



## Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 02:39 PM EST

PDB ID : 3J3S  
EMDB ID : EMD-5608  
Title : Structural dynamics of the MecA-ClpC complex revealed by cryo-EM  
Authors : Liu, J.; Mei, Z.; Li, N.; Qi, Y.; Xu, Y.; Shi, Y.; Wang, F.; Lei, J.; Gao, N.  
Deposited on : 2013-04-18  
Resolution : 11.00 Å(reported)  
Based on initial model : 3PXI

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

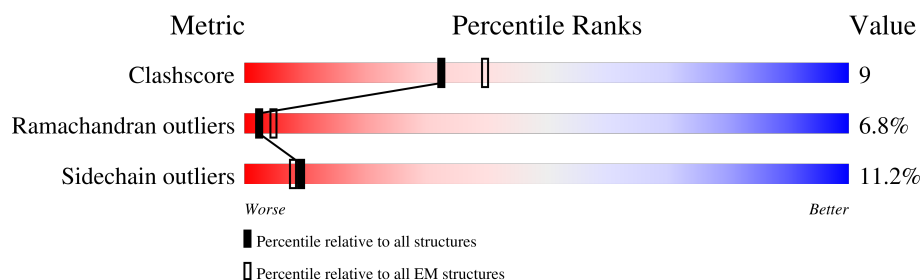
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 11.00 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) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 158937                      | 4297                        |
| Ramachandran outliers | 154571                      | 4023                        |
| Sidechain outliers    | 154315                      | 3826                        |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 1     | 218    |                  |
| 1   | 2     | 218    |                  |
| 1   | 3     | 218    |                  |
| 1   | 4     | 218    |                  |
| 1   | 5     | 218    |                  |
| 1   | 6     | 218    |                  |
| 2   | A     | 810    |                  |
| 2   | B     | 810    |                  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 2   | C     | 810    | <div><div></div><div>6%</div><div>70%</div><div>23%</div><div>5% ..</div></div> |
| 2   | D     | 810    | <div><div></div><div>6%</div><div>65%</div><div>28%</div><div>5% ..</div></div> |
| 2   | E     | 810    | <div><div></div><div>7%</div><div>69%</div><div>22%</div><div>6% ..</div></div> |
| 2   | F     | 810    | <div><div></div><div>7%</div><div>68%</div><div>25%</div><div>. ..</div></div>  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41862 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 Adapter protein MecA 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | 1     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 777   | 498 | 123 | 154 | 2 |         |       |
| 1   | 2     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 777   | 498 | 123 | 154 | 2 |         |       |
| 1   | 3     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 777   | 498 | 123 | 154 | 2 |         |       |
| 1   | 4     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 777   | 498 | 123 | 154 | 2 |         |       |
| 1   | 5     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 777   | 498 | 123 | 154 | 2 |         |       |
| 1   | 6     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 777   | 498 | 123 | 154 | 2 |         |       |

- Molecule 2 is a protein called Negative regulator of genetic competence ClpC/MecB.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | A     | 798      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6200  | 3850 | 1120 | 1215 | 15 |         |       |
| 2   | B     | 798      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6200  | 3850 | 1120 | 1215 | 15 |         |       |
| 2   | C     | 798      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6200  | 3850 | 1120 | 1215 | 15 |         |       |
| 2   | D     | 798      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6200  | 3850 | 1120 | 1215 | 15 |         |       |
| 2   | E     | 798      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6200  | 3850 | 1120 | 1215 | 15 |         |       |
| 2   | F     | 798      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6200  | 3850 | 1120 | 1215 | 15 |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 618     | ALA      | GLU    | engineered mutation | UNP P37571 |
| B     | 618     | ALA      | GLU    | engineered mutation | UNP P37571 |

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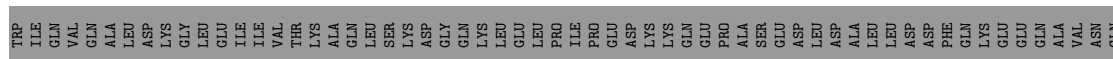
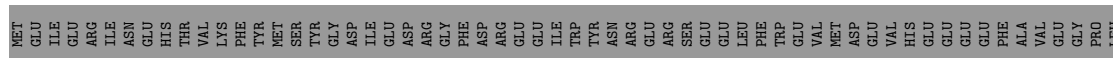
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| C     | 618     | ALA      | GLU    | engineered mutation | UNP P37571 |
| D     | 618     | ALA      | GLU    | engineered mutation | UNP P37571 |
| E     | 618     | ALA      | GLU    | engineered mutation | UNP P37571 |
| F     | 618     | ALA      | GLU    | engineered mutation | UNP P37571 |





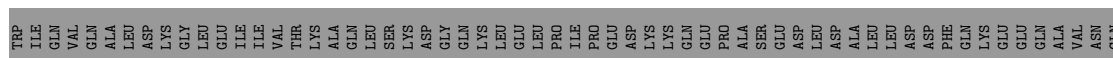
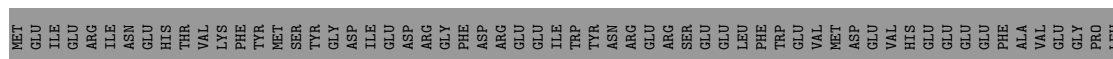
• Molecule 1: Adapter protein MecA 1

Chain 4: 31% 10% 57%



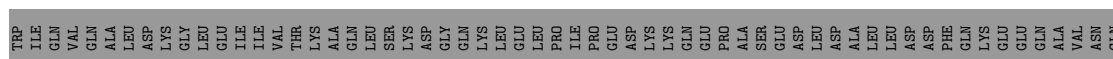
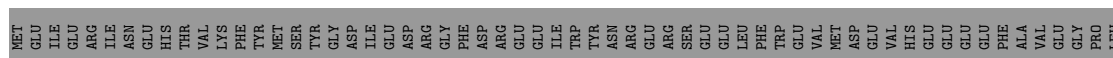
• Molecule 1: Adapter protein MecA 1

Chain 5: 30% 11% 57%



• Molecule 1: Adapter protein MecA 1

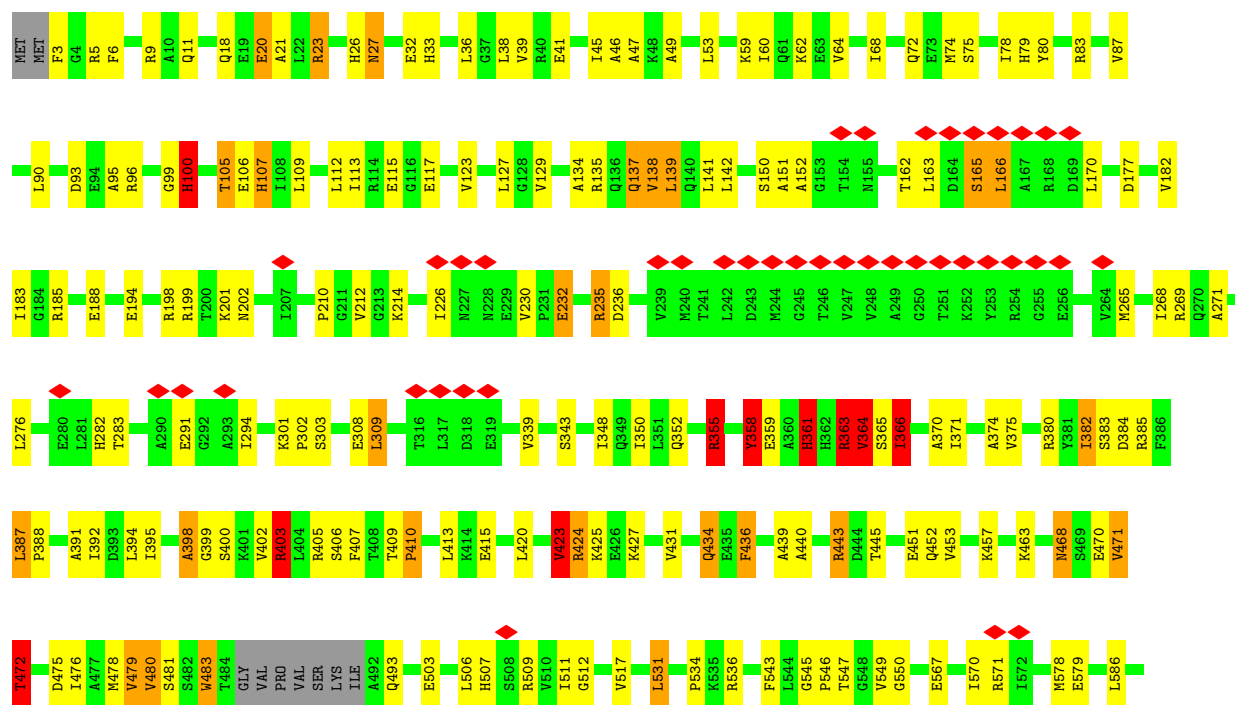
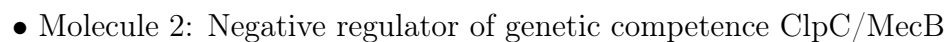
Chain 6: 31% 10% 57%



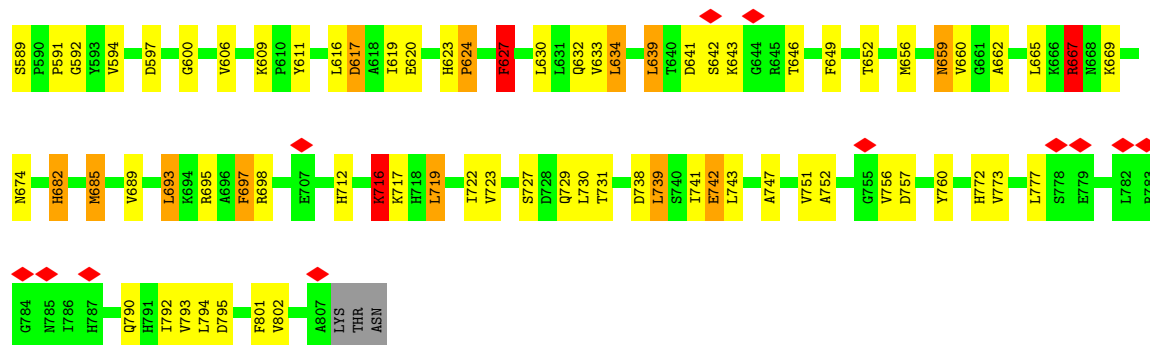
• Molecule 2: Negative regulator of genetic competence ClpC/MecB

