 (100%)  | 0        | 100         | 100 |
| 1   | K     | 421/431 (98%)   | 421 (100%)  | 0        | 100         | 100 |
| 1   | L     | 421/431 (98%)   | 419 (100%)  | 2 (0%)   | 81          | 82  |
| 1   | M     | 421/431 (98%)   | 421 (100%)  | 0        | 100         | 100 |
| 1   | N     | 421/431 (98%)   | 421 (100%)  | 0        | 100         | 100 |
| All | All   | 5894/6034 (98%) | 5889 (100%) | 5 (0%)   | 87          | 89  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 194 | ASP  |
| 1   | F     | 485 | MET  |
| 1   | L     | 10  | ASP  |
| 1   | L     | 194 | ASP  |
| 1   | G     | 138 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 81  | ASN  |
| 1   | A     | 263 | ASN  |
| 1   | B     | 81  | ASN  |
| 1   | B     | 96  | GLN  |
| 1   | B     | 241 | GLN  |
| 1   | B     | 263 | ASN  |
| 1   | C     | 96  | GLN  |
| 1   | C     | 263 | ASN  |
| 1   | C     | 503 | ASN  |
| 1   | I     | 81  | ASN  |
| 1   | I     | 241 | GLN  |
| 1   | I     | 263 | ASN  |
| 1   | I     | 468 | ASN  |
| 1   | I     | 503 | ASN  |
| 1   | D     | 81  | ASN  |
| 1   | D     | 263 | ASN  |
| 1   | J     | 81  | ASN  |
| 1   | J     | 263 | ASN  |
| 1   | J     | 468 | ASN  |
| 1   | E     | 263 | ASN  |
| 1   | K     | 81  | ASN  |
| 1   | K     | 241 | GLN  |
| 1   | K     | 263 | ASN  |
| 1   | K     | 399 | ASN  |
| 1   | K     | 468 | ASN  |
| 1   | F     | 263 | ASN  |
| 1   | L     | 81  | ASN  |
| 1   | L     | 263 | ASN  |
| 1   | L     | 503 | ASN  |
| 1   | G     | 81  | ASN  |
| 1   | G     | 96  | GLN  |
| 1   | G     | 241 | GLN  |
| 1   | G     | 263 | ASN  |
| 1   | M     | 81  | ASN  |
| 1   | M     | 96  | GLN  |
| 1   | M     | 263 | ASN  |
| 1   | H     | 263 | ASN  |
| 1   | N     | 81  | ASN  |
| 1   | N     | 96  | GLN  |
| 1   | N     | 241 | GLN  |
| 1   | N     | 263 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 468 | ASN  |
| 1   | N     | 503 | ASN  |

### 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.

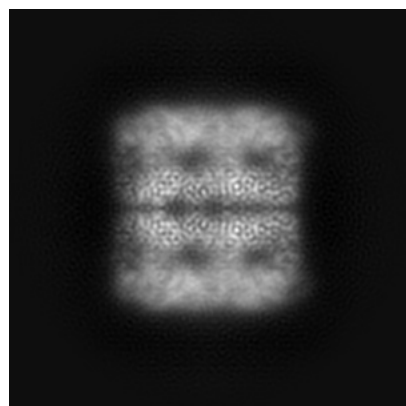
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45080. These allow visual inspection of the internal detail of the map and identification of artifacts.

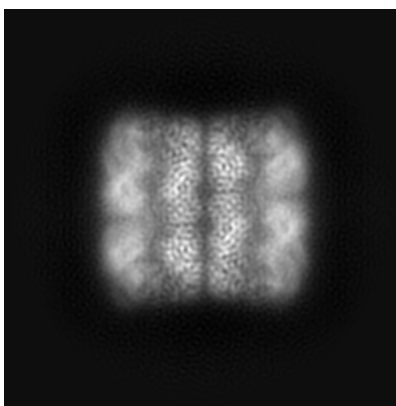
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