Chain A: 7% 66% 28%

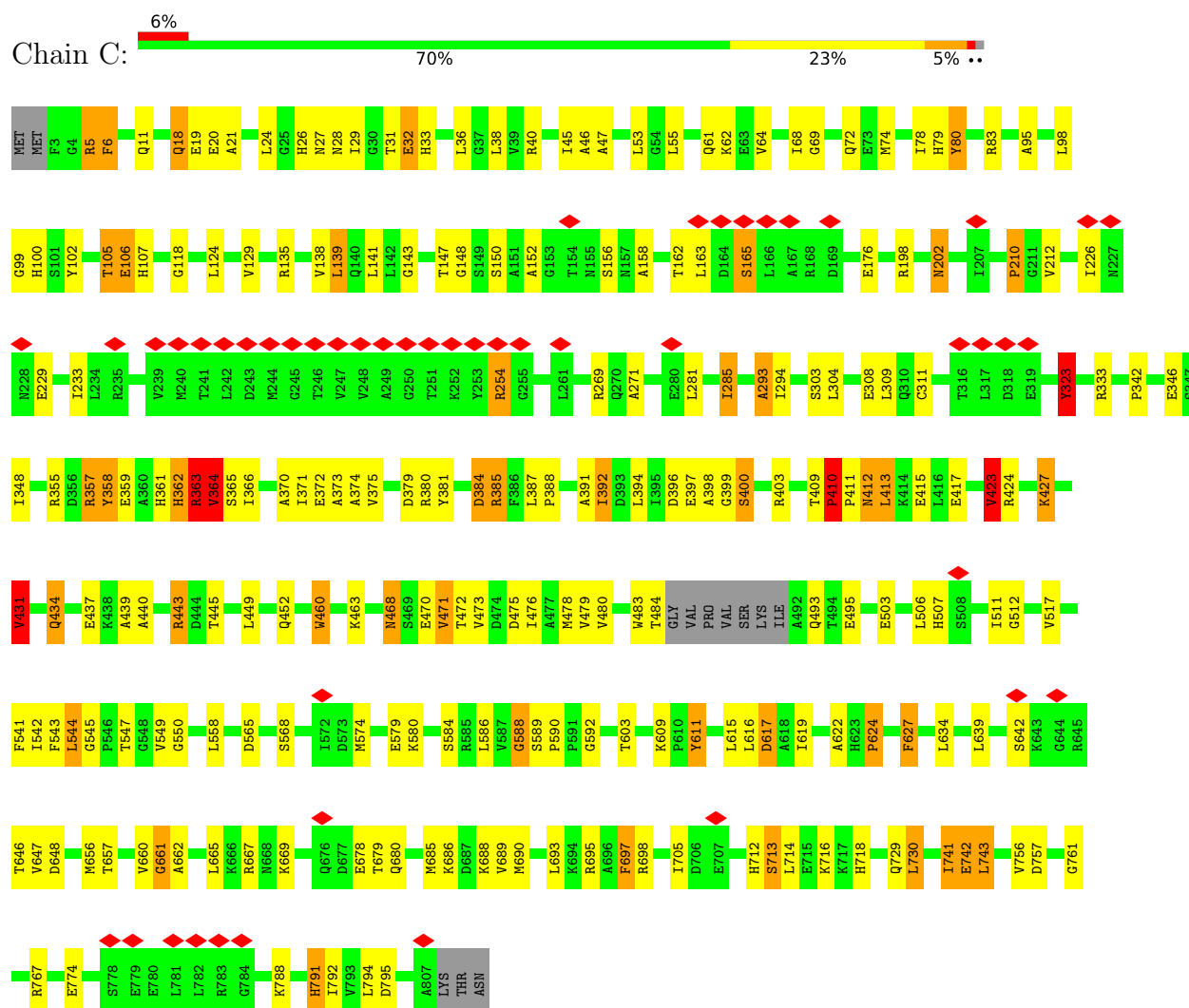




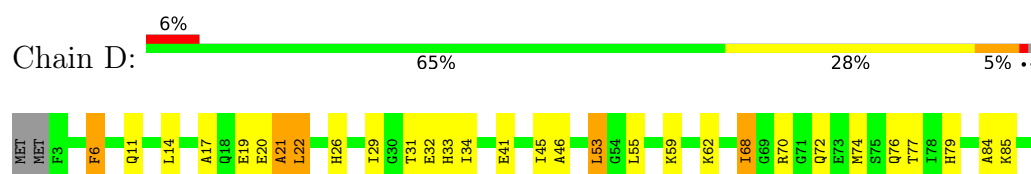


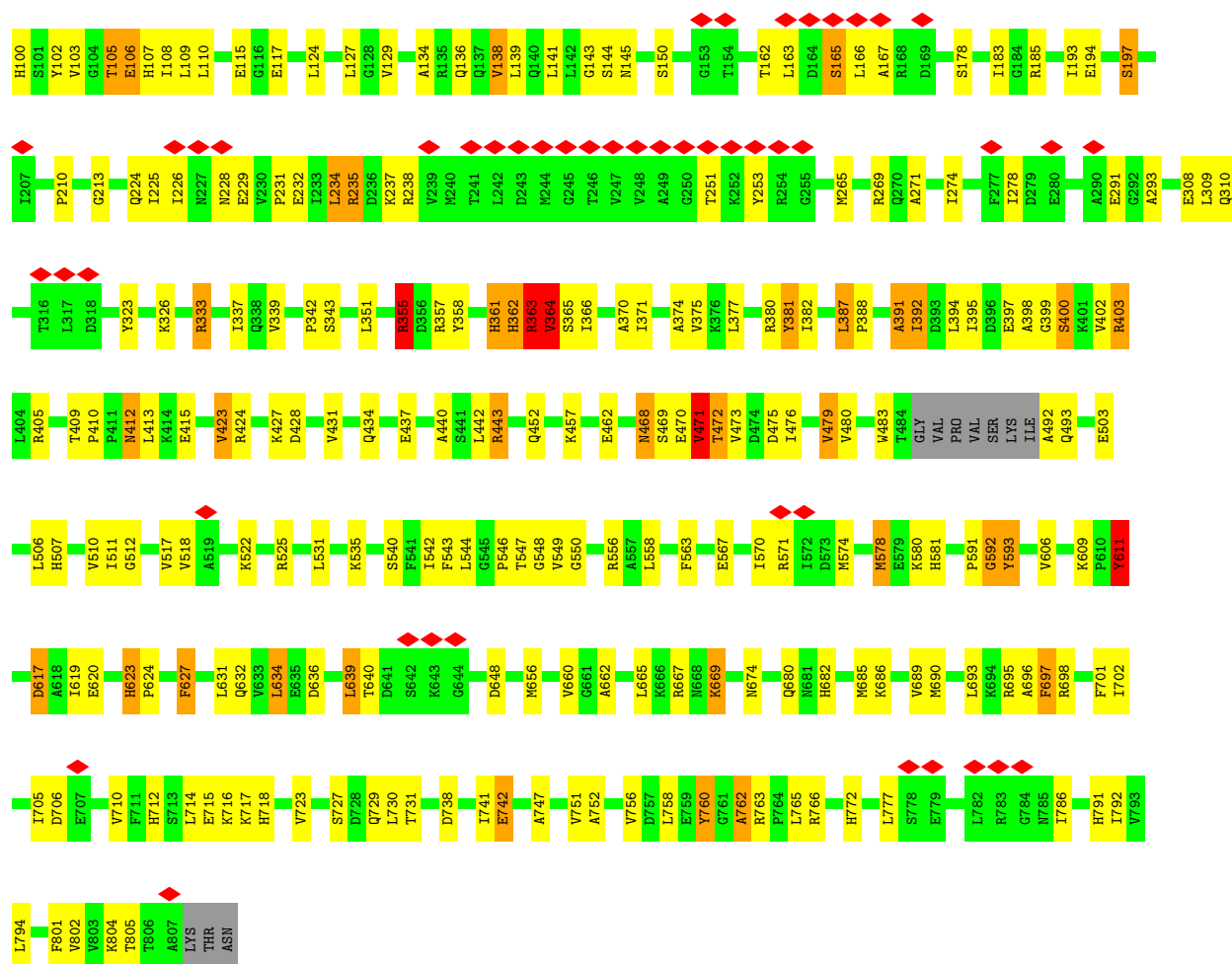


• Molecule 2: Negative regulator of genetic competence ClpC/MecB

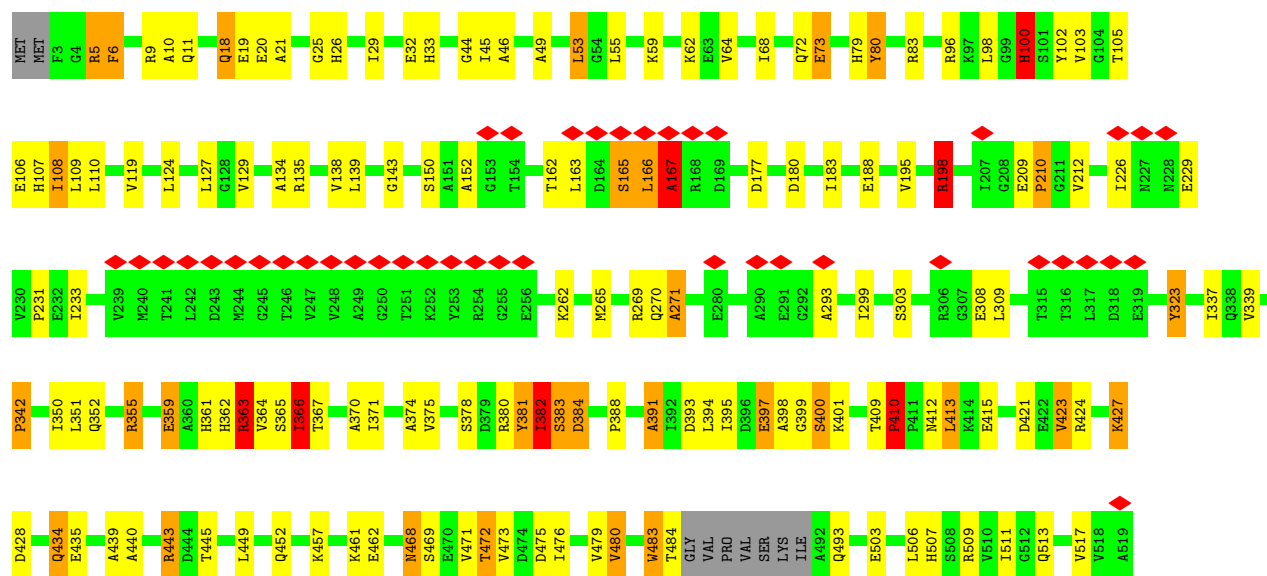


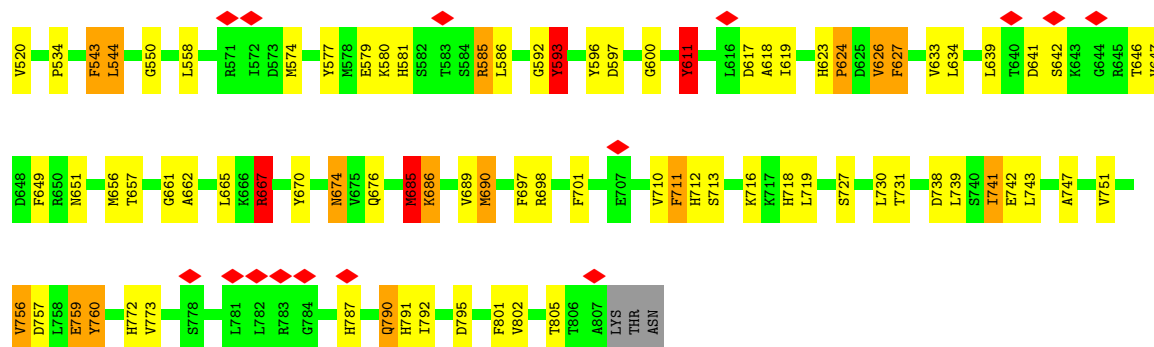
• Molecule 2: Negative regulator of genetic competence ClpC/MecB



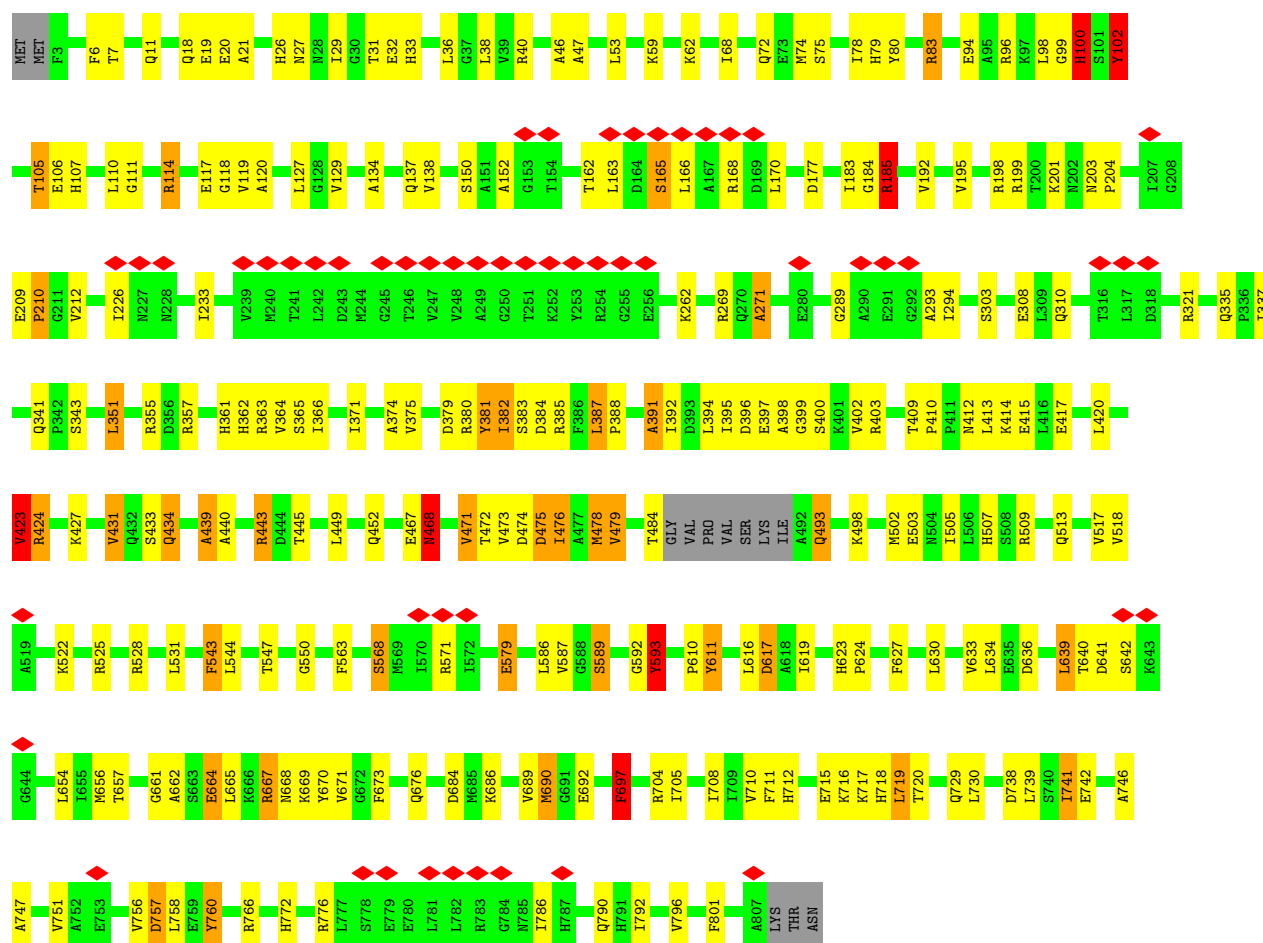


● Molecule 2: Negative regulator of genetic competence ClpC/MecB





• Molecule 2: Negative regulator of genetic competence ClpC/MecB



## 4 Experimental information

| Property                             | Value                          | Source    |
|--------------------------------------|--------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                | Depositor |
| Imposed symmetry                     | POINT, C1                      | Depositor |
| Number of particles used             | 41902                          | Depositor |
| Resolution determination method      | FSC 0.5 CUT-OFF                | Depositor |
| CTF correction method                | each defocus group on 3D level | Depositor |
| Microscope                           | FEI TITAN KRIOS                | Depositor |
| Voltage (kV)                         | 300                            | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 20                             | Depositor |
| Minimum defocus (nm)                 | 1500                           | Depositor |
| Maximum defocus (nm)                 | 3000                           | Depositor |
| Magnification                        | 59000                          | Depositor |
| Image detector                       | FEI EAGLE (4k x 4k)            | Depositor |
| Maximum map value                    | 7.059                          | Depositor |
| Minimum map value                    | -4.200                         | Depositor |
| Average map value                    | 0.002                          | Depositor |
| Map value standard deviation         | 0.997                          | Depositor |
| Recommended contour level            | 1.5                            | Depositor |
| Map size ( $\text{\AA}$ )            | 225.0, 225.0, 225.0            | wwPDB     |
| Map dimensions                       | 150, 150, 150                  | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0               | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.5, 1.5, 1.5                  | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |             | Bond angles |                  |
|-----|-------|--------------|-------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$      |
| 1   | 1     | 0.98         | 0/791       | 1.31        | 4/1064 (0.4%)    |
| 1   | 2     | 0.97         | 0/791       | 1.28        | 3/1064 (0.3%)    |
| 1   | 3     | 0.97         | 0/791       | 1.34        | 5/1064 (0.5%)    |
| 1   | 4     | 0.99         | 0/791       | 1.26        | 3/1064 (0.3%)    |
| 1   | 5     | 0.96         | 0/791       | 1.29        | 4/1064 (0.4%)    |
| 1   | 6     | 0.99         | 0/791       | 1.36        | 5/1064 (0.5%)    |
| 2   | A     | 1.00         | 0/6269      | 1.26        | 27/8441 (0.3%)   |
| 2   | B     | 1.00         | 0/6269      | 1.30        | 32/8441 (0.4%)   |
| 2   | C     | 0.99         | 0/6269      | 1.27        | 28/8441 (0.3%)   |
| 2   | D     | 1.00         | 0/6269      | 1.28        | 29/8441 (0.3%)   |
| 2   | E     | 0.99         | 0/6269      | 1.29        | 36/8441 (0.4%)   |
| 2   | F     | 1.01         | 0/6269      | 1.28        | 24/8441 (0.3%)   |
| All | All   | 1.00         | 0/42360     | 1.28        | 200/57030 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | 1     | 0                   | 1                   |
| 1   | 2     | 0                   | 1                   |
| 1   | 3     | 0                   | 4                   |
| 1   | 4     | 0                   | 1                   |
| 1   | 5     | 0                   | 1                   |
| 1   | 6     | 0                   | 2                   |
| 2   | A     | 0                   | 19                  |
| 2   | B     | 0                   | 20                  |
| 2   | C     | 0                   | 12                  |
| 2   | D     | 0                   | 17                  |
| 2   | E     | 0                   | 15                  |
| 2   | F     | 0                   | 14                  |
| All | All   | 0                   | 107                 |

There are no bond length outliers.

All (200) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | F     | 593 | TYR  | CB-CG-CD2 | 9.71  | 126.83      | 121.00   |
| 2   | F     | 593 | TYR  | CB-CG-CD1 | -8.53 | 115.88      | 121.00   |
| 2   | E     | 167 | ALA  | N-CA-CB   | 8.31  | 121.74      | 110.10   |
| 2   | C     | 588 | GLY  | N-CA-C    | -8.22 | 92.55       | 113.10   |
| 2   | E     | 611 | TYR  | CB-CG-CD2 | -7.59 | 116.44      | 121.00   |
| 2   | E     | 543 | PHE  | CB-CG-CD1 | 7.53  | 126.07      | 120.80   |
| 2   | A     | 165 | SER  | C-N-CA    | 7.49  | 140.43      | 121.70   |
| 2   | F     | 760 | TYR  | CB-CG-CD2 | 7.49  | 125.49      | 121.00   |
| 2   | E     | 760 | TYR  | CB-CG-CD1 | -7.40 | 116.56      | 121.00   |
| 2   | F     | 760 | TYR  | CB-CG-CD1 | -7.38 | 116.57      | 121.00   |
| 2   | E     | 381 | TYR  | CB-CG-CD1 | -7.34 | 116.59      | 121.00   |
| 1   | 1     | 136 | PHE  | CB-CG-CD1 | 7.34  | 125.94      | 120.80   |
| 2   | F     | 543 | PHE  | CB-CG-CD2 | -7.32 | 115.68      | 120.80   |
| 2   | C     | 543 | PHE  | CB-CG-CD2 | -7.14 | 115.80      | 120.80   |
| 2   | B     | 165 | SER  | C-N-CA    | 7.08  | 139.40      | 121.70   |
| 2   | E     | 543 | PHE  | CB-CG-CD2 | -7.08 | 115.85      | 120.80   |
| 1   | 3     | 199 | TYR  | CB-CG-CD1 | -7.07 | 116.76      | 121.00   |
| 2   | F     | 165 | SER  | C-N-CA    | 7.06  | 139.35      | 121.70   |
| 2   | D     | 253 | TYR  | CB-CG-CD2 | 7.06  | 125.24      | 121.00   |
| 2   | D     | 165 | SER  | C-N-CA    | 6.99  | 139.17      | 121.70   |
| 2   | A     | 627 | PHE  | CB-CG-CD2 | -6.89 | 115.97      | 120.80   |
| 2   | B     | 543 | PHE  | CB-CG-CD2 | -6.89 | 115.98      | 120.80   |
| 2   | D     | 423 | VAL  | CA-CB-CG1 | -6.87 | 100.59      | 110.90   |
| 2   | E     | 760 | TYR  | CB-CG-CD2 | 6.87  | 125.12      | 121.00   |
| 2   | E     | 364 | VAL  | C-N-CA    | 6.86  | 138.86      | 121.70   |
| 2   | E     | 6   | PHE  | CB-CG-CD1 | -6.78 | 116.06      | 120.80   |
| 2   | E     | 423 | VAL  | CA-CB-CG1 | -6.78 | 100.74      | 110.90   |
| 1   | 6     | 136 | PHE  | CB-CG-CD1 | 6.76  | 125.54      | 120.80   |
| 1   | 6     | 215 | HIS  | CA-CB-CG  | 6.75  | 125.08      | 113.60   |
| 2   | F     | 543 | PHE  | CB-CG-CD1 | 6.72  | 125.50      | 120.80   |
| 2   | C     | 165 | SER  | C-N-CA    | 6.69  | 138.42      | 121.70   |
| 2   | D     | 364 | VAL  | C-N-CA    | 6.68  | 138.41      | 121.70   |
| 2   | E     | 611 | TYR  | CB-CG-CD1 | 6.67  | 125.00      | 121.00   |
| 2   | B     | 364 | VAL  | C-N-CA    | 6.63  | 138.28      | 121.70   |
| 2   | A     | 6   | PHE  | CB-CG-CD1 | -6.63 | 116.16      | 120.80   |
| 2   | D     | 611 | TYR  | CB-CG-CD1 | -6.59 | 117.04      | 121.00   |
| 2   | D     | 543 | PHE  | CB-CG-CD2 | -6.56 | 116.21      | 120.80   |
| 2   | F     | 102 | TYR  | CB-CG-CD2 | 6.53  | 124.92      | 121.00   |
| 1   | 3     | 199 | TYR  | CB-CG-CD2 | 6.51  | 124.91      | 121.00   |
| 2   | E     | 577 | TYR  | CB-CG-CD2 | -6.47 | 117.12      | 121.00   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | B     | 423 | VAL  | CA-CB-CG1 | -6.45 | 101.22      | 110.90   |
| 1   | 6     | 130 | VAL  | N-CA-C    | -6.41 | 93.70       | 111.00   |
| 2   | B     | 543 | PHE  | CB-CG-CD1 | 6.35  | 125.25      | 120.80   |
| 1   | 6     | 216 | PHE  | CB-CG-CD1 | -6.34 | 116.36      | 120.80   |
| 2   | A     | 6   | PHE  | CB-CG-CD2 | 6.34  | 125.24      | 120.80   |
| 2   | C     | 423 | VAL  | CA-CB-CG1 | -6.33 | 101.41      | 110.90   |
| 2   | E     | 165 | SER  | C-N-CA    | 6.31  | 137.49      | 121.70   |
| 2   | B     | 358 | TYR  | CB-CG-CD2 | -6.28 | 117.23      | 121.00   |
| 2   | F     | 697 | PHE  | CB-CG-CD1 | 6.28  | 125.20      | 120.80   |
| 2   | F     | 102 | TYR  | CB-CG-CD1 | -6.27 | 117.24      | 121.00   |
| 2   | A     | 543 | PHE  | CB-CG-CD2 | -6.26 | 116.42      | 120.80   |
| 2   | B     | 627 | PHE  | CB-CG-CD2 | -6.21 | 116.45      | 120.80   |
| 2   | C     | 543 | PHE  | CB-CG-CD1 | 6.21  | 125.15      | 120.80   |
| 2   | A     | 366 | ILE  | C-N-CA    | 6.20  | 137.20      | 121.70   |
| 1   | 5     | 199 | TYR  | CB-CG-CD1 | 6.18  | 124.71      | 121.00   |
| 2   | C     | 410 | PRO  | N-CA-CB   | -6.15 | 95.83       | 102.60   |
| 2   | D     | 213 | GLY  | N-CA-C    | -6.14 | 97.75       | 113.10   |
| 2   | A     | 669 | LYS  | N-CA-C    | -6.13 | 94.44       | 111.00   |
| 2   | C     | 106 | GLU  | N-CA-CB   | 6.12  | 121.62      | 110.60   |
| 2   | D     | 543 | PHE  | CB-CG-CD1 | 6.12  | 125.09      | 120.80   |
| 2   | A     | 402 | VAL  | CA-CB-CG2 | -6.12 | 101.72      | 110.90   |
| 2   | E     | 44  | GLY  | N-CA-C    | -6.11 | 97.81       | 113.10   |
| 2   | A     | 382 | ILE  | C-N-CA    | 6.10  | 136.95      | 121.70   |
| 2   | E     | 366 | ILE  | C-N-CA    | 6.05  | 136.82      | 121.70   |
| 2   | C     | 363 | ARG  | N-CA-CB   | 5.98  | 121.37      | 110.60   |
| 2   | C     | 431 | VAL  | CB-CA-C   | -5.97 | 100.05      | 111.40   |
| 2   | D     | 253 | TYR  | CB-CG-CD1 | -5.97 | 117.42      | 121.00   |
| 2   | A     | 627 | PHE  | CB-CG-CD1 | 5.97  | 124.98      | 120.80   |
| 2   | C     | 364 | VAL  | C-N-CA    | 5.92  | 136.50      | 121.70   |
| 2   | E     | 6   | PHE  | CB-CG-CD2 | 5.90  | 124.93      | 120.80   |
| 2   | B     | 6   | PHE  | CB-CG-CD1 | -5.89 | 116.68      | 120.80   |
| 2   | C     | 80  | TYR  | CA-CB-CG  | -5.87 | 102.24      | 113.40   |
| 2   | A     | 543 | PHE  | CB-CG-CD1 | 5.85  | 124.90      | 120.80   |
| 1   | 1     | 199 | TYR  | CB-CG-CD2 | 5.83  | 124.50      | 121.00   |
| 2   | F     | 79  | HIS  | N-CA-C    | -5.81 | 95.31       | 111.00   |
| 2   | C     | 511 | ILE  | N-CA-C    | -5.81 | 95.31       | 111.00   |
| 2   | D     | 632 | GLN  | CB-CA-C   | -5.81 | 98.78       | 110.40   |
| 2   | A     | 423 | VAL  | CA-CB-CG1 | -5.80 | 102.19      | 110.90   |
| 2   | D     | 802 | VAL  | N-CA-C    | -5.80 | 95.34       | 111.00   |
| 2   | E     | 381 | TYR  | CB-CG-CD2 | 5.79  | 124.48      | 121.00   |
| 2   | D     | 310 | GLN  | N-CA-C    | -5.78 | 95.39       | 111.00   |
| 2   | F     | 433 | SER  | C-N-CA    | 5.78  | 136.14      | 121.70   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | A     | 760 | TYR  | CB-CG-CD1 | -5.76 | 117.55      | 121.00   |
| 2   | A     | 690 | MET  | CG-SD-CE  | -5.75 | 91.00       | 100.20   |
| 2   | D     | 669 | LYS  | N-CA-CB   | 5.75  | 120.95      | 110.60   |
| 2   | A     | 568 | SER  | N-CA-C    | -5.75 | 95.48       | 111.00   |
| 2   | E     | 577 | TYR  | CB-CG-CD1 | 5.70  | 124.42      | 121.00   |
| 2   | F     | 757 | ASP  | N-CA-CB   | 5.70  | 120.86      | 110.60   |
| 1   | 3     | 195 | ARG  | NE-CZ-NH2 | 5.70  | 123.15      | 120.30   |
| 2   | B     | 802 | VAL  | N-CA-C    | -5.69 | 95.63       | 111.00   |
| 2   | B     | 79  | HIS  | N-CA-C    | -5.69 | 95.64       | 111.00   |
| 1   | 3     | 130 | VAL  | N-CA-C    | -5.68 | 95.66       | 111.00   |
| 2   | C     | 6   | PHE  | CB-CG-CD1 | -5.66 | 116.84      | 120.80   |
| 2   | D     | 611 | TYR  | CB-CG-CD2 | 5.64  | 124.39      | 121.00   |
| 2   | D     | 805 | THR  | N-CA-C    | -5.62 | 95.81       | 111.00   |
| 2   | A     | 102 | TYR  | CB-CG-CD2 | 5.62  | 124.37      | 121.00   |
| 2   | E     | 79  | HIS  | N-CA-C    | -5.62 | 95.83       | 111.00   |
| 2   | E     | 166 | LEU  | C-N-CA    | 5.62  | 135.74      | 121.70   |
| 2   | C     | 358 | TYR  | CB-CG-CD2 | -5.61 | 117.63      | 121.00   |
| 2   | D     | 6   | PHE  | CB-CG-CD1 | -5.59 | 116.88      | 120.80   |
| 1   | 5     | 199 | TYR  | CB-CG-CD2 | -5.59 | 117.64      | 121.00   |
| 2   | C     | 79  | HIS  | N-CA-C    | -5.57 | 95.95       | 111.00   |
| 2   | D     | 690 | MET  | CG-SD-CE  | -5.55 | 91.32       | 100.20   |
| 1   | 1     | 156 | SER  | N-CA-C    | -5.54 | 96.03       | 111.00   |
| 2   | E     | 19  | GLU  | N-CA-CB   | 5.54  | 120.58      | 110.60   |
| 2   | B     | 410 | PRO  | CA-C-N    | 5.54  | 132.62      | 117.10   |
| 2   | C     | 743 | LEU  | N-CA-C    | -5.51 | 96.13       | 111.00   |
| 2   | F     | 711 | PHE  | N-CA-C    | -5.49 | 96.18       | 111.00   |
| 2   | F     | 440 | ALA  | CB-CA-C   | -5.49 | 101.87      | 110.10   |
| 2   | F     | 439 | ALA  | N-CA-CB   | 5.48  | 117.77      | 110.10   |
| 2   | F     | 568 | SER  | N-CA-C    | -5.47 | 96.23       | 111.00   |
| 2   | C     | 293 | ALA  | N-CA-CB   | 5.47  | 117.76      | 110.10   |
| 2   | E     | 742 | GLU  | N-CA-CB   | 5.46  | 120.43      | 110.60   |
| 2   | A     | 596 | TYR  | CB-CG-CD1 | -5.46 | 117.72      | 121.00   |
| 2   | B     | 382 | ILE  | C-N-CA    | 5.45  | 135.33      | 121.70   |
| 1   | 2     | 199 | TYR  | CB-CG-CD2 | 5.44  | 124.27      | 121.00   |
| 2   | F     | 478 | MET  | CG-SD-CE  | -5.44 | 91.50       | 100.20   |
| 1   | 1     | 199 | TYR  | CB-CG-CD1 | -5.43 | 117.74      | 121.00   |
| 2   | B     | 398 | ALA  | C-N-CA    | 5.43  | 133.70      | 122.30   |
| 1   | 2     | 156 | SER  | N-CA-C    | -5.43 | 96.35       | 111.00   |
| 2   | D     | 333 | ARG  | N-CA-C    | -5.41 | 96.39       | 111.00   |
| 1   | 4     | 216 | PHE  | N-CA-CB   | 5.40  | 120.31      | 110.60   |
| 2   | A     | 79  | HIS  | N-CA-C    | -5.39 | 96.45       | 111.00   |
| 1   | 5     | 217 | ALA  | N-CA-CB   | 5.38  | 117.64      | 110.10   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | C     | 6   | PHE  | CB-CG-CD2 | 5.38  | 124.57      | 120.80   |
| 2   | C     | 176 | GLU  | N-CA-C    | -5.36 | 96.53       | 111.00   |
| 2   | F     | 423 | VAL  | CA-CB-CG1 | -5.36 | 102.86      | 110.90   |
| 2   | D     | 21  | ALA  | CB-CA-C   | -5.36 | 102.07      | 110.10   |
| 2   | D     | 469 | SER  | N-CA-CB   | 5.35  | 118.53      | 110.50   |
| 2   | A     | 102 | TYR  | CB-CG-CD1 | -5.34 | 117.79      | 121.00   |
| 2   | C     | 358 | TYR  | CB-CG-CD1 | 5.33  | 124.20      | 121.00   |
| 2   | B     | 611 | TYR  | CB-CG-CD2 | -5.33 | 117.80      | 121.00   |
| 2   | C     | 333 | ARG  | N-CA-C    | -5.33 | 96.61       | 111.00   |
| 2   | E     | 711 | PHE  | N-CA-CB   | 5.33  | 120.19      | 110.60   |
| 2   | E     | 685 | MET  | N-CA-CB   | 5.32  | 120.18      | 110.60   |
| 1   | 3     | 167 | PHE  | CB-CG-CD1 | 5.31  | 124.52      | 120.80   |
| 2   | A     | 29  | ILE  | N-CA-C    | -5.31 | 96.66       | 111.00   |
| 2   | D     | 403 | ARG  | NE-CZ-NH1 | 5.31  | 122.95      | 120.30   |
| 2   | C     | 363 | ARG  | N-CA-C    | -5.31 | 96.67       | 111.00   |
| 2   | B     | 6   | PHE  | CB-CG-CD2 | 5.29  | 124.51      | 120.80   |
| 2   | E     | 323 | TYR  | CB-CG-CD1 | -5.29 | 117.82      | 121.00   |
| 2   | F     | 6   | PHE  | CB-CG-CD2 | 5.29  | 124.51      | 120.80   |
| 2   | D     | 669 | LYS  | N-CA-C    | -5.29 | 96.73       | 111.00   |
| 2   | C     | 646 | THR  | N-CA-C    | -5.28 | 96.75       | 111.00   |
| 2   | D     | 6   | PHE  | CB-CG-CD2 | 5.28  | 124.49      | 120.80   |
| 2   | A     | 802 | VAL  | N-CA-C    | -5.26 | 96.80       | 111.00   |
| 2   | B     | 403 | ARG  | NE-CZ-NH1 | 5.26  | 122.93      | 120.30   |
| 2   | B     | 358 | TYR  | CB-CG-CD1 | 5.25  | 124.15      | 121.00   |
| 2   | E     | 382 | ILE  | C-N-CA    | 5.25  | 134.83      | 121.70   |
| 2   | C     | 544 | LEU  | N-CA-C    | -5.25 | 96.83       | 111.00   |
| 2   | F     | 617 | ASP  | CB-CG-OD2 | 5.23  | 123.01      | 118.30   |
| 2   | D     | 617 | ASP  | CB-CG-OD2 | 5.23  | 123.01      | 118.30   |
| 2   | F     | 106 | GLU  | N-CA-CB   | 5.23  | 120.01      | 110.60   |
| 2   | E     | 80  | TYR  | CA-CB-CG  | -5.22 | 103.47      | 113.40   |
| 2   | C     | 617 | ASP  | CB-CG-OD2 | 5.21  | 122.98      | 118.30   |
| 2   | B     | 617 | ASP  | CB-CG-OD2 | 5.20  | 122.98      | 118.30   |
| 2   | E     | 617 | ASP  | CB-CG-OD2 | 5.20  | 122.98      | 118.30   |
| 2   | E     | 805 | THR  | N-CA-C    | -5.20 | 96.97       | 111.00   |
| 2   | B     | 634 | LEU  | CB-CG-CD1 | 5.19  | 119.83      | 111.00   |
| 2   | C     | 678 | GLU  | CB-CA-C   | -5.19 | 100.02      | 110.40   |
| 2   | D     | 363 | ARG  | N-CA-CB   | 5.19  | 119.94      | 110.60   |
| 1   | 4     | 156 | SER  | N-CA-C    | -5.18 | 97.00       | 111.00   |
| 2   | E     | 198 | ARG  | NE-CZ-NH2 | -5.18 | 117.71      | 120.30   |
| 2   | B     | 358 | TYR  | CA-CB-CG  | 5.17  | 123.23      | 113.40   |
| 1   | 4     | 166 | ASP  | N-CA-C    | -5.17 | 97.05       | 111.00   |
| 1   | 6     | 164 | TYR  | N-CA-CB   | 5.17  | 119.91      | 110.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | E     | 596 | TYR  | CB-CG-CD2 | -5.17 | 117.90      | 121.00   |
| 2   | A     | 617 | ASP  | CB-CG-OD2 | 5.17  | 122.95      | 118.30   |
| 2   | C     | 143 | GLY  | N-CA-C    | -5.17 | 100.19      | 113.10   |
| 2   | B     | 472 | THR  | N-CA-CB   | 5.16  | 120.11      | 110.30   |
| 2   | B     | 436 | PHE  | CB-CG-CD1 | -5.15 | 117.19      | 120.80   |
| 2   | E     | 383 | SER  | N-CA-CB   | 5.14  | 118.22      | 110.50   |
| 2   | A     | 165 | SER  | CA-C-N    | 5.14  | 128.51      | 117.20   |
| 2   | E     | 483 | TRP  | CB-CG-CD2 | -5.14 | 119.92      | 126.60   |
| 2   | F     | 711 | PHE  | N-CA-CB   | 5.13  | 119.84      | 110.60   |
| 2   | F     | 440 | ALA  | N-CA-CB   | 5.13  | 117.28      | 110.10   |
| 2   | B     | 410 | PRO  | N-CA-C    | -5.12 | 98.78       | 112.10   |
| 2   | B     | 685 | MET  | CG-SD-CE  | -5.12 | 92.01       | 100.20   |
| 2   | B     | 165 | SER  | CA-C-N    | 5.11  | 128.44      | 117.20   |
| 2   | E     | 646 | THR  | N-CA-C    | -5.10 | 97.23       | 111.00   |
| 1   | 2     | 199 | TYR  | CB-CG-CD1 | -5.09 | 117.95      | 121.00   |
| 2   | A     | 471 | VAL  | C-N-CA    | 5.08  | 134.41      | 121.70   |
| 2   | C     | 627 | PHE  | CB-CG-CD1 | 5.08  | 124.36      | 120.80   |
| 2   | E     | 802 | VAL  | N-CA-C    | -5.08 | 97.29       | 111.00   |
| 2   | B     | 646 | THR  | N-CA-C    | -5.07 | 97.32       | 111.00   |
| 2   | D     | 358 | TYR  | CB-CG-CD2 | -5.06 | 117.96      | 121.00   |
| 2   | B     | 659 | ASN  | N-CA-CB   | 5.06  | 119.71      | 110.60   |
| 2   | A     | 166 | LEU  | N-CA-CB   | 5.06  | 120.52      | 110.40   |
| 2   | B     | 201 | LYS  | N-CA-C    | -5.05 | 97.37       | 111.00   |
| 2   | B     | 471 | VAL  | CA-CB-CG1 | -5.04 | 103.34      | 110.90   |
| 1   | 5     | 166 | ASP  | N-CA-C    | -5.04 | 97.39       | 111.00   |
| 2   | A     | 270 | GLN  | C-N-CA    | 5.04  | 134.29      | 121.70   |
| 2   | A     | 742 | GLU  | N-CA-CB   | 5.03  | 119.65      | 110.60   |
| 2   | B     | 667 | ARG  | N-CA-C    | -5.03 | 97.43       | 111.00   |
| 2   | B     | 361 | HIS  | CA-CB-CG  | 5.02  | 122.14      | 113.60   |
| 2   | B     | 366 | ILE  | C-N-CA    | 5.01  | 134.22      | 121.70   |
| 2   | D     | 627 | PHE  | CB-CG-CD2 | -5.01 | 117.29      | 120.80   |
| 2   | D     | 355 | ARG  | NE-CZ-NH2 | -5.01 | 117.80      | 120.30   |
| 2   | E     | 483 | TRP  | CB-CG-CD1 | 5.01  | 133.51      | 127.00   |
| 2   | D     | 470 | GLU  | N-CA-C    | -5.00 | 97.49       | 111.00   |