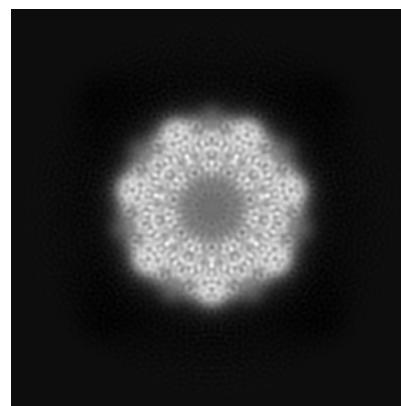
#### 6.1.1 Primary map



X

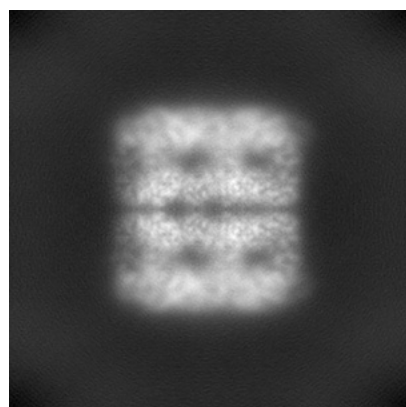


Y

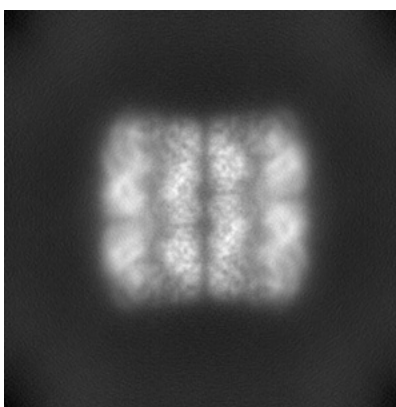


Z

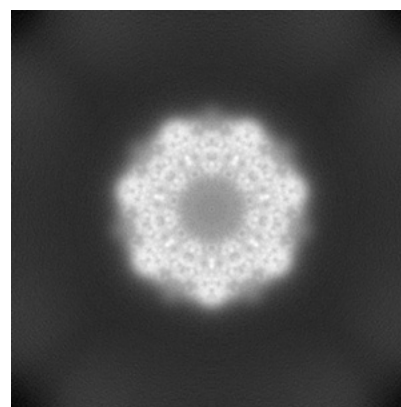
#### 6.1.2 Raw map



X



Y

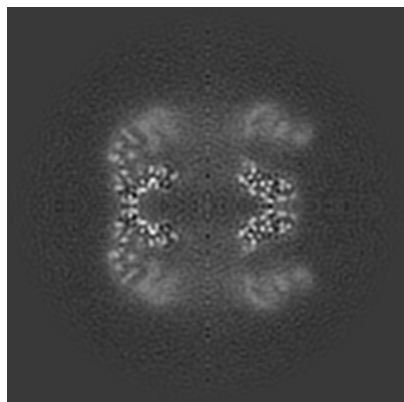


Z

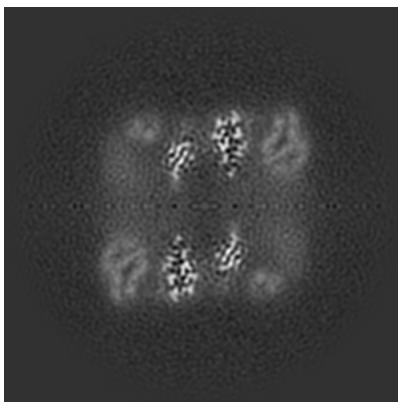
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

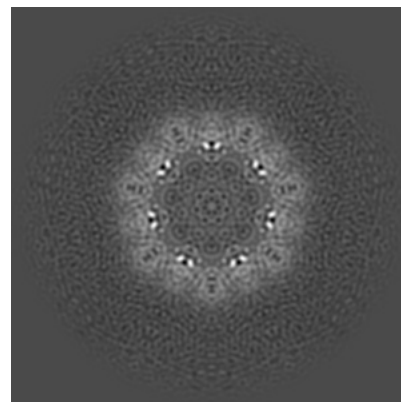
### 6.2.1 Primary map



X Index: 128

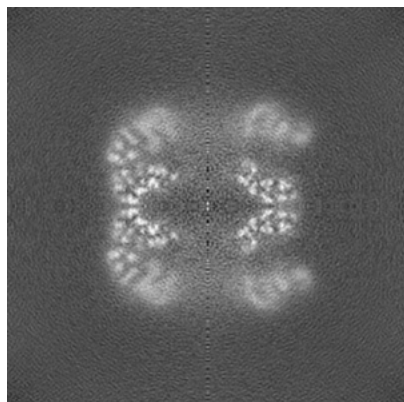


Y Index: 128

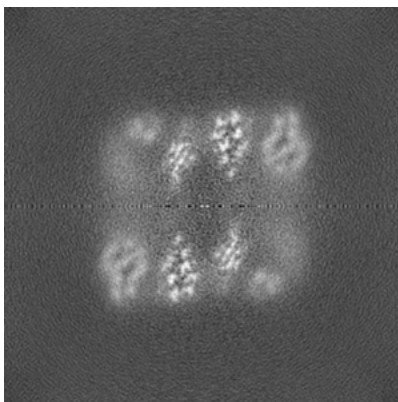


Z Index: 128

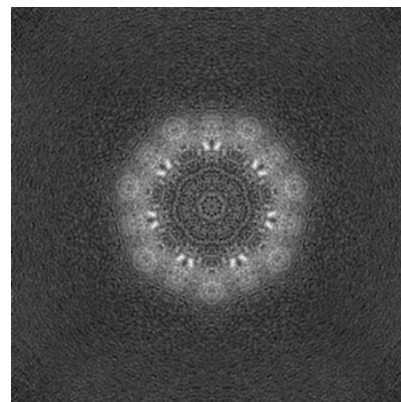
### 6.2.2 Raw map



X Index: 128



Y Index: 128

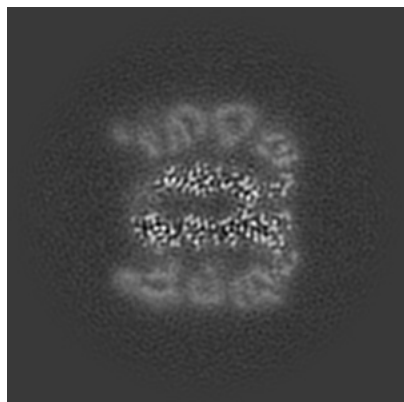


Z Index: 128

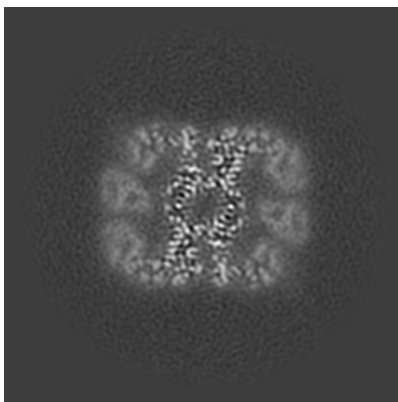
The images above show central slices of the map in three orthogonal directions.

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

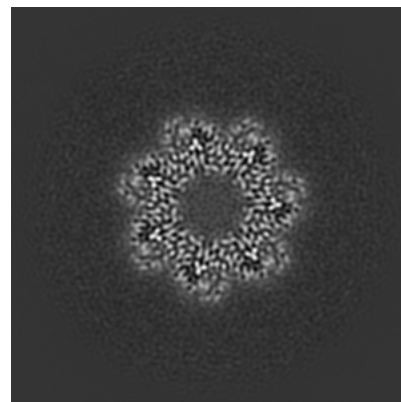
### 6.3.1 Primary map



X Index: 100

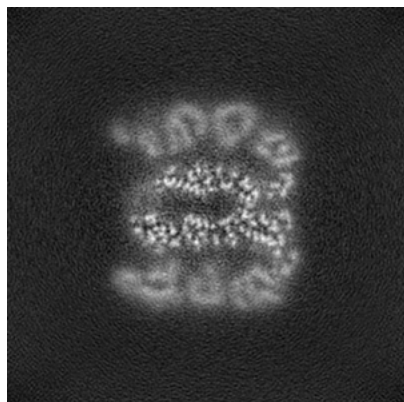


Y Index: 93

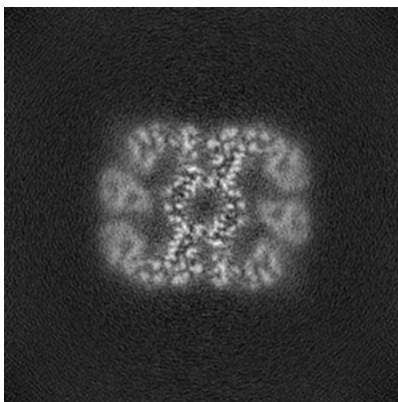


Z Index: 142

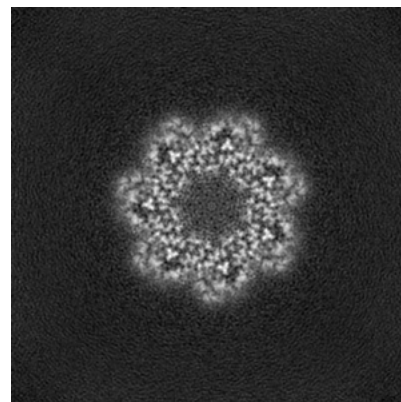
### 6.3.2 Raw map



X Index: 100



Y Index: 93

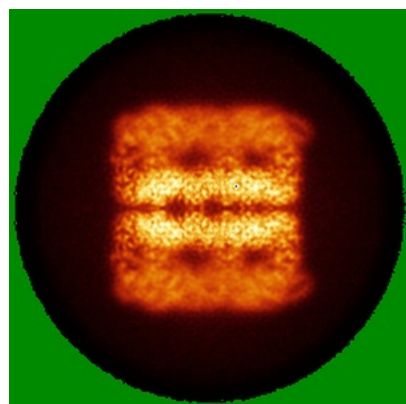


Z Index: 114

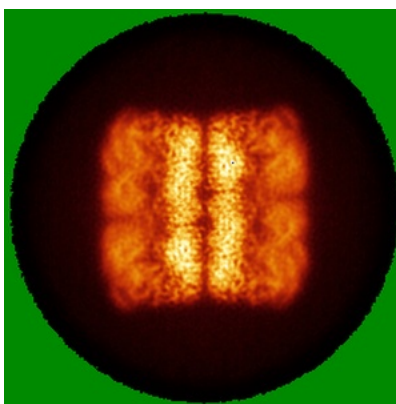
The images above show the largest variance slices of the map in three orthogonal directions.