There are no chirality outliers.

All (107) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | 1     | 161 | TYR  | Sidechain |
| 1   | 2     | 199 | TYR  | Sidechain |
| 1   | 3     | 164 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | 3     | 185 | TYR  | Sidechain         |
| 1   | 3     | 194 | HIS  | Sidechain         |
| 1   | 3     | 216 | PHE  | Sidechain         |
| 1   | 4     | 161 | TYR  | Sidechain         |
| 1   | 5     | 185 | TYR  | Sidechain         |
| 1   | 6     | 164 | TYR  | Sidechain         |
| 1   | 6     | 215 | HIS  | Sidechain         |
| 2   | A     | 185 | ARG  | Sidechain         |
| 2   | A     | 210 | PRO  | Peptide           |
| 2   | A     | 355 | ARG  | Sidechain         |
| 2   | A     | 363 | ARG  | Sidechain         |
| 2   | A     | 409 | THR  | Peptide           |
| 2   | A     | 424 | ARG  | Sidechain         |
| 2   | A     | 468 | ASN  | Peptide           |
| 2   | A     | 592 | GLY  | Peptide           |
| 2   | A     | 596 | TYR  | Sidechain         |
| 2   | A     | 627 | PHE  | Sidechain         |
| 2   | A     | 667 | ARG  | Sidechain         |
| 2   | A     | 697 | PHE  | Sidechain         |
| 2   | A     | 716 | LYS  | Mainchain,Peptide |
| 2   | A     | 756 | VAL  | Peptide           |
| 2   | A     | 760 | TYR  | Sidechain         |
| 2   | A     | 767 | ARG  | Sidechain         |
| 2   | A     | 776 | ARG  | Sidechain         |
| 2   | A     | 80  | TYR  | Sidechain         |
| 2   | B     | 107 | HIS  | Sidechain         |
| 2   | B     | 199 | ARG  | Sidechain         |
| 2   | B     | 210 | PRO  | Peptide           |
| 2   | B     | 23  | ARG  | Sidechain         |
| 2   | B     | 355 | ARG  | Sidechain         |
| 2   | B     | 358 | TYR  | Sidechain         |
| 2   | B     | 363 | ARG  | Sidechain         |
| 2   | B     | 403 | ARG  | Sidechain         |
| 2   | B     | 409 | THR  | Peptide           |
| 2   | B     | 468 | ASN  | Peptide           |
| 2   | B     | 536 | ARG  | Sidechain         |
| 2   | B     | 592 | GLY  | Peptide           |
| 2   | B     | 627 | PHE  | Sidechain         |
| 2   | B     | 667 | ARG  | Sidechain         |
| 2   | B     | 697 | PHE  | Sidechain         |
| 2   | B     | 716 | LYS  | Mainchain,Peptide |
| 2   | B     | 756 | VAL  | Peptide           |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 2   | B     | 760 | TYR  | Sidechain         |
| 2   | B     | 80  | TYR  | Sidechain         |
| 2   | C     | 210 | PRO  | Peptide           |
| 2   | C     | 28  | ASN  | Mainchain         |
| 2   | C     | 358 | TYR  | Sidechain         |
| 2   | C     | 409 | THR  | Peptide           |
| 2   | C     | 468 | ASN  | Peptide           |
| 2   | C     | 541 | PHE  | Peptide           |
| 2   | C     | 592 | GLY  | Peptide           |
| 2   | C     | 697 | PHE  | Sidechain         |
| 2   | C     | 716 | LYS  | Peptide           |
| 2   | C     | 756 | VAL  | Peptide           |
| 2   | C     | 791 | HIS  | Sidechain         |
| 2   | C     | 80  | TYR  | Sidechain         |
| 2   | D     | 210 | PRO  | Peptide           |
| 2   | D     | 355 | ARG  | Sidechain         |
| 2   | D     | 363 | ARG  | Sidechain         |
| 2   | D     | 381 | TYR  | Sidechain         |
| 2   | D     | 405 | ARG  | Sidechain         |
| 2   | D     | 409 | THR  | Peptide           |
| 2   | D     | 468 | ASN  | Peptide           |
| 2   | D     | 556 | ARG  | Sidechain         |
| 2   | D     | 592 | GLY  | Peptide           |
| 2   | D     | 593 | TYR  | Sidechain         |
| 2   | D     | 611 | TYR  | Sidechain         |
| 2   | D     | 667 | ARG  | Sidechain         |
| 2   | D     | 697 | PHE  | Sidechain         |
| 2   | D     | 716 | LYS  | Mainchain,Peptide |
| 2   | D     | 756 | VAL  | Peptide           |
| 2   | D     | 760 | TYR  | Sidechain         |
| 2   | E     | 198 | ARG  | Sidechain         |
| 2   | E     | 210 | PRO  | Peptide           |
| 2   | E     | 381 | TYR  | Sidechain         |
| 2   | E     | 409 | THR  | Peptide           |
| 2   | E     | 468 | ASN  | Peptide           |
| 2   | E     | 5   | ARG  | Sidechain         |
| 2   | E     | 592 | GLY  | Peptide           |
| 2   | E     | 593 | TYR  | Sidechain         |
| 2   | E     | 627 | PHE  | Sidechain         |
| 2   | E     | 667 | ARG  | Sidechain         |
| 2   | E     | 716 | LYS  | Mainchain,Peptide |
| 2   | E     | 756 | VAL  | Peptide           |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 2   | E     | 80  | TYR  | Sidechain         |
| 2   | E     | 96  | ARG  | Sidechain         |
| 2   | F     | 102 | TYR  | Sidechain         |
| 2   | F     | 114 | ARG  | Sidechain         |
| 2   | F     | 210 | PRO  | Peptide           |
| 2   | F     | 381 | TYR  | Sidechain         |
| 2   | F     | 409 | THR  | Peptide           |
| 2   | F     | 424 | ARG  | Sidechain         |
| 2   | F     | 468 | ASN  | Peptide           |
| 2   | F     | 592 | GLY  | Peptide           |
| 2   | F     | 667 | ARG  | Sidechain         |
| 2   | F     | 697 | PHE  | Sidechain         |
| 2   | F     | 716 | LYS  | Mainchain,Peptide |
| 2   | F     | 756 | VAL  | Peptide           |
| 2   | F     | 80  | TYR  | Sidechain         |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 777   | 0        | 758      | 17      | 0            |
| 1   | 2     | 777   | 0        | 758      | 15      | 0            |
| 1   | 3     | 777   | 0        | 758      | 20      | 0            |
| 1   | 4     | 777   | 0        | 758      | 13      | 0            |
| 1   | 5     | 777   | 0        | 758      | 14      | 0            |
| 1   | 6     | 777   | 0        | 758      | 12      | 0            |
| 2   | A     | 6200  | 0        | 6290     | 116     | 0            |
| 2   | B     | 6200  | 0        | 6290     | 133     | 0            |
| 2   | C     | 6200  | 0        | 6290     | 110     | 0            |
| 2   | D     | 6200  | 0        | 6290     | 137     | 0            |
| 2   | E     | 6200  | 0        | 6290     | 116     | 0            |
| 2   | F     | 6200  | 0        | 6290     | 119     | 0            |
| All | All   | 41862 | 0        | 42288    | 771     | 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 9.

All (771) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:619:ILE:CD1  | 2:A:656:MET:HB3  | 1.24                     | 1.66              |
| 2:A:619:ILE:CD1  | 2:A:656:MET:CB   | 2.18                     | 1.21              |
| 2:F:619:ILE:HD12 | 2:F:656:MET:HB3  | 1.23                     | 1.21              |
| 2:E:619:ILE:CD1  | 2:E:656:MET:HB3  | 1.69                     | 1.20              |
| 2:F:619:ILE:CG2  | 2:F:627:PHE:CZ   | 2.27                     | 1.18              |
| 2:C:615:LEU:HD22 | 2:C:617:ASP:OD1  | 1.47                     | 1.13              |
| 2:E:619:ILE:HG23 | 2:E:627:PHE:CZ   | 1.84                     | 1.12              |
| 2:D:619:ILE:HD12 | 2:D:656:MET:HB3  | 1.15                     | 1.11              |
| 2:F:619:ILE:HG21 | 2:F:627:PHE:CE1  | 1.85                     | 1.11              |
| 2:A:619:ILE:HD11 | 2:A:656:MET:HB3  | 1.20                     | 1.10              |
| 2:E:619:ILE:CG2  | 2:E:627:PHE:CZ   | 2.34                     | 1.09              |
| 2:F:619:ILE:CG2  | 2:F:627:PHE:HZ   | 1.64                     | 1.09              |
| 2:C:616:LEU:HB3  | 2:C:619:ILE:HD11 | 1.36                     | 1.08              |
| 2:A:619:ILE:HD12 | 2:A:656:MET:CB   | 1.81                     | 1.04              |
| 2:E:619:ILE:HD12 | 2:E:656:MET:HB3  | 1.10                     | 1.04              |
| 2:B:619:ILE:CD1  | 2:B:656:MET:HB3  | 1.87                     | 1.03              |
| 2:E:619:ILE:HG23 | 2:E:627:PHE:HZ   | 1.14                     | 1.03              |
| 2:B:619:ILE:HD12 | 2:B:656:MET:HB3  | 1.01                     | 1.01              |
| 2:E:619:ILE:HG21 | 2:E:627:PHE:CE1  | 1.99                     | 0.98              |
| 2:F:619:ILE:HG22 | 2:F:627:PHE:HZ   | 1.31                     | 0.96              |
| 2:F:619:ILE:HG21 | 2:F:627:PHE:HE1  | 1.24                     | 0.94              |
| 2:D:619:ILE:CG2  | 2:D:627:PHE:HE1  | 1.81                     | 0.94              |
| 2:A:619:ILE:HD12 | 2:A:656:MET:HB3  | 0.94                     | 0.93              |
| 2:B:619:ILE:HD12 | 2:B:656:MET:CB   | 1.97                     | 0.93              |
| 2:A:619:ILE:HD11 | 2:A:656:MET:CB   | 1.90                     | 0.93              |
| 2:E:619:ILE:CG2  | 2:E:627:PHE:CE1  | 2.51                     | 0.93              |
| 2:F:619:ILE:CG2  | 2:F:627:PHE:CE1  | 2.49                     | 0.93              |
| 2:B:616:LEU:HB2  | 2:B:619:ILE:HD11 | 1.53                     | 0.90              |
| 2:D:619:ILE:CG2  | 2:D:627:PHE:CE1  | 2.54                     | 0.89              |
| 2:D:619:ILE:HG23 | 2:D:627:PHE:HE1  | 1.37                     | 0.89              |
| 2:F:619:ILE:HG22 | 2:F:627:PHE:CZ   | 2.07                     | 0.88              |
| 2:A:394:LEU:HD13 | 2:A:480:VAL:HG22 | 1.54                     | 0.86              |
| 2:B:619:ILE:CG2  | 2:B:627:PHE:HE1  | 1.89                     | 0.86              |
| 2:C:616:LEU:CB   | 2:C:619:ILE:HD11 | 2.05                     | 0.85              |
| 2:C:619:ILE:HG22 | 2:C:619:ILE:O    | 1.76                     | 0.85              |
| 2:D:619:ILE:CD1  | 2:D:656:MET:HB3  | 2.05                     | 0.84              |
| 2:B:619:ILE:CG2  | 2:B:627:PHE:CE1  | 2.62                     | 0.83              |
| 2:C:615:LEU:CD2  | 2:C:617:ASP:OD1  | 2.26                     | 0.82              |
| 2:C:619:ILE:CG2  | 2:C:627:PHE:HE1  | 1.92                     | 0.82              |
| 2:F:619:ILE:HG23 | 2:F:627:PHE:CZ   | 2.18                     | 0.79              |
| 2:C:394:LEU:HD13 | 2:C:480:VAL:HG22 | 1.64                     | 0.79              |
| 2:F:571:ARG:CZ   | 2:F:617:ASP:OD2  | 2.31                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:619:ILE:HG22 | 2:B:627:PHE:CE1  | 2.18                     | 0.77              |
| 2:E:619:ILE:HD12 | 2:E:656:MET:CB   | 2.05                     | 0.76              |
| 2:C:26:HIS:CD2   | 2:C:33:HIS:CE1   | 2.75                     | 0.75              |
| 2:E:619:ILE:HG21 | 2:E:627:PHE:HE1  | 1.52                     | 0.72              |
| 2:F:619:ILE:CD1  | 2:F:656:MET:HB3  | 2.13                     | 0.72              |
| 2:F:513:GLN:H    | 2:F:718:HIS:CD2  | 2.08                     | 0.72              |
| 2:D:619:ILE:HG22 | 2:D:627:PHE:CE1  | 2.25                     | 0.72              |
| 2:E:619:ILE:HG22 | 2:E:619:ILE:O    | 1.91                     | 0.71              |
| 2:F:26:HIS:CD2   | 2:F:33:HIS:CE1   | 2.79                     | 0.71              |
| 2:B:21:ALA:HA    | 2:B:33:HIS:CE1   | 2.25                     | 0.71              |
| 2:D:619:ILE:HG22 | 2:D:697:PHE:HE1  | 1.55                     | 0.71              |
| 2:F:619:ILE:HD12 | 2:F:656:MET:CB   | 2.14                     | 0.71              |
| 2:E:107:HIS:HA   | 2:E:110:LEU:HD12 | 1.73                     | 0.70              |
| 2:F:619:ILE:HG22 | 2:F:619:ILE:O    | 1.90                     | 0.70              |
| 2:D:55:LEU:HD13  | 2:D:124:LEU:HD22 | 1.74                     | 0.69              |
| 2:C:574:MET:HG3  | 2:C:619:ILE:HG12 | 1.74                     | 0.69              |
| 2:B:619:ILE:HG23 | 2:B:627:PHE:HE1  | 1.57                     | 0.68              |
| 2:C:693:LEU:HD12 | 2:C:697:PHE:CD2  | 2.28                     | 0.68              |
| 2:B:363:ARG:HH11 | 2:B:399:GLY:HA2  | 1.59                     | 0.68              |
| 2:C:26:HIS:CG    | 2:C:33:HIS:CE1   | 2.81                     | 0.68              |
| 2:D:363:ARG:HH11 | 2:D:399:GLY:HA2  | 1.60                     | 0.67              |
| 2:D:363:ARG:HH12 | 2:D:471:VAL:HA   | 1.60                     | 0.67              |
| 2:A:544:LEU:HD21 | 2:A:693:LEU:HD13 | 1.77                     | 0.66              |
| 2:A:682:HIS:CD2  | 2:A:712:HIS:CE1  | 2.84                     | 0.66              |
| 2:D:53:LEU:HD21  | 2:D:134:ALA:HA   | 1.77                     | 0.66              |
| 2:D:197:SER:HA   | 2:D:234:LEU:HD23 | 1.77                     | 0.66              |
| 2:D:544:LEU:HD11 | 2:D:693:LEU:HD13 | 1.77                     | 0.66              |
| 2:C:619:ILE:O    | 2:C:619:ILE:CG2  | 2.43                     | 0.66              |
| 2:E:507:HIS:CD2  | 2:E:517:VAL:HG11 | 2.32                     | 0.65              |
| 2:F:26:HIS:CG    | 2:F:33:HIS:CE1   | 2.84                     | 0.65              |
| 1:4:142:LEU:HD23 | 1:4:185:TYR:CD2  | 2.30                     | 0.65              |
| 2:F:619:ILE:HG23 | 2:F:627:PHE:HZ   | 1.56                     | 0.65              |
| 2:C:55:LEU:HD13  | 2:C:124:LEU:HD22 | 1.79                     | 0.65              |
| 2:A:21:ALA:HA    | 2:A:33:HIS:CE1   | 2.33                     | 0.64              |
| 2:F:751:VAL:HG22 | 2:F:772:HIS:CB   | 2.27                     | 0.64              |
| 2:A:394:LEU:HD21 | 2:A:483:TRP:CE2  | 2.32                     | 0.64              |
| 2:F:741:ILE:HG22 | 2:F:792:ILE:HD12 | 1.80                     | 0.64              |
| 2:C:619:ILE:HG23 | 2:C:622:ALA:HB3  | 1.80                     | 0.64              |
| 2:E:619:ILE:HD11 | 2:E:656:MET:HB3  | 1.77                     | 0.64              |
| 2:C:24:LEU:HD11  | 2:C:61:GLN:HE22  | 1.62                     | 0.63              |
| 2:C:619:ILE:CG2  | 2:C:627:PHE:CE1  | 2.78                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:163:LEU:HD11 | 1:1:209:LEU:HD21 | 1.79                     | 0.63              |
| 2:B:669:LYS:H    | 2:B:685:MET:HE1  | 1.64                     | 0.63              |
| 2:F:351:LEU:HD13 | 2:F:391:ALA:HB1  | 1.79                     | 0.63              |
| 1:5:154:LEU:HB3  | 1:5:204:ILE:HD12 | 1.81                     | 0.63              |
| 2:A:619:ILE:CG2  | 2:A:627:PHE:CE1  | 2.82                     | 0.63              |
| 2:A:727:SER:O    | 2:A:731:THR:HG23 | 1.99                     | 0.62              |
| 2:B:26:HIS:CD2   | 2:B:33:HIS:HE2   | 2.16                     | 0.62              |
| 2:D:619:ILE:HD12 | 2:D:656:MET:CB   | 2.10                     | 0.62              |
| 2:C:619:ILE:HG22 | 2:C:697:PHE:HE1  | 1.64                     | 0.62              |
| 2:D:665:LEU:HD23 | 2:D:685:MET:HG3  | 1.82                     | 0.62              |
| 2:D:682:HIS:CG   | 2:D:712:HIS:CE1  | 2.88                     | 0.62              |
| 2:F:427:LYS:HG3  | 2:F:443:ARG:HA   | 1.81                     | 0.62              |
| 2:C:544:LEU:HD11 | 2:C:693:LEU:HD13 | 1.80                     | 0.62              |
| 2:A:544:LEU:HD23 | 2:A:658:SER:HB2  | 1.82                     | 0.61              |
| 2:D:21:ALA:HB2   | 2:D:29:ILE:CG1   | 2.30                     | 0.61              |
| 2:D:26:HIS:CE1   | 2:D:68:ILE:HB    | 2.35                     | 0.61              |
| 2:F:21:ALA:HA    | 2:F:33:HIS:CE1   | 2.34                     | 0.61              |
| 2:B:20:GLU:HB2   | 2:B:33:HIS:CD2   | 2.35                     | 0.61              |
| 2:E:55:LEU:HD13  | 2:E:124:LEU:HD22 | 1.83                     | 0.61              |
| 2:F:363:ARG:HH11 | 2:F:399:GLY:HA2  | 1.65                     | 0.61              |
| 2:C:693:LEU:HD12 | 2:C:697:PHE:HD2  | 1.64                     | 0.61              |
| 2:B:507:HIS:CD2  | 2:B:517:VAL:HG11 | 2.36                     | 0.60              |
| 2:D:46:ALA:HB1   | 2:D:109:LEU:HB2  | 1.83                     | 0.60              |
| 2:A:476:ILE:O    | 2:A:480:VAL:HG23 | 2.01                     | 0.60              |
| 2:C:198:ARG:N    | 2:C:233:ILE:HG21 | 2.17                     | 0.60              |
| 2:D:786:ILE:HG21 | 2:D:792:ILE:HG23 | 1.83                     | 0.60              |
| 2:F:233:ILE:H    | 2:F:233:ILE:HD12 | 1.66                     | 0.60              |
| 2:B:633:VAL:HG23 | 2:B:639:LEU:HD23 | 1.83                     | 0.60              |
| 2:E:507:HIS:CG   | 2:E:517:VAL:HG11 | 2.37                     | 0.60              |
| 2:A:363:ARG:HH12 | 2:A:471:VAL:HA   | 1.67                     | 0.60              |
| 2:A:383:SER:H    | 2:A:390:LYS:HD2  | 1.67                     | 0.59              |
| 2:C:364:VAL:H    | 2:C:470:GLU:H    | 1.50                     | 0.59              |
| 2:D:685:MET:O    | 2:D:689:VAL:HG23 | 2.02                     | 0.59              |
| 2:B:723:VAL:HG21 | 2:B:752:ALA:HA   | 1.83                     | 0.59              |
| 2:D:363:ARG:HH21 | 2:D:402:VAL:HG11 | 1.66                     | 0.59              |
| 2:A:395:ILE:HA   | 2:A:476:ILE:HD12 | 1.85                     | 0.59              |
| 2:D:507:HIS:CD2  | 2:D:517:VAL:HG11 | 2.38                     | 0.59              |
| 2:A:786:ILE:HG21 | 2:A:792:ILE:HG23 | 1.85                     | 0.59              |
| 2:D:387:LEU:H    | 2:D:387:LEU:HD22 | 1.67                     | 0.59              |
| 2:F:715:GLU:HB2  | 2:F:718:HIS:CD2  | 2.38                     | 0.59              |
| 1:2:142:LEU:HD13 | 1:2:209:LEU:HD21 | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:619:ILE:HG22 | 2:A:697:PHE:HE1  | 1.68                     | 0.58              |
| 2:E:25:GLY:HA3   | 2:E:73:GLU:HA    | 1.85                     | 0.58              |
| 2:B:633:VAL:HG13 | 2:B:649:PHE:HB3  | 1.85                     | 0.58              |
| 2:D:547:THR:H    | 2:D:763:ARG:HH21 | 1.51                     | 0.58              |
| 2:F:351:LEU:CD1  | 2:F:391:ALA:HB1  | 2.33                     | 0.58              |
| 1:5:164:TYR:CG   | 1:5:193:ILE:HD13 | 2.39                     | 0.58              |
| 2:B:106:GLU:CD   | 2:B:142:LEU:HD11 | 2.24                     | 0.58              |
| 2:E:574:MET:HG2  | 2:E:619:ILE:HG12 | 1.85                     | 0.58              |
| 2:E:633:VAL:HG13 | 2:E:649:PHE:HB3  | 1.85                     | 0.58              |
| 2:B:665:LEU:HD11 | 2:B:689:VAL:HG11 | 1.86                     | 0.58              |
| 2:D:437:GLU:HA   | 2:D:440:ALA:HB3  | 1.84                     | 0.58              |
| 2:C:21:ALA:HB2   | 2:C:29:ILE:HG12  | 1.86                     | 0.58              |
| 2:E:619:ILE:CD1  | 2:E:656:MET:CB   | 2.64                     | 0.58              |
| 2:F:719:LEU:HD12 | 2:F:720:THR:H    | 1.68                     | 0.58              |
| 2:F:747:ALA:O    | 2:F:751:VAL:HG23 | 2.03                     | 0.58              |
| 2:A:624:PRO:HA   | 2:A:627:PHE:CD2  | 2.39                     | 0.58              |
| 2:F:522:LYS:HA   | 2:F:525:ARG:HE   | 1.69                     | 0.58              |
| 2:F:289:GLY:H    | 2:F:321:ARG:HH12 | 1.49                     | 0.57              |
| 2:B:627:PHE:HB2  | 2:B:698:ARG:HE   | 1.70                     | 0.57              |
| 2:D:619:ILE:HG22 | 2:D:697:PHE:CE1  | 2.39                     | 0.57              |
| 2:A:723:VAL:HG21 | 2:A:752:ALA:HA   | 1.86                     | 0.57              |
| 2:E:21:ALA:HA    | 2:E:33:HIS:CE1   | 2.39                     | 0.57              |
| 2:A:28:ASN:HB2   | 2:A:81:THR:HG23  | 1.86                     | 0.57              |
| 2:A:233:ILE:HA   | 2:F:361:HIS:HA   | 1.87                     | 0.57              |
| 2:D:548:GLY:O    | 2:D:762:ALA:HB3  | 2.04                     | 0.57              |
| 2:A:402:VAL:HG13 | 2:A:405:ARG:HE   | 1.69                     | 0.57              |
| 2:E:427:LYS:HG3  | 2:E:443:ARG:HA   | 1.86                     | 0.57              |
| 2:B:616:LEU:CB   | 2:B:619:ILE:HD11 | 2.31                     | 0.57              |
| 2:B:624:PRO:HA   | 2:B:627:PHE:CD2  | 2.40                     | 0.57              |
| 1:3:136:PHE:CD1  | 2:C:431:VAL:HG11 | 2.40                     | 0.57              |
| 2:A:427:LYS:HG3  | 2:A:443:ARG:HA   | 1.87                     | 0.57              |
| 1:3:216:PHE:CZ   | 2:C:439:ALA:HB3  | 2.40                     | 0.56              |