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

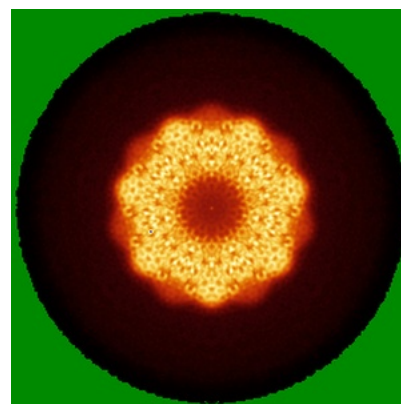
### 6.4.1 Primary map



X

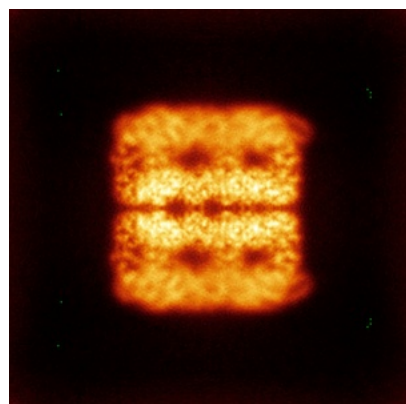


Y

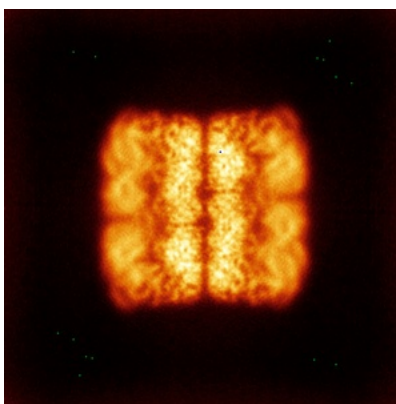


Z

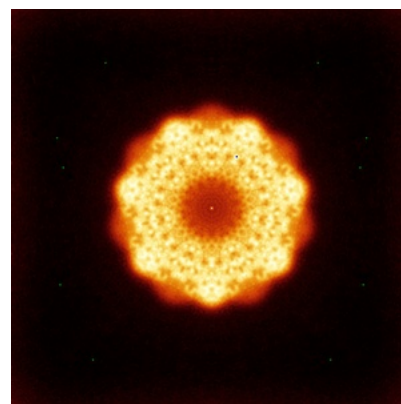
### 6.4.2 Raw map



X



Y

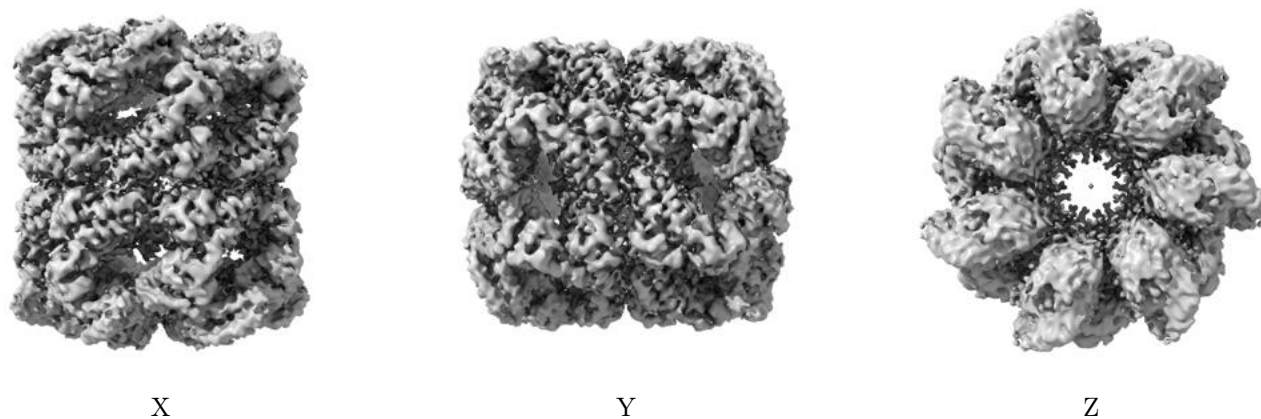


Z

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.

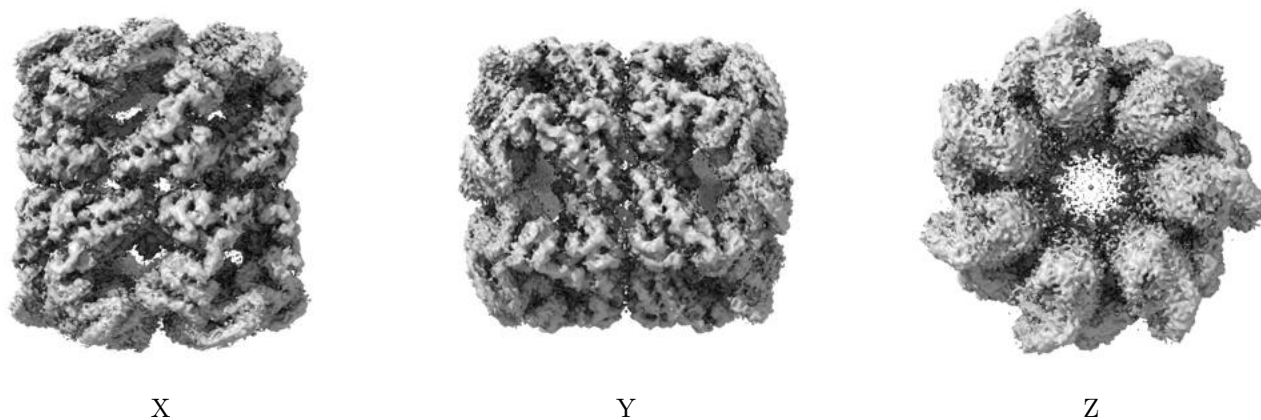
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.175. 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.

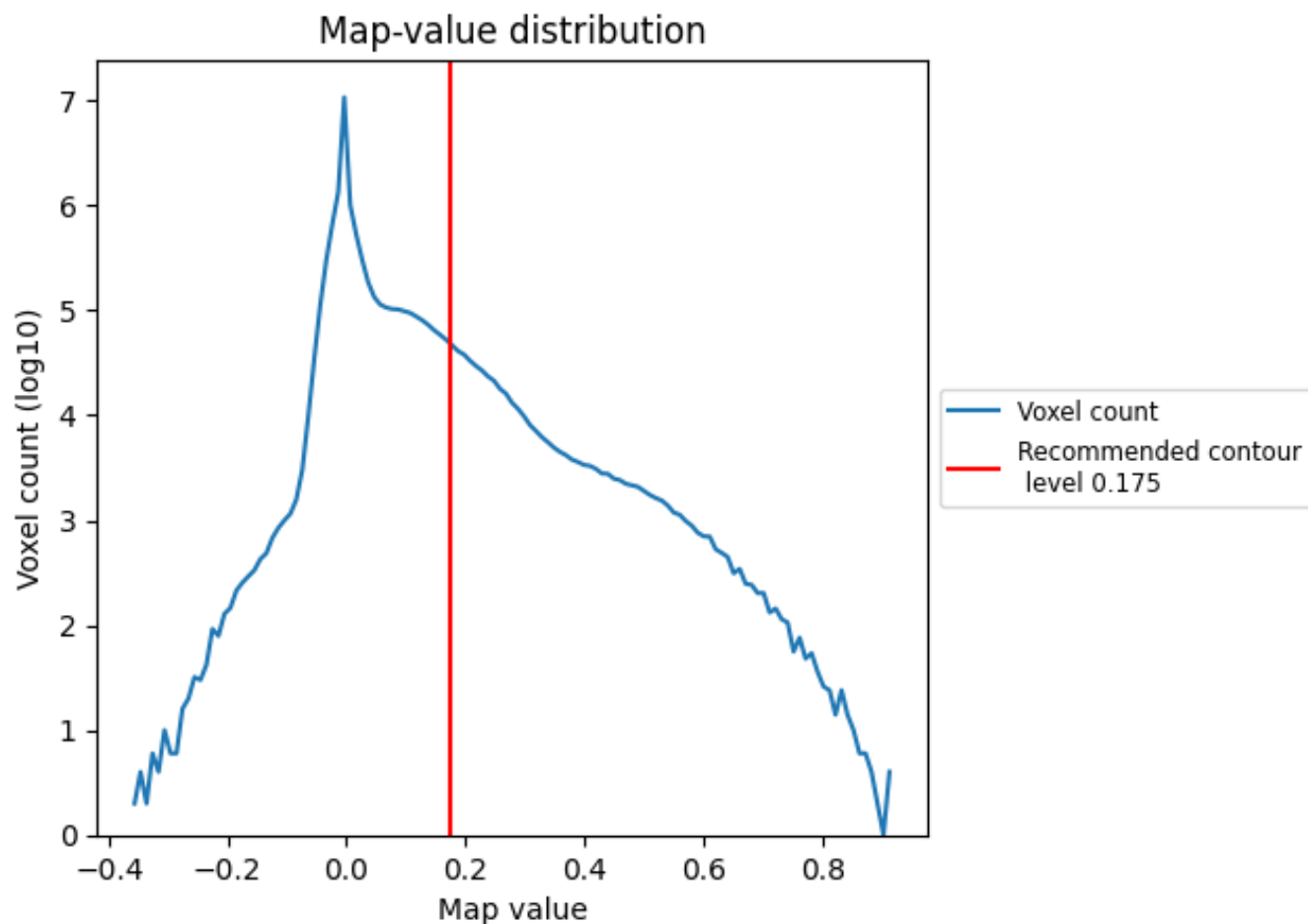
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

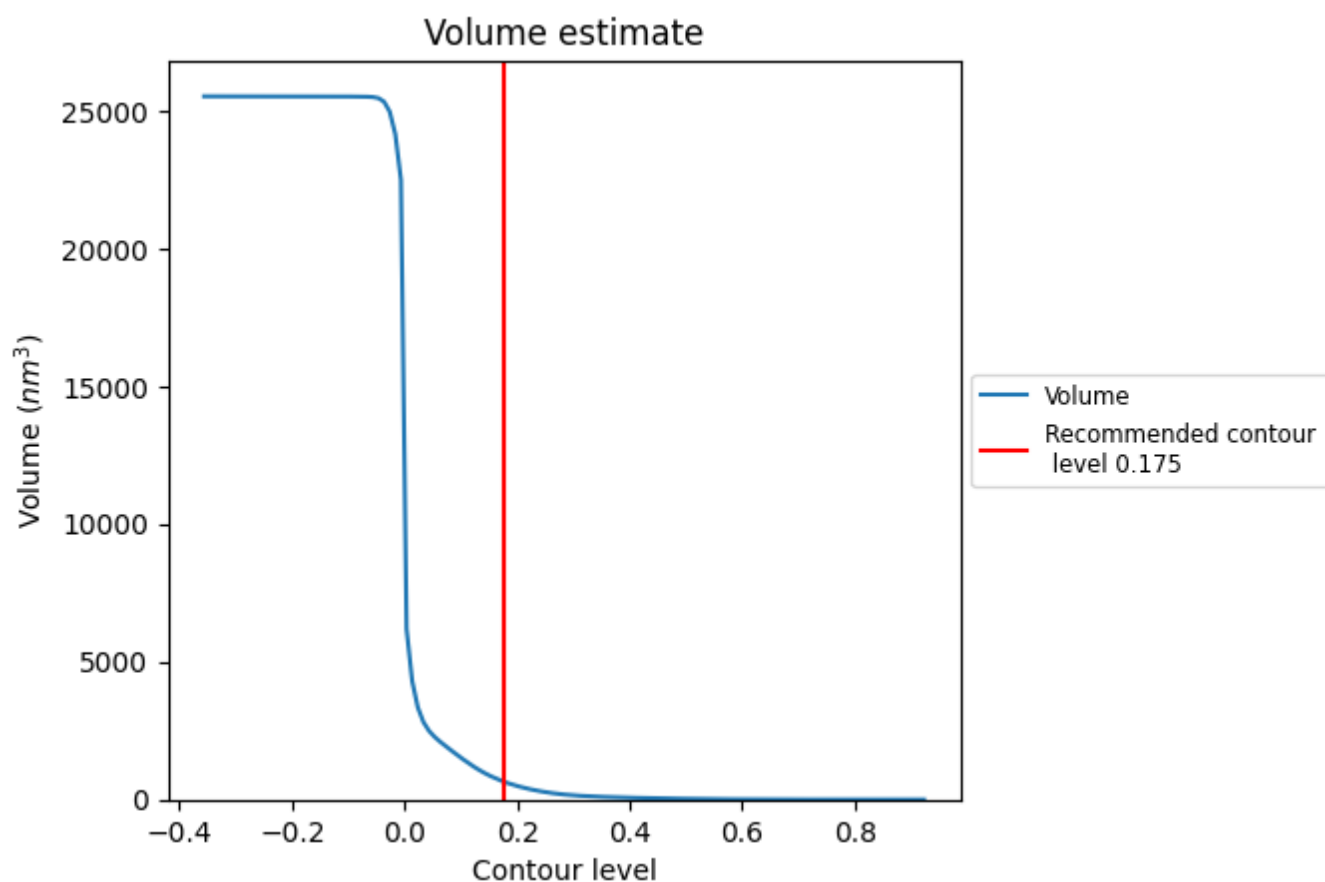
This section contains the results of statistical analysis of the map.