| 1:4:142:LEU:HD21 | 1:4:182:LEU:HA   | 1.86                     | 0.56              |
| 1:2:194:HIS:CE1  | 2:C:141:LEU:HD22 | 2.40                     | 0.56              |
| 1:3:142:LEU:HD23 | 1:3:142:LEU:O    | 2.05                     | 0.56              |
| 2:B:276:LEU:HD23 | 2:B:309:LEU:HA   | 1.88                     | 0.56              |
| 2:D:399:GLY:O    | 2:E:233:ILE:HD13 | 2.05                     | 0.56              |
| 1:2:133:PHE:CZ   | 1:2:142:LEU:HD12 | 2.40                     | 0.56              |
| 2:D:398:ALA:HB1  | 2:D:475:ASP:HB3  | 1.87                     | 0.56              |
| 1:1:140:ILE:HD13 | 1:1:216:PHE:CE1  | 2.41                     | 0.56              |
| 2:C:403:ARG:HH21 | 2:D:232:GLU:H    | 1.54                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:351:LEU:HD13 | 2:D:391:ALA:HB1  | 1.87                     | 0.56              |
| 2:E:685:MET:HG3  | 2:E:712:HIS:CG   | 2.41                     | 0.56              |
| 2:F:627:PHE:CD2  | 2:F:697:PHE:HA   | 2.40                     | 0.56              |
| 2:C:507:HIS:CD2  | 2:C:517:VAL:HG11 | 2.41                     | 0.55              |
| 2:F:26:HIS:CE1   | 2:F:68:ILE:HB    | 2.41                     | 0.55              |
| 1:1:140:ILE:HD13 | 1:1:216:PHE:CD1  | 2.42                     | 0.55              |
| 2:A:619:ILE:CD1  | 2:A:656:MET:CG   | 2.83                     | 0.55              |
| 2:B:545:GLY:H    | 2:B:665:LEU:HD13 | 1.70                     | 0.55              |
| 2:E:619:ILE:CG2  | 2:E:619:ILE:O    | 2.54                     | 0.55              |
| 2:E:685:MET:HG3  | 2:E:712:HIS:CD2  | 2.42                     | 0.55              |
| 1:3:130:VAL:HG22 | 1:3:164:TYR:CE1  | 2.41                     | 0.55              |
| 2:A:484:THR:HG23 | 2:A:611:TYR:CE1  | 2.42                     | 0.55              |
| 2:B:49:ALA:HB1   | 2:B:137:GLN:HB3  | 1.88                     | 0.55              |
| 2:E:363:ARG:HB3  | 2:E:399:GLY:HA2  | 1.89                     | 0.55              |
| 1:2:208:ALA:O    | 1:2:212:ILE:HD13 | 2.07                     | 0.55              |
| 1:3:142:LEU:HD21 | 1:3:182:LEU:HD22 | 1.87                     | 0.55              |
| 2:B:512:GLY:HA2  | 2:B:722:ILE:HD11 | 1.88                     | 0.55              |
| 2:E:751:VAL:HG22 | 2:E:772:HIS:CG   | 2.42                     | 0.55              |
| 2:F:21:ALA:HB2   | 2:F:29:ILE:HG12  | 1.89                     | 0.55              |
| 2:F:633:VAL:HG11 | 2:F:654:LEU:HD11 | 1.88                     | 0.55              |
| 2:A:542:ILE:HG13 | 2:A:705:ILE:HD13 | 1.89                     | 0.55              |
| 2:F:776:ARG:HE   | 2:F:801:PHE:HB3  | 1.72                     | 0.54              |
| 2:C:394:LEU:HD23 | 2:C:479:VAL:HG22 | 1.90                     | 0.54              |
| 2:F:661:GLY:H    | 2:F:689:VAL:HG13 | 1.73                     | 0.54              |
| 1:5:216:PHE:HA   | 2:E:440:ALA:HB2  | 1.89                     | 0.54              |
| 2:D:17:ALA:HB1   | 2:D:29:ILE:HG21  | 1.88                     | 0.54              |
| 2:D:21:ALA:HB2   | 2:D:29:ILE:HG13  | 1.89                     | 0.54              |
| 2:D:394:LEU:HD13 | 2:D:480:VAL:HG22 | 1.89                     | 0.54              |
| 2:A:26:HIS:CD2   | 2:A:33:HIS:CE1   | 2.95                     | 0.54              |
| 2:B:741:ILE:HG21 | 2:B:777:LEU:HD13 | 1.89                     | 0.54              |
| 2:E:351:LEU:CD1  | 2:E:391:ALA:HB1  | 2.38                     | 0.54              |
| 1:5:142:LEU:HD13 | 1:5:209:LEU:HD21 | 1.89                     | 0.54              |
| 2:B:90:LEU:HA    | 2:C:156:SER:H    | 1.73                     | 0.54              |
| 2:A:387:LEU:HD12 | 2:A:387:LEU:H    | 1.72                     | 0.54              |
| 1:1:137:GLU:HA   | 1:1:140:ILE:HD12 | 1.89                     | 0.53              |
| 2:A:437:GLU:HA   | 2:A:440:ALA:HB3  | 1.90                     | 0.53              |
| 2:E:53:LEU:HD21  | 2:E:134:ALA:HA   | 1.90                     | 0.53              |
| 2:F:616:LEU:HB2  | 2:F:619:ILE:HD11 | 1.88                     | 0.53              |
| 1:5:140:ILE:HD11 | 1:5:216:PHE:CD1  | 2.42                     | 0.53              |
| 2:A:556:ARG:HE   | 2:A:571:ARG:HH22 | 1.56                     | 0.53              |
| 2:B:9:ARG:HB3    | 2:B:105:THR:H    | 1.72                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:682:HIS:CE1  | 2:B:712:HIS:CE1  | 2.96                     | 0.53              |
| 2:C:624:PRO:HA   | 2:C:627:PHE:CD2  | 2.43                     | 0.53              |
| 2:D:26:HIS:CG    | 2:D:33:HIS:CE1   | 2.97                     | 0.53              |
| 2:D:106:GLU:HG2  | 2:D:107:HIS:CD2  | 2.43                     | 0.53              |
| 2:D:374:ALA:HA   | 2:D:394:LEU:HD12 | 1.90                     | 0.53              |
| 2:F:199:ARG:HH21 | 2:F:310:GLN:HE22 | 1.55                     | 0.53              |
| 2:E:26:HIS:HB2   | 2:E:33:HIS:CE1   | 2.43                     | 0.53              |
| 2:B:630:LEU:O    | 2:B:634:LEU:HD13 | 2.08                     | 0.53              |
| 2:C:361:HIS:CG   | 2:C:361:HIS:O    | 2.61                     | 0.53              |
| 2:D:45:ILE:HG23  | 2:D:141:LEU:HB2  | 1.91                     | 0.53              |
| 2:E:351:LEU:HD13 | 2:E:391:ALA:HB1  | 1.91                     | 0.53              |
| 2:D:355:ARG:HE   | 2:D:364:VAL:HG12 | 1.73                     | 0.53              |
| 2:E:371:ILE:HD12 | 2:E:395:ILE:HD13 | 1.91                     | 0.53              |
| 2:E:667:ARG:H    | 2:E:667:ARG:HH11 | 1.57                     | 0.53              |
| 1:6:142:LEU:HD21 | 1:6:182:LEU:HD22 | 1.90                     | 0.53              |
| 2:A:619:ILE:HG22 | 2:A:627:PHE:CE1  | 2.44                     | 0.53              |
| 2:C:100:HIS:CG   | 2:C:102:TYR:O    | 2.61                     | 0.53              |
| 2:E:195:VAL:HG13 | 2:E:198:ARG:HH11 | 1.73                     | 0.53              |
| 2:C:542:ILE:HG13 | 2:C:705:ILE:HD13 | 1.91                     | 0.53              |
| 2:C:545:GLY:H    | 2:C:661:GLY:HA3  | 1.73                     | 0.53              |
| 2:D:476:ILE:O    | 2:D:480:VAL:HG23 | 2.09                     | 0.53              |
| 2:D:542:ILE:HG13 | 2:D:705:ILE:HD13 | 1.91                     | 0.53              |
| 2:F:619:ILE:CG2  | 2:F:619:ILE:O    | 2.55                     | 0.53              |
| 1:3:216:PHE:HA   | 2:C:440:ALA:HB2  | 1.91                     | 0.53              |
| 2:C:95:ALA:HA    | 2:C:107:HIS:CD2  | 2.44                     | 0.53              |
| 2:F:571:ARG:NH2  | 2:F:617:ASP:OD2  | 2.41                     | 0.53              |
| 2:B:361:HIS:CG   | 2:C:233:ILE:HG12 | 2.44                     | 0.53              |
| 2:F:387:LEU:H    | 2:F:387:LEU:HD22 | 1.73                     | 0.53              |
| 1:5:133:PHE:CZ   | 1:5:142:LEU:HD12 | 2.45                     | 0.52              |
| 2:B:53:LEU:HD21  | 2:B:134:ALA:HA   | 1.90                     | 0.52              |
| 2:E:46:ALA:HB1   | 2:E:109:LEU:HB2  | 1.91                     | 0.52              |
| 2:E:747:ALA:HB1  | 2:E:801:PHE:CZ   | 2.45                     | 0.52              |
| 1:1:216:PHE:CE1  | 2:A:440:ALA:HA   | 2.44                     | 0.52              |
| 2:C:506:LEU:HD21 | 2:C:558:LEU:HD23 | 1.91                     | 0.52              |
| 2:D:26:HIS:HB2   | 2:D:33:HIS:CE1   | 2.44                     | 0.52              |
| 2:B:619:ILE:HG22 | 2:B:697:PHE:HE1  | 1.74                     | 0.52              |
| 2:F:362:HIS:HB2  | 2:F:403:ARG:HH21 | 1.74                     | 0.52              |
| 2:A:374:ALA:HA   | 2:A:476:ILE:HG21 | 1.90                     | 0.52              |
| 2:D:26:HIS:CD2   | 2:D:33:HIS:NE2   | 2.77                     | 0.52              |
| 2:E:361:HIS:HA   | 2:F:233:ILE:HA   | 1.90                     | 0.52              |
| 2:B:394:LEU:HD13 | 2:B:480:VAL:HG22 | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:630:LEU:O    | 2:F:634:LEU:HD13 | 2.09                     | 0.52              |
| 2:C:21:ALA:HA    | 2:C:33:HIS:CE1   | 2.45                     | 0.52              |
| 2:F:423:VAL:HG11 | 2:F:445:THR:HB   | 1.92                     | 0.52              |
| 2:F:639:LEU:HD13 | 2:F:640:THR:H    | 1.74                     | 0.52              |
| 1:6:203:ILE:HA   | 2:F:434:GLN:HE22 | 1.74                     | 0.52              |
| 2:E:342:PRO:HG2  | 2:E:350:ILE:HD11 | 1.92                     | 0.52              |
| 2:B:355:ARG:HD3  | 2:B:366:ILE:H    | 1.75                     | 0.51              |
| 2:B:669:LYS:HD3  | 2:B:712:HIS:CD2  | 2.44                     | 0.51              |
| 2:D:394:LEU:HD23 | 2:D:479:VAL:HG22 | 1.92                     | 0.51              |
| 2:D:702:ILE:HA   | 2:D:705:ILE:HD12 | 1.91                     | 0.51              |
| 2:F:786:ILE:HD12 | 2:F:792:ILE:HD13 | 1.91                     | 0.51              |
| 1:2:216:PHE:HA   | 2:B:440:ALA:HB2  | 1.92                     | 0.51              |
| 2:A:619:ILE:HG22 | 2:A:619:ILE:O    | 2.09                     | 0.51              |
| 2:B:26:HIS:CG    | 2:B:33:HIS:CE1   | 2.98                     | 0.51              |
| 2:D:21:ALA:HA    | 2:D:33:HIS:CE1   | 2.45                     | 0.51              |
| 2:D:540:SER:HB2  | 2:D:706:ASP:H    | 1.74                     | 0.51              |
| 2:F:111:GLY:HA2  | 2:F:114:ARG:HH11 | 1.75                     | 0.51              |
| 2:A:26:HIS:CG    | 2:A:33:HIS:CE1   | 2.98                     | 0.51              |
| 2:B:427:LYS:O    | 2:B:431:VAL:HG23 | 2.09                     | 0.51              |
| 2:B:741:ILE:HG22 | 2:B:792:ILE:HB   | 1.92                     | 0.51              |
| 2:D:701:PHE:CE2  | 2:D:705:ILE:HD11 | 2.46                     | 0.51              |
| 1:1:154:LEU:HD11 | 1:1:161:TYR:HB3  | 1.92                     | 0.51              |
| 2:A:423:VAL:HG11 | 2:A:445:THR:HB   | 1.92                     | 0.51              |
| 2:D:46:ALA:HB2   | 2:D:105:THR:O    | 2.09                     | 0.51              |
| 2:D:235:ARG:HH22 | 2:D:238:ARG:HH22 | 1.58                     | 0.51              |
| 2:F:26:HIS:CD2   | 2:F:33:HIS:HE1   | 2.26                     | 0.51              |
| 2:C:46:ALA:H     | 2:C:105:THR:HB   | 1.75                     | 0.51              |
| 2:C:403:ARG:HE   | 2:D:231:PRO:HB2  | 1.76                     | 0.51              |
| 2:A:26:HIS:CE1   | 2:A:68:ILE:HB    | 2.46                     | 0.51              |
| 2:A:363:ARG:HD2  | 2:A:403:ARG:HB2  | 1.93                     | 0.51              |
| 2:A:777:LEU:HD22 | 2:A:792:ILE:HG21 | 1.93                     | 0.51              |
| 2:C:303:SER:HB3  | 2:C:309:LEU:HB2  | 1.92                     | 0.51              |
| 2:D:619:ILE:HG23 | 2:D:627:PHE:CE1  | 2.26                     | 0.51              |
| 2:C:254:ARG:HD3  | 2:C:254:ARG:H    | 1.76                     | 0.51              |
| 2:D:109:LEU:HD23 | 2:D:138:VAL:HG22 | 1.92                     | 0.51              |
| 2:E:363:ARG:CZ   | 2:E:471:VAL:HA   | 2.41                     | 0.51              |
| 2:A:731:THR:HG22 | 2:A:741:ILE:O    | 2.10                     | 0.51              |
| 2:F:507:HIS:CD2  | 2:F:517:VAL:HG11 | 2.46                     | 0.51              |
| 2:F:355:ARG:HB3  | 2:F:365:SER:HA   | 1.92                     | 0.50              |
| 1:3:142:LEU:HD22 | 1:3:209:LEU:HD13 | 1.93                     | 0.50              |
| 2:F:398:ALA:HB1  | 2:F:475:ASP:HB3  | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:4:140:ILE:HG21 | 2:D:443:ARG:HE   | 1.76                     | 0.50              |
| 2:C:742:GLU:HB3  | 2:C:791:HIS:CE1  | 2.46                     | 0.50              |
| 2:A:192:VAL:HG13 | 2:A:204:PRO:HG2  | 1.93                     | 0.50              |
| 2:B:423:VAL:HG11 | 2:B:445:THR:HB   | 1.94                     | 0.50              |
| 2:B:743:LEU:HD21 | 2:B:773:VAL:HG22 | 1.93                     | 0.50              |
| 2:C:743:LEU:HG   | 2:C:794:LEU:HD23 | 1.93                     | 0.50              |
| 2:E:394:LEU:HD13 | 2:E:480:VAL:HG22 | 1.92                     | 0.50              |
| 1:4:164:TYR:CG   | 1:4:193:ILE:HD13 | 2.46                     | 0.50              |
| 2:B:93:ASP:HB3   | 2:C:158:ALA:H    | 1.77                     | 0.50              |
| 2:C:26:HIS:CE1   | 2:C:68:ILE:HB    | 2.46                     | 0.50              |
| 2:C:619:ILE:HG23 | 2:C:622:ALA:CB   | 2.41                     | 0.50              |
| 2:E:543:PHE:HB2  | 2:E:657:THR:HA   | 1.92                     | 0.50              |
| 2:B:38:LEU:O     | 2:B:47:ALA:HB2   | 2.12                     | 0.50              |
| 2:E:685:MET:O    | 2:E:689:VAL:HG23 | 2.11                     | 0.50              |
| 2:F:195:VAL:HA   | 2:F:198:ARG:HE   | 1.76                     | 0.50              |
| 2:F:498:LYS:HB2  | 2:F:528:ARG:HH12 | 1.76                     | 0.50              |
| 1:3:136:PHE:CG   | 2:C:431:VAL:HG11 | 2.47                     | 0.50              |
| 2:A:544:LEU:HD22 | 2:A:660:VAL:HG12 | 1.93                     | 0.50              |
| 2:E:29:ILE:HA    | 2:E:33:HIS:HD1   | 1.77                     | 0.50              |
| 2:A:348:ILE:HG22 | 2:A:352:GLN:HE21 | 1.77                     | 0.50              |
| 2:B:424:ARG:HE   | 2:B:427:LYS:HD3  | 1.77                     | 0.50              |
| 2:B:727:SER:HB3  | 2:B:743:LEU:HD13 | 1.94                     | 0.50              |
| 2:D:45:ILE:HG22  | 2:D:138:VAL:HG12 | 1.94                     | 0.50              |
| 2:E:371:ILE:O    | 2:E:374:ALA:HB3  | 2.12                     | 0.50              |
| 2:F:18:GLN:O     | 2:F:21:ALA:HB3   | 2.12                     | 0.50              |
| 2:F:36:LEU:HB3   | 2:F:40:ARG:HE    | 1.77                     | 0.50              |
| 2:D:627:PHE:HB2  | 2:D:698:ARG:HE   | 1.77                     | 0.49              |
| 2:A:46:ALA:HB2   | 2:A:105:THR:O    | 2.12                     | 0.49              |
| 2:C:370:ALA:HB1  | 2:C:471:VAL:HG13 | 1.94                     | 0.49              |
| 2:E:98:LEU:CD1   | 2:E:110:LEU:HD13 | 2.42                     | 0.49              |
| 2:F:394:LEU:HD23 | 2:F:479:VAL:HG22 | 1.94                     | 0.49              |
| 1:5:142:LEU:HD11 | 1:5:182:LEU:HD22 | 1.94                     | 0.49              |
| 2:F:184:GLY:HA2  | 2:F:185:ARG:HB2  | 1.94                     | 0.49              |
| 1:2:203:ILE:HG23 | 2:B:434:GLN:HE21 | 1.78                     | 0.49              |
| 2:A:20:GLU:HB3   | 2:A:33:HIS:CD2   | 2.47                     | 0.49              |
| 2:B:39:VAL:HG11  | 2:B:60:ILE:HD12  | 1.93                     | 0.49              |
| 2:B:571:ARG:NE   | 2:B:617:ASP:OD2  | 2.46                     | 0.49              |
| 2:C:36:LEU:HB3   | 2:C:40:ARG:HE    | 1.78                     | 0.49              |
| 2:D:371:ILE:O    | 2:D:374:ALA:HB3  | 2.13                     | 0.49              |
| 2:E:18:GLN:O     | 2:E:21:ALA:HB3   | 2.12                     | 0.49              |
| 1:2:136:PHE:CE2  | 1:2:216:PHE:CD2  | 3.00                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:777:LEU:CD2  | 2:A:792:ILE:HG21 | 2.43                     | 0.49              |
| 2:B:506:LEU:HB2  | 2:B:517:VAL:HG13 | 1.95                     | 0.49              |
| 2:E:49:ALA:O     | 2:E:53:LEU:HD22  | 2.13                     | 0.49              |
| 2:B:303:SER:HB3  | 2:B:309:LEU:HB2  | 1.95                     | 0.49              |
| 1:5:216:PHE:CE1  | 2:E:440:ALA:HA   | 2.48                     | 0.49              |
| 2:B:355:ARG:CD   | 2:B:366:ILE:H    | 2.25                     | 0.49              |
| 2:B:355:ARG:CG   | 2:B:366:ILE:H    | 2.26                     | 0.49              |
| 2:C:355:ARG:HB2  | 2:C:364:VAL:HG12 | 1.94                     | 0.49              |
| 1:4:195:ARG:HA   | 1:4:195:ARG:HH21 | 1.78                     | 0.49              |
| 2:A:631:LEU:HD13 | 2:A:698:ARG:HH12 | 1.78                     | 0.49              |
| 2:B:36:LEU:HD11  | 2:B:64:VAL:HG11  | 1.95                     | 0.49              |
| 2:D:398:ALA:HB1  | 2:D:475:ASP:CB   | 2.42                     | 0.49              |
| 1:3:152:THR:OG1  | 1:3:163:LEU:HD21 | 2.13                     | 0.48              |
| 2:C:285:ILE:HD11 | 2:C:323:TYR:CE1  | 2.47                     | 0.48              |
| 2:E:98:LEU:HD12  | 2:E:110:LEU:HD13 | 1.94                     | 0.48              |
| 2:E:544:LEU:HD23 | 2:E:689:VAL:HG11 | 1.95                     | 0.48              |
| 2:F:26:HIS:CG    | 2:F:33:HIS:HE1   | 2.30                     | 0.48              |
| 2:A:743:LEU:HD11 | 2:A:773:VAL:CG2  | 2.43                     | 0.48              |
| 2:B:46:ALA:HB2   | 2:B:105:THR:O    | 2.13                     | 0.48              |
| 2:B:198:ARG:HB2  | 2:B:202:ASN:HA   | 1.95                     | 0.48              |
| 2:D:522:LYS:HA   | 2:D:525:ARG:HE   | 1.78                     | 0.48              |
| 2:D:741:ILE:HD13 | 2:D:777:LEU:CD1  | 2.43                     | 0.48              |
| 1:1:142:LEU:HD23 | 1:1:185:TYR:CE2  | 2.48                     | 0.48              |
| 1:4:136:PHE:CE2  | 1:4:216:PHE:CE2  | 3.02                     | 0.48              |
| 2:C:364:VAL:HG22 | 2:C:471:VAL:CG2  | 2.43                     | 0.48              |
| 2:C:387:LEU:HD12 | 2:C:387:LEU:H    | 1.78                     | 0.48              |
| 1:6:139:VAL:HG11 | 1:6:154:LEU:HD13 | 1.96                     | 0.48              |
| 2:A:77:THR:HG21  | 2:A:450:ARG:HH22 | 1.79                     | 0.48              |
| 2:A:619:ILE:HG22 | 2:A:697:PHE:CE1  | 2.47                     | 0.48              |
| 2:D:639:LEU:HD13 | 2:D:640:THR:H    | 1.79                     | 0.48              |
| 2:B:619:ILE:CD1  | 2:B:656:MET:CB   | 2.75                     | 0.48              |
| 2:D:715:GLU:HB3  | 2:D:717:LYS:HZ3  | 1.79                     | 0.48              |
| 2:E:21:ALA:HB2   | 2:E:29:ILE:HG12  | 1.94                     | 0.48              |
| 2:E:46:ALA:HB2   | 2:E:105:THR:O    | 2.13                     | 0.48              |
| 2:F:667:ARG:HH22 | 2:F:684:ASP:HB2  | 1.78                     | 0.48              |
| 1:3:164:TYR:CD1  | 1:3:193:ILE:HD13 | 2.48                     | 0.48              |
| 2:D:627:PHE:HB3  | 2:D:701:PHE:CG   | 2.48                     | 0.48              |
| 1:5:203:ILE:HG23 | 2:E:434:GLN:OE1  | 2.14                     | 0.48              |
| 2:A:53:LEU:HD21  | 2:A:134:ALA:HA   | 1.95                     | 0.48              |
| 2:B:361:HIS:HA   | 2:C:233:ILE:HA   | 1.96                     | 0.48              |
| 2:D:377:LEU:HD21 | 2:D:492:ALA:HA   | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:751:VAL:HG22 | 2:D:772:HIS:CD2  | 2.49                     | 0.48              |
| 2:D:762:ALA:HB1  | 2:D:765:LEU:CD1  | 2.43                     | 0.48              |
| 2:D:483:TRP:HE1  | 2:E:198:ARG:HH22 | 1.62                     | 0.48              |
| 2:E:188:GLU:HG3  | 2:E:339:VAL:HA   | 1.95                     | 0.48              |
| 1:3:136:PHE:CE2  | 1:3:216:PHE:CD2  | 3.02                     | 0.47              |
| 1:3:153:THR:O    | 1:3:163:LEU:HD22 | 2.14                     | 0.47              |
| 2:A:49:ALA:O     | 2:A:53:LEU:HD22  | 2.14                     | 0.47              |
| 2:F:38:LEU:O     | 2:F:47:ALA:HB2   | 2.14                     | 0.47              |
| 2:F:705:ILE:HG21 | 2:F:708:ILE:HD13 | 1.95                     | 0.47              |
| 1:1:142:LEU:HD23 | 1:1:185:TYR:CD2  | 2.49                     | 0.47              |
| 2:C:38:LEU:O     | 2:C:47:ALA:HB2   | 2.13                     | 0.47              |
| 2:C:619:ILE:HD12 | 2:C:656:MET:HB3  | 1.95                     | 0.47              |
| 2:E:100:HIS:HB2  | 2:E:107:HIS:CE1  | 2.48                     | 0.47              |
| 2:E:506:LEU:HB2  | 2:E:517:VAL:HG13 | 1.96                     | 0.47              |
| 2:F:751:VAL:HG22 | 2:F:772:HIS:HB3  | 1.95                     | 0.47              |
| 2:F:563:PHE:CE1  | 2:F:611:TYR:CD1  | 3.02                     | 0.47              |
| 2:A:507:HIS:CD2  | 2:A:517:VAL:HG11 | 2.50                     | 0.47              |
| 2:C:98:LEU:HD11  | 2:C:139:LEU:HD22 | 1.96                     | 0.47              |
| 2:F:27:ASN:HA    | 2:F:75:SER:HA    | 1.97                     | 0.47              |
| 2:A:394:LEU:HD11 | 2:A:483:TRP:CZ3  | 2.49                     | 0.47              |
| 2:B:370:ALA:HB1  | 2:B:476:ILE:HD12 | 1.96                     | 0.47              |
| 2:C:484:THR:HG23 | 2:C:611:TYR:CE2  | 2.48                     | 0.47              |
| 2:F:543:PHE:HB2  | 2:F:657:THR:HG22 | 1.95                     | 0.47              |
| 1:1:140:ILE:HG21 | 2:A:443:ARG:HD2  | 1.97                     | 0.47              |
| 1:1:180:SER:HB3  | 2:A:68:ILE:HD11  | 1.96                     | 0.47              |
| 2:B:27:ASN:HA    | 2:B:75:SER:HA    | 1.97                     | 0.47              |
| 2:F:431:VAL:HG22 | 2:F:439:ALA:HB1  | 1.97                     | 0.47              |
| 1:3:154:LEU:HD22 | 1:3:212:ILE:HD11 | 1.96                     | 0.47              |
| 1:3:195:ARG:HH21 | 2:D:144:SER:H    | 1.62                     | 0.47              |
| 1:3:204:ILE:HD11 | 1:3:212:ILE:HD11 | 1.96                     | 0.47              |
| 2:A:363:ARG:HE   | 2:A:467:GLU:HB3  | 1.79                     | 0.47              |
| 2:A:364:VAL:HG11 | 2:A:471:VAL:HG21 | 1.96                     | 0.47              |
| 2:A:743:LEU:HD12 | 2:A:794:LEU:HD13 | 1.96                     | 0.47              |
| 2:D:623:HIS:CD2  | 2:D:624:PRO:HD2  | 2.49                     | 0.47              |
| 2:E:271:ALA:HB2  | 2:E:308:GLU:HA   | 1.96                     | 0.47              |
| 2:A:747:ALA:HB1  | 2:A:801:PHE:CZ   | 2.50                     | 0.47              |
| 2:B:403:ARG:HG2  | 2:B:403:ARG:HH11 | 1.80                     | 0.47              |
| 2:E:670:TYR:CE1  | 2:E:756:VAL:HG13 | 2.50                     | 0.47              |
| 2:C:18:GLN:O     | 2:C:21:ALA:HB3   | 2.14                     | 0.47              |
| 2:C:403:ARG:HE   | 2:D:231:PRO:CB   | 2.27                     | 0.47              |
| 2:E:623:HIS:CD2  | 2:E:624:PRO:HD2  | 2.50                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:743:LEU:HD11 | 2:E:773:VAL:HG22 | 1.97                     | 0.47              |
| 2:F:786:ILE:HG21 | 2:F:792:ILE:HG23 | 1.97                     | 0.47              |
| 2:A:381:TYR:HB2  | 2:A:484:THR:HG21 | 1.97                     | 0.46              |
| 2:B:95:ALA:HB2   | 2:B:107:HIS:CG   | 2.50                     | 0.46              |
| 2:B:100:HIS:HB2  | 2:B:107:HIS:CE1  | 2.50                     | 0.46              |
| 2:C:363:ARG:HH21 | 2:C:470:GLU:CD   | 2.18                     | 0.46              |
| 2:D:362:HIS:O    | 2:E:233:ILE:HD11 | 2.15                     | 0.46              |
| 2:B:60:ILE:HG23  | 2:B:123:VAL:HG11 | 1.97                     | 0.46              |
| 2:B:751:VAL:HG22 | 2:B:772:HIS:HB2  | 1.97                     | 0.46              |
| 2:E:109:LEU:HD23 | 2:E:138:VAL:CG2  | 2.45                     | 0.46              |
| 2:A:413:LEU:HB2  | 2:A:460:TRP:HE1  | 1.81                     | 0.46              |
| 2:A:563:PHE:CD2  | 2:A:611:TYR:CD1  | 3.04                     | 0.46              |
| 2:D:427:LYS:HA   | 2:D:442:LEU:HB2  | 1.98                     | 0.46              |
| 2:A:276:LEU:HD23 | 2:A:309:LEU:HA   | 1.97                     | 0.46              |
| 2:B:402:VAL:HG23 | 2:B:475:ASP:OD1  | 2.16                     | 0.46              |
| 2:A:420:LEU:O    | 2:A:420:LEU:HD23 | 2.16                     | 0.46              |
| 2:C:423:VAL:HG11 | 2:C:445:THR:HB   | 1.97                     | 0.46              |
| 2:F:31:THR:HB    | 2:F:120:ALA:HB2  | 1.96                     | 0.46              |
| 1:2:142:LEU:HD21 | 1:2:182:LEU:HG   | 1.98                     | 0.46              |
| 2:B:139:LEU:O    | 2:B:142:LEU:HD13 | 2.16                     | 0.46              |
| 2:C:660:VAL:HG21 | 2:C:697:PHE:CE2  | 2.51                     | 0.46              |
| 2:E:787:HIS:H    | 2:E:790:GLN:HG2  | 1.80                     | 0.46              |
| 2:A:559:ALA:HA   | 2:A:563:PHE:CD1  | 2.51                     | 0.46              |
| 2:C:619:ILE:HG21 | 2:C:627:PHE:HE1  | 1.78                     | 0.46              |
| 2:D:17:ALA:HB1   | 2:D:29:ILE:CG2   | 2.46                     | 0.46              |
| 2:E:727:SER:O    | 2:E:731:THR:HG23 | 2.16                     | 0.46              |
| 1:2:142:LEU:HD22 | 1:2:146:ASN:HB2  | 1.98                     | 0.46              |
| 1:4:154:LEU:HD22 | 1:4:212:ILE:HD11 | 1.98                     | 0.46              |
| 2:A:109:LEU:HD23 | 2:A:138:VAL:HG22 | 1.97                     | 0.46              |
| 2:B:623:HIS:CD2  | 2:B:624:PRO:HD2  | 2.51                     | 0.46              |
| 2:B:747:ALA:HB1  | 2:B:801:PHE:CE1  | 2.51                     | 0.46              |
| 2:D:363:ARG:NH1  | 2:D:399:GLY:HA2  | 2.30                     | 0.46              |
| 2:F:665:LEU:HG   | 2:F:689:VAL:HG21 | 1.98                     | 0.46              |
| 1:2:136:PHE:CD1  | 2:B:431:VAL:HG11 | 2.51                     | 0.46              |
| 2:A:374:ALA:CA   | 2:A:476:ILE:HG21 | 2.45                     | 0.46              |
| 2:A:396:ASP:HB3  | 2:B:198:ARG:HB3  | 1.96                     | 0.46              |
| 2:A:619:ILE:CG2  | 2:A:619:ILE:O    | 2.63                     | 0.46              |
| 2:B:87:VAL:HG13  | 2:B:112:LEU:HA   | 1.97                     | 0.46              |
| 2:B:20:GLU:HB3   | 2:B:23:ARG:HH21  | 1.80                     | 0.45              |
| 2:B:26:HIS:CE1   | 2:B:68:ILE:HB    | 2.50                     | 0.45              |
| 2:D:34:ILE:HD11  | 2:D:84:ALA:HB1   | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:571:ARG:NE   | 2:D:617:ASP:OD2  | 2.49                     | 0.45              |
| 2:D:777:LEU:HD21 | 2:D:794:LEU:HD11 | 1.97                     | 0.45              |
| 2:E:574:MET:SD   | 2:E:626:VAL:HG11 | 2.56                     | 0.45              |
| 2:E:739:LEU:HD11 | 2:E:792:ILE:HD11 | 1.98                     | 0.45              |
| 2:B:406:SER:HB3  | 2:B:407:PHE:CD1  | 2.51                     | 0.45              |
| 2:B:727:SER:O    | 2:B:731:THR:HG23 | 2.16                     | 0.45              |
| 2:C:542:ILE:CG1  | 2:C:705:ILE:HD13 | 2.46                     | 0.45              |
| 2:D:21:ALA:HB2   | 2:D:29:ILE:HD11  | 1.98                     | 0.45              |
| 2:D:370:ALA:HB1  | 2:D:471:VAL:HG13 | 1.99                     | 0.45              |
| 2:D:723:VAL:HG21 | 2:D:752:ALA:HA   | 1.97                     | 0.45              |
| 2:E:352:GLN:HG3  | 2:E:371:ILE:HG21 | 1.98                     | 0.45              |
| 2:F:751:VAL:HA   | 2:F:772:HIS:CD2  | 2.52                     | 0.45              |
| 1:2:164:TYR:CD1  | 1:2:193:ILE:HD13 | 2.50                     | 0.45              |
| 2:A:199:ARG:H    | 2:F:396:ASP:HB3  | 1.80                     | 0.45              |
| 2:B:26:HIS:HE1   | 2:B:68:ILE:HB    | 1.81                     | 0.45              |
| 2:E:32:GLU:HB2   | 2:E:64:VAL:HG13  | 1.97                     | 0.45              |
| 1:4:137:GLU:HA   | 1:4:140:ILE:HD12 | 1.99                     | 0.45              |
| 1:4:203:ILE:CG2  | 2:D:434:GLN:HE21 | 2.29                     | 0.45              |
| 1:5:136:PHE:CE2  | 1:5:203:ILE:HG21 | 2.51                     | 0.45              |
| 2:A:355:ARG:HD3  | 2:A:366:ILE:H    | 1.82                     | 0.45              |
| 2:C:410:PRO:HG2  | 2:C:412:ASN:H    | 1.82                     | 0.45              |
| 2:E:106:GLU:HG3  | 2:E:107:HIS:CD2  | 2.52                     | 0.45              |
| 2:F:100:HIS:CD2  | 2:F:107:HIS:CE1  | 3.04                     | 0.45              |
| 2:F:751:VAL:HG22 | 2:F:772:HIS:HB2  | 1.99                     | 0.45              |
| 2:A:38:LEU:O     | 2:A:47:ALA:HB2   | 2.17                     | 0.45              |
| 2:B:348:ILE:HG22 | 2:B:352:GLN:HE21 | 1.82                     | 0.45              |
| 2:B:394:LEU:HD23 | 2:B:479:VAL:HG22 | 1.97                     | 0.45              |
| 2:A:685:MET:HA   | 2:A:689:VAL:HG23 | 1.99                     | 0.45              |
| 2:C:661:GLY:HA2  | 2:C:689:VAL:HG22 | 1.99                     | 0.45              |
| 2:A:363:ARG:HA   | 2:A:468:ASN:HA   | 1.99                     | 0.45              |
| 2:B:743:LEU:HB3  | 2:B:747:ALA:HB3  | 1.98                     | 0.45              |
| 2:E:483:TRP:HE1  | 2:F:198:ARG:HH12 | 1.63                     | 0.45              |
| 2:E:674:ASN:HB3  | 2:E:676:GLN:H    | 1.82                     | 0.45              |
| 2:F:100:HIS:HB3  | 2:F:107:HIS:CE1  | 2.51                     | 0.45              |
| 2:F:587:VAL:HG22 | 2:F:589:SER:H    | 1.82                     | 0.45              |
| 2:F:616:LEU:CB   | 2:F:619:ILE:HD11 | 2.46                     | 0.45              |
| 2:C:363:ARG:HG3  | 2:C:403:ARG:HB2  | 1.98                     | 0.45              |
| 2:E:476:ILE:O    | 2:E:480:VAL:HG23 | 2.17                     | 0.45              |
| 1:6:142:LEU:HD23 | 1:6:182:LEU:HA   | 1.97                     | 0.45              |
| 2:C:403:ARG:HG3  | 2:D:231:PRO:HB3  | 1.99                     | 0.45              |
| 2:C:574:MET:CG   | 2:C:619:ILE:HG12 | 2.46                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:394:LEU:HD23 | 2:E:479:VAL:HG22 | 1.99                     | 0.45              |
| 2:D:53:LEU:HB3   | 2:D:129:VAL:HG21 | 1.99                     | 0.45              |
| 2:D:278:ILE:HD11 | 2:D:309:LEU:HD23 | 1.99                     | 0.45              |
| 1:1:133:PHE:CE2  | 1:1:163:LEU:HD12 | 2.52                     | 0.44              |
| 2:A:32:GLU:HG2   | 2:A:33:HIS:CD2   | 2.52                     | 0.44              |
| 2:A:371:ILE:O    | 2:A:374:ALA:HB3  | 2.17                     | 0.44              |
| 2:A:619:ILE:HG23 | 2:A:627:PHE:HE1  | 1.81                     | 0.44              |
| 2:B:363:ARG:HH12 | 2:B:471:VAL:HA   | 1.82                     | 0.44              |
| 2:D:731:THR:HG22 | 2:D:741:ILE:HD12 | 1.99                     | 0.44              |
| 2:D:777:LEU:CD2  | 2:D:792:ILE:HG21 | 2.47                     | 0.44              |
| 2:E:26:HIS:CE1   | 2:E:68:ILE:HB    | 2.52                     | 0.44              |
| 2:F:623:HIS:CD2  | 2:F:624:PRO:HD2  | 2.52                     | 0.44              |
| 1:6:204:ILE:HG21 | 1:6:211:THR:HB   | 2.00                     | 0.44              |
| 2:A:113:ILE:HG21 | 2:A:135:ARG:HB2  | 2.00                     | 0.44              |
| 2:A:510:VAL:HG21 | 2:A:554:LEU:HA   | 1.99                     | 0.44              |
| 2:E:355:ARG:HG3  | 2:E:371:ILE:HD11 | 1.99                     | 0.44              |
| 1:4:181:ILE:H    | 1:4:181:ILE:HD12 | 1.81                     | 0.44              |
| 2:A:665:LEU:HD21 | 2:A:689:VAL:HG21 | 1.99                     | 0.44              |
| 2:C:714:LEU:HD22 | 2:C:718:HIS:CD2  | 2.51                     | 0.44              |
| 2:D:77:THR:HB    | 2:D:79:HIS:CD2   | 2.53                     | 0.44              |
| 2:D:624:PRO:HA   | 2:D:627:PHE:CD2  | 2.52                     | 0.44              |
| 2:E:394:LEU:HD21 | 2:E:483:TRP:CZ2  | 2.53                     | 0.44              |
| 2:F:100:HIS:CD2  | 2:F:107:HIS:HE1  | 2.35                     | 0.44              |
| 2:F:669:LYS:HG2  | 2:F:712:HIS:CE1  | 2.52                     | 0.44              |
| 2:A:665:LEU:CD2  | 2:A:689:VAL:HG21 | 2.48                     | 0.44              |
| 2:B:420:LEU:HD13 | 2:B:453:VAL:HG21 | 1.99                     | 0.44              |
| 2:B:693:LEU:O    | 2:B:697:PHE:CD2  | 2.70                     | 0.44              |
| 2:D:394:LEU:CD1  | 2:D:480:VAL:HG22 | 2.47                     | 0.44              |
| 2:F:417:GLU:H    | 2:F:417:GLU:CD   | 2.21                     | 0.44              |
| 2:F:420:LEU:O    | 2:F:420:LEU:HD23 | 2.18                     | 0.44              |
| 1:3:139:VAL:CG1  | 1:3:212:ILE:HD13 | 2.47                     | 0.44              |
| 2:D:26:HIS:HB2   | 2:D:33:HIS:HE1   | 1.83                     | 0.44              |
| 2:E:55:LEU:HD11  | 2:E:129:VAL:HG11 | 2.00                     | 0.44              |
| 1:1:203:ILE:HG22 | 1:1:204:ILE:HD13 | 1.99                     | 0.44              |
| 1:5:204:ILE:HD11 | 1:5:212:ILE:HD11 | 1.99                     | 0.44              |
| 2:A:431:VAL:HG13 | 2:A:439:ALA:HB1  | 1.99                     | 0.44              |
| 2:B:45:ILE:HG22  | 2:B:138:VAL:HG12 | 2.00                     | 0.44              |
| 2:B:282:HIS:CE1  | 2:B:283:THR:HG23 | 2.52                     | 0.44              |
| 2:C:6:PHE:HA     | 2:C:102:TYR:HA   | 2.00                     | 0.44              |
| 2:C:371:ILE:O    | 2:C:374:ALA:HB3  | 2.17                     | 0.44              |
| 2:E:10:ALA:HB1   | 2:E:108:ILE:HD11 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:579:GLU:HA   | 2:E:593:TYR:CD2  | 2.53                     | 0.44              |
| 2:A:363:ARG:HH11 | 2:A:399:GLY:HA2  | 1.82                     | 0.44              |
| 2:A:631:LEU:HA   | 2:A:634:LEU:HD22 | 2.00                     | 0.44              |
| 2:D:660:VAL:HG21 | 2:D:696:ALA:HB2  | 1.99                     | 0.44              |
| 2:E:382:ILE:HG12 | 2:E:651:ASN:HD21 | 1.82                     | 0.44              |
| 2:F:468:ASN:HD22 | 2:F:468:ASN:H    | 1.65                     | 0.44              |
| 2:F:739:LEU:HD11 | 2:F:792:ILE:HD11 | 1.98                     | 0.44              |
| 2:A:20:GLU:HB2   | 2:A:33:HIS:CG    | 2.52                     | 0.44              |
| 2:A:53:LEU:HD11  | 2:A:137:GLN:HB2  | 2.00                     | 0.44              |
| 2:B:59:LYS:HG2   | 2:B:127:LEU:HD22 | 1.99                     | 0.44              |
| 2:C:32:GLU:HB2   | 2:C:64:VAL:HG13  | 1.99                     | 0.44              |
| 2:C:476:ILE:O    | 2:C:480:VAL:HG23 | 2.18                     | 0.44              |
| 2:E:20:GLU:HB3   | 2:E:33:HIS:CD2   | 2.52                     | 0.44              |
| 2:B:619:ILE:HG22 | 2:B:619:ILE:O    | 2.18                     | 0.44              |
| 2:C:55:LEU:HD11  | 2:C:129:VAL:HG11 | 1.99                     | 0.44              |
| 2:E:398:ALA:HB1  | 2:E:475:ASP:HB3  | 2.00                     | 0.44              |
| 2:A:351:LEU:HD22 | 2:A:392:ILE:HG12 | 1.99                     | 0.43              |
| 2:B:32:GLU:HB2   | 2:B:64:VAL:HG13  | 2.00                     | 0.43              |
| 2:B:402:VAL:HG22 | 2:B:405:ARG:CZ   | 2.48                     | 0.43              |
| 2:C:24:LEU:HD13  | 2:C:69:GLY:HA2   | 2.00                     | 0.43              |
| 2:C:384:ASP:HB3  | 2:C:385:ARG:HE   | 1.82                     | 0.43              |
| 2:A:510:VAL:HG12 | 2:A:512:GLY:H    | 1.84                     | 0.43              |
| 2:A:639:LEU:HD23 | 2:A:640:THR:H    | 1.83                     | 0.43              |
| 2:A:702:ILE:HA   | 2:A:705:ILE:HD12 | 2.01                     | 0.43              |
| 2:C:398:ALA:C    | 2:C:400:SER:H    | 2.21                     | 0.43              |
| 2:D:394:LEU:HD21 | 2:D:483:TRP:CH2  | 2.53                     | 0.43              |
| 2:D:619:ILE:HG22 | 2:D:619:ILE:O    | 2.17                     | 0.43              |
| 2:A:231:PRO:HB2  | 2:F:403:ARG:HD3  | 2.00                     | 0.43              |
| 2:B:371:ILE:O    | 2:B:374:ALA:HB3  | 2.18                     | 0.43              |
| 2:B:399:GLY:O    | 2:C:233:ILE:HD11 | 2.17                     | 0.43              |
| 2:C:198:ARG:HD2  | 2:C:202:ASN:HA   | 1.99                     | 0.43              |
| 2:E:59:LYS:HG2   | 2:E:127:LEU:HD22 | 1.99                     | 0.43              |
| 2:F:21:ALA:HA    | 2:F:33:HIS:ND1   | 2.33                     | 0.43              |
| 1:6:133:PHE:CZ   | 1:6:186:ALA:HB2  | 2.52                     | 0.43              |
| 1:6:153:THR:O    | 1:6:163:LEU:HD22 | 2.18                     | 0.43              |
| 2:A:402:VAL:HG21 | 2:A:475:ASP:CG   | 2.38                     | 0.43              |
| 2:D:193:ILE:HD13 | 2:D:225:ILE:HG12 | 2.00                     | 0.43              |
| 2:D:701:PHE:CZ   | 2:D:705:ILE:HD11 | 2.54                     | 0.43              |
| 2:E:623:HIS:CG   | 2:E:624:PRO:HD2  | 2.53                     | 0.43              |
| 2:F:59:LYS:HG2   | 2:F:127:LEU:HD22 | 1.99                     | 0.43              |
| 1:3:133:PHE:CD2  | 1:3:139:VAL:HG22 | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:301:LYS:HB2  | 2:B:302:PRO:HD3  | 2.00                     | 0.43              |
| 2:C:348:ILE:HG21 | 2:C:372:GLU:HG2  | 2.01                     | 0.43              |
| 2:C:627:PHE:HB2  | 2:C:698:ARG:HE   | 1.83                     | 0.43              |
| 2:D:712:HIS:H    | 2:D:712:HIS:CD2  | 2.35                     | 0.43              |
| 2:E:6:PHE:HA     | 2:E:102:TYR:HA   | 2.00                     | 0.43              |
| 2:E:520:VAL:HG11 | 2:E:558:LEU:HD11 | 2.01                     | 0.43              |
| 2:E:627:PHE:HB3  | 2:E:701:PHE:CG   | 2.53                     | 0.43              |
| 2:A:588:GLY:HA3  | 2:B:594:VAL:H    | 1.84                     | 0.43              |
| 2:B:374:ALA:HA   | 2:B:394:LEU:HD12 | 2.01                     | 0.43              |
| 2:C:381:TYR:HB2  | 2:C:611:TYR:CE2  | 2.54                     | 0.43              |
| 2:E:21:ALA:CB    | 2:E:29:ILE:HG12  | 2.49                     | 0.43              |
| 2:E:110:LEU:HD23 | 2:E:135:ARG:HG2  | 2.00                     | 0.43              |
| 1:3:140:ILE:HD11 | 1:3:216:PHE:CD1  | 2.54                     | 0.43              |
| 1:6:137:GLU:HA   | 1:6:140:ILE:HD12 | 2.00                     | 0.43              |
| 2:C:730:LEU:HD11 | 2:C:774:GLU:HG2  | 2.00                     | 0.43              |
| 2:D:580:LYS:HD3  | 2:D:581:HIS:CE1  | 2.54                     | 0.43              |
| 2:D:665:LEU:HD22 | 2:D:712:HIS:HA   | 2.00                     | 0.43              |
| 2:B:394:LEU:HD21 | 2:B:483:TRP:CH2  | 2.54                     | 0.43              |
| 2:B:406:SER:HB2  | 2:B:463:LYS:HE2  | 2.01                     | 0.43              |
| 2:F:31:THR:HG23  | 2:F:83:ARG:HG3   | 2.01                     | 0.43              |
| 2:F:402:VAL:HG12 | 2:F:467:GLU:HB3  | 2.00                     | 0.43              |
| 2:F:664:GLU:HA   | 2:F:667:ARG:HE   | 1.84                     | 0.43              |
| 2:B:742:GLU:OE1  | 2:B:793:VAL:HG13 | 2.19                     | 0.43              |
| 2:C:363:ARG:HH12 | 2:C:475:ASP:HB3  | 1.84                     | 0.43              |
| 2:D:22:LEU:HD12  | 2:D:22:LEU:H     | 1.82                     | 0.43              |
| 2:D:510:VAL:HG12 | 2:D:512:GLY:H    | 1.84                     | 0.43              |
| 2:C:410:PRO:HB2  | 2:C:411:PRO:HD2  | 2.00                     | 0.43              |
| 2:E:367:THR:O    | 2:E:370:ALA:HB3  | 2.19                     | 0.43              |
| 2:E:394:LEU:HD21 | 2:E:483:TRP:CE2  | 2.54                     | 0.43              |
| 2:F:53:LEU:HD21  | 2:F:134:ALA:HA   | 2.00                     | 0.43              |
| 2:A:363:ARG:HD2  | 2:A:403:ARG:H    | 1.83                     | 0.42              |
| 2:A:398:ALA:C    | 2:A:400:SER:H    | 2.22                     | 0.42              |
| 2:A:619:ILE:HD11 | 2:A:656:MET:CG   | 2.44                     | 0.42              |
| 2:B:407:PHE:CD1  | 2:C:229:GLU:HB3  | 2.53                     | 0.42              |
| 2:D:747:ALA:O    | 2:D:751:VAL:HG23 | 2.19                     | 0.42              |
| 2:A:20:GLU:CB    | 2:A:33:HIS:CD2   | 3.02                     | 0.42              |
| 2:D:6:PHE:CD2    | 2:D:103:VAL:HG23 | 2.54                     | 0.42              |
| 2:D:370:ALA:HB2  | 2:D:472:THR:HA   | 2.01                     | 0.42              |
| 2:E:359:GLU:HA   | 2:E:362:HIS:CD2  | 2.54                     | 0.42              |
| 2:E:397:GLU:CB   | 2:E:479:VAL:HG21 | 2.50                     | 0.42              |
| 2:F:192:VAL:HG13 | 2:F:204:PRO:HG2  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:5:144:LYS:HZ1  | 1:5:213:LYS:HA   | 1.85                     | 0.42              |
| 2:B:53:LEU:HD12  | 2:B:129:VAL:HG13 | 2.01                     | 0.42              |
| 2:B:546:PRO:HD2  | 2:B:549:VAL:HG21 | 1.99                     | 0.42              |
| 2:C:46:ALA:HB2   | 2:C:105:THR:O    | 2.19                     | 0.42              |
| 2:D:26:HIS:CD2   | 2:D:33:HIS:CE1   | 3.07                     | 0.42              |
| 2:E:410:PRO:HG2  | 2:E:413:LEU:H    | 1.85                     | 0.42              |
| 2:E:513:GLN:HA   | 2:E:718:HIS:CE1  | 2.54                     | 0.42              |
| 2:F:98:LEU:HD12  | 2:F:110:LEU:HD13 | 2.00                     | 0.42              |
| 1:5:175:VAL:HA   | 1:5:178:GLN:HE21 | 1.84                     | 0.42              |
| 2:A:46:