### 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.

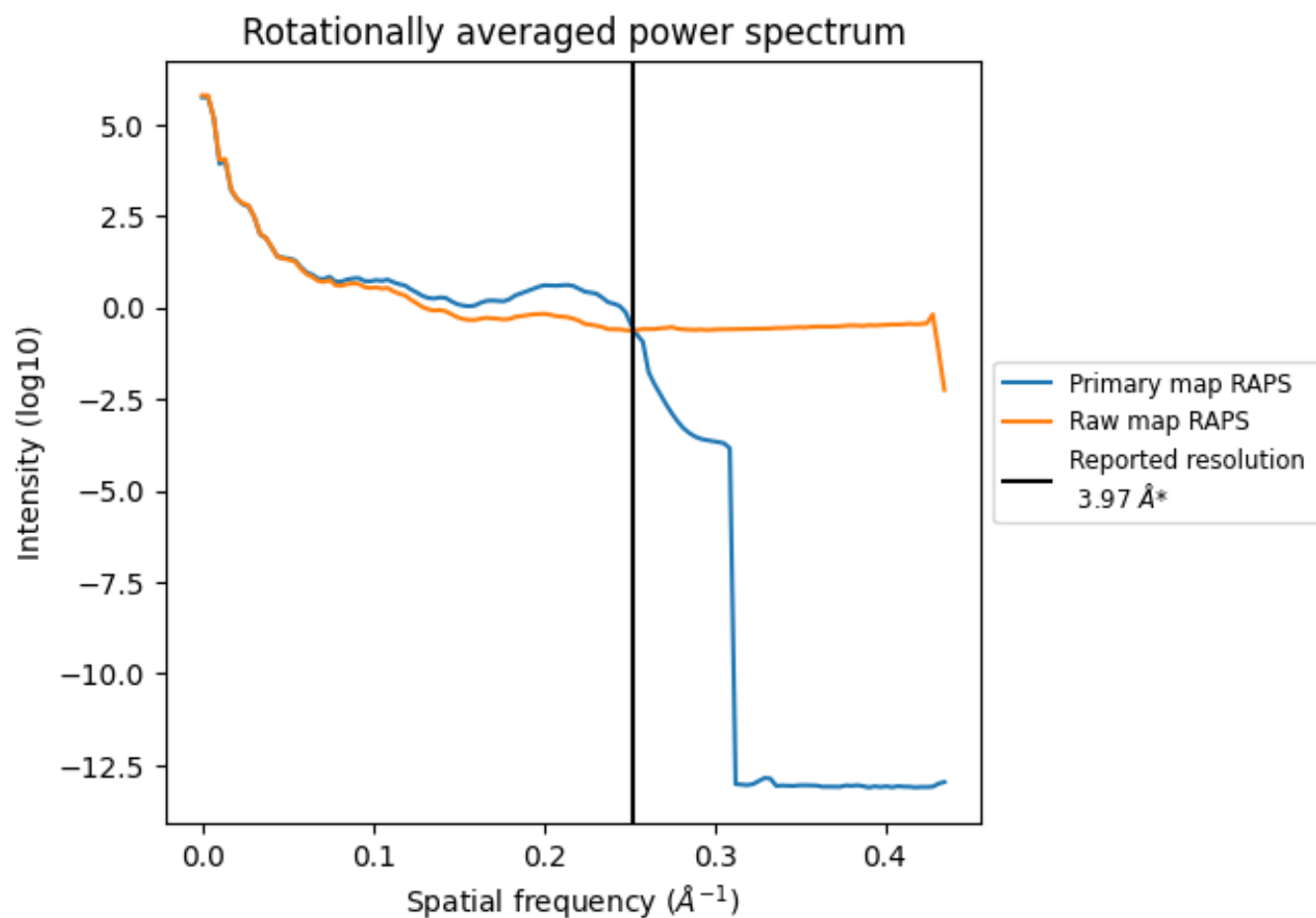
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 659 nm<sup>3</sup>; this corresponds to an approximate mass of 595 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 ⓘ

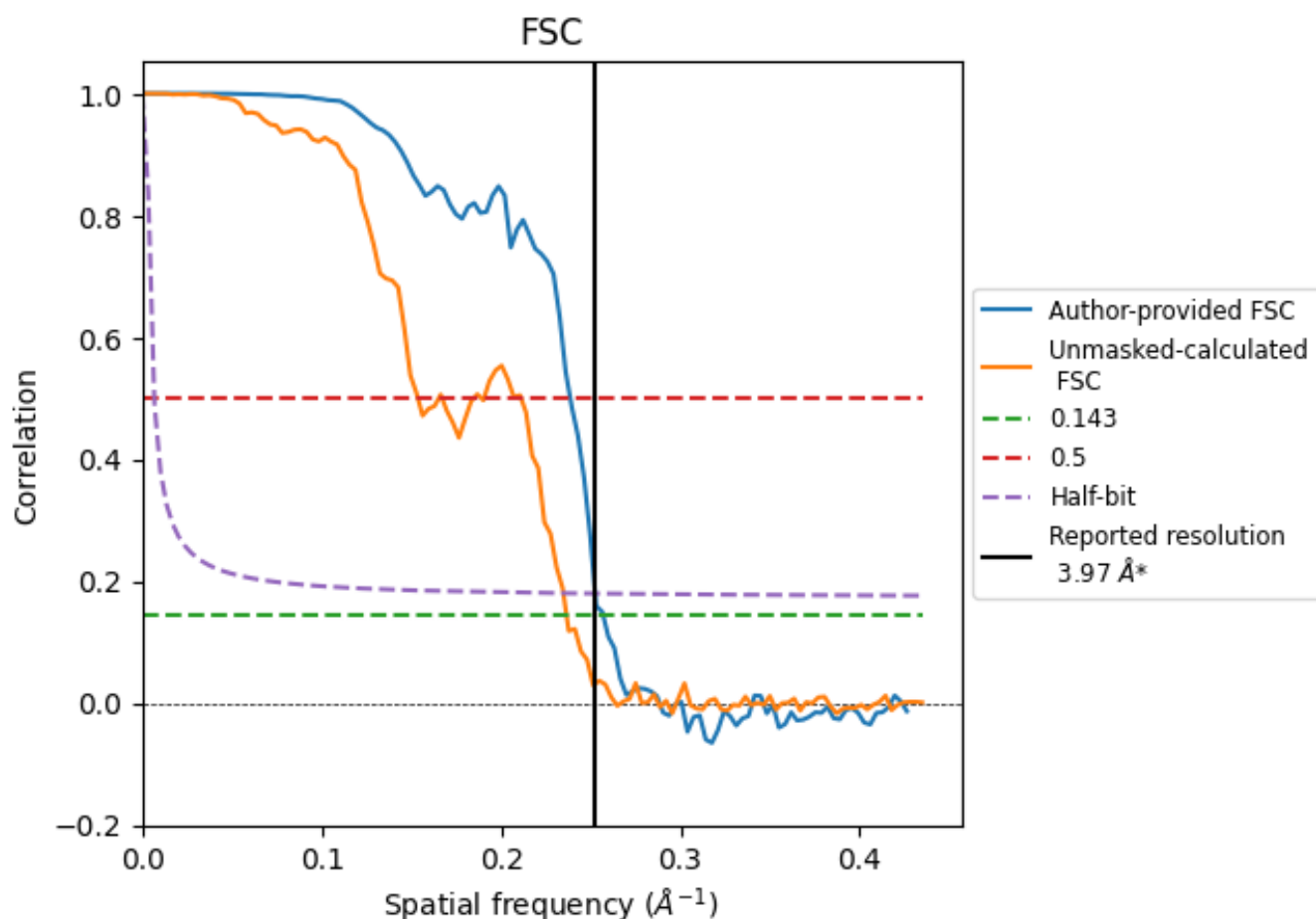


\*Reported resolution corresponds to spatial frequency of 0.252 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.252  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

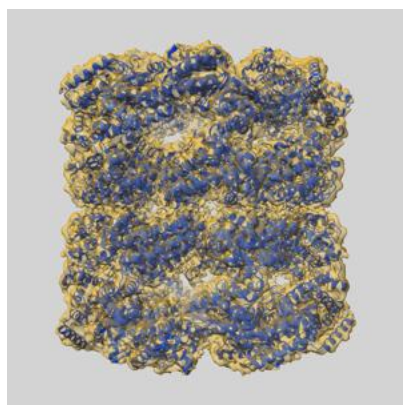
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.97                               | -    | -        |
| Author-provided FSC curve | 3.89                               | 4.19 | 3.96     |
| Unmasked-calculated*      | 4.23                               | 6.51 | 4.26     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

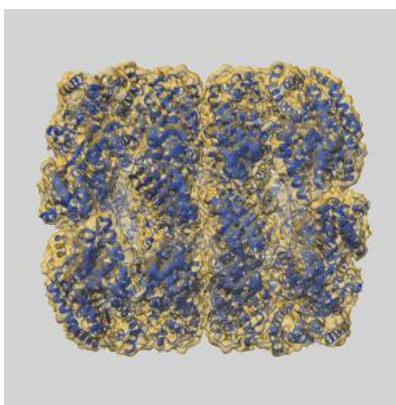
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45080 and PDB model 9C0D. Per-residue inclusion information can be found in section [3](#) on page [5](#).

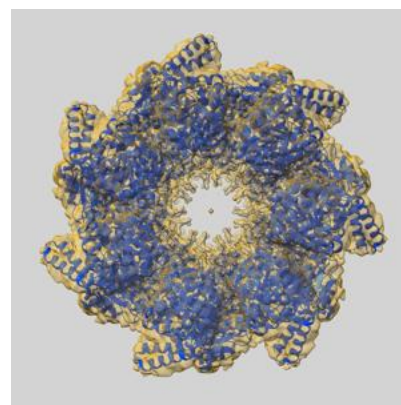
### 9.1 Map-model overlay [i](#)



X



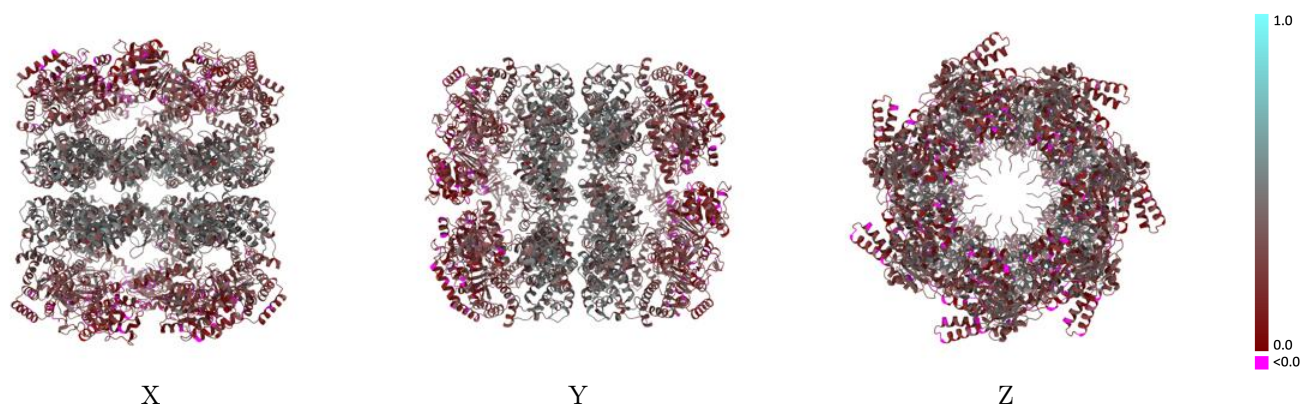
Y



Z

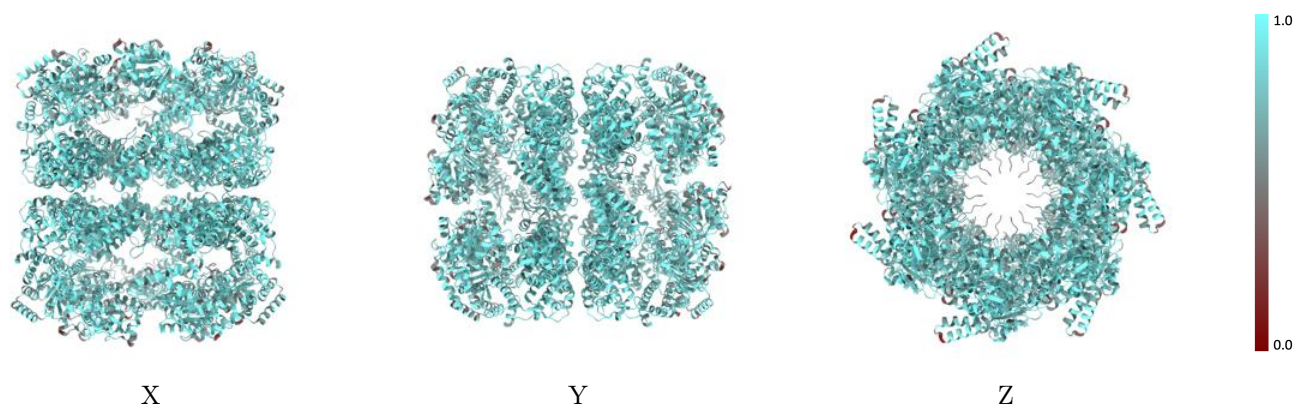
The images above show the 3D surface view of the map at the recommended contour level 0.175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



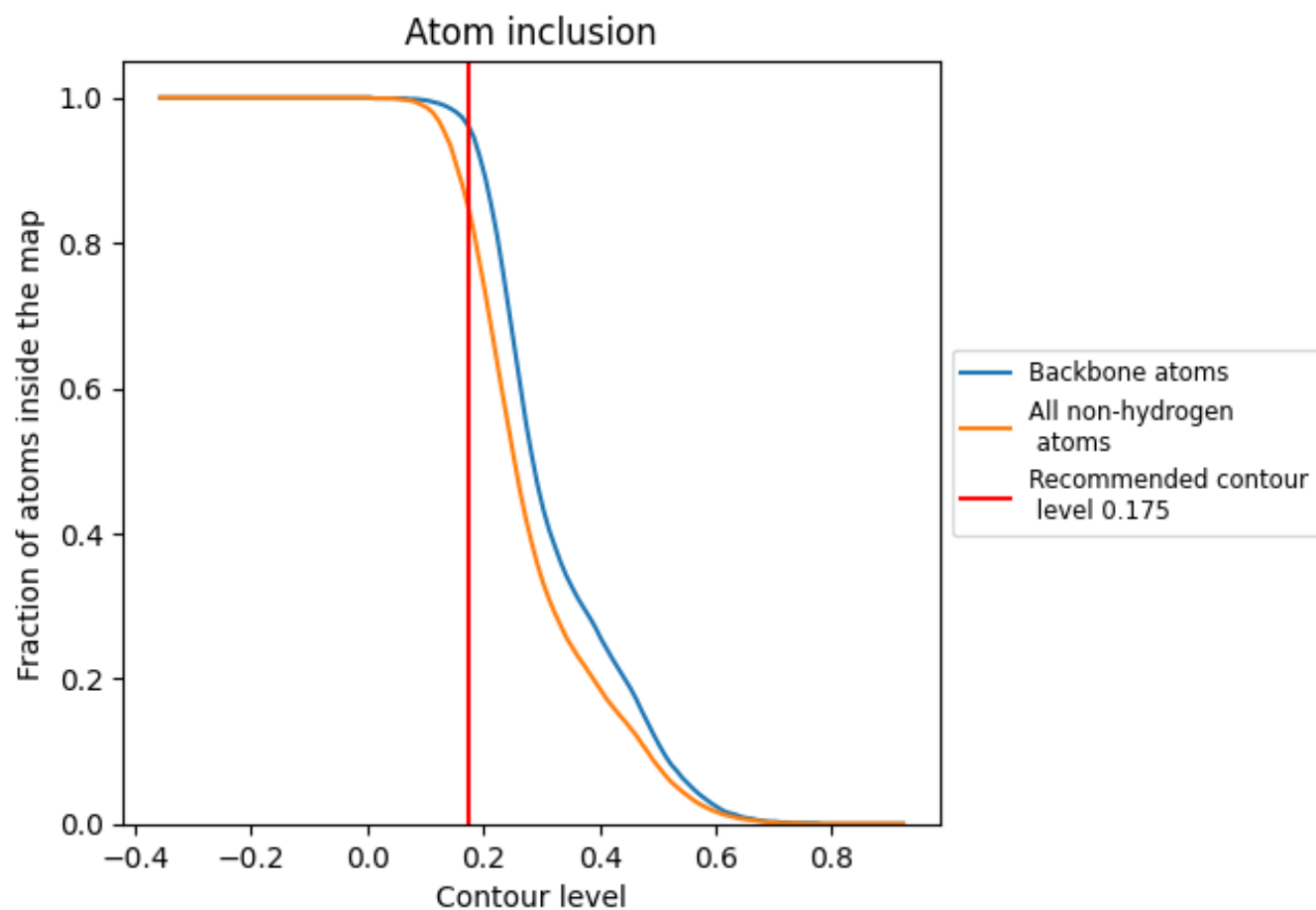
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.175).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 85% 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 (0.175) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion               | Q-score                      |
|-------|------------------------------|------------------------------|
| All   | <div><div></div>0.8460</div> | <div><div></div>0.3030</div> |
| A     | <div><div></div>0.8520</div> | <div><div></div>0.3100</div> |
| B     | <div><div></div>0.8530</div> | <div><div></div>0.3080</div> |
| C     | <div><div></div>0.8500</div> | <div><div></div>0.3090</div> |
| D     | <div><div></div>0.8460</div> | <div><div></div>0.3050</div> |
| E     | <div><div></div>0.8430</div> | <div><div></div>0.3040</div> |
| F     | <div><div></div>0.8330</div> | <div><div></div>0.2830</div> |
| G     | <div><div></div>0.8450</div> | <div><div></div>0.3030</div> |
| H     | <div><div></div>0.8540</div> | <div><div></div>0.3080</div> |
| I     | <div><div></div>0.8480</div> | <div><div></div>0.3020</div> |
| J     | <div><div></div>0.8460</div> | <div><div></div>0.3020</div> |
| K     | <div><div></div>0.8380</div> | <div><div></div>0.2980</div> |
| L     | <div><div></div>0.8500</div> | <div><div></div>0.3080</div> |
| M     | <div><div></div>0.8460</div> | <div><div></div>0.3040</div> |
| N     | <div><div></div>0.8410</div> | <div><div></div>0.2990</div> |

1.0

0.0

<0.0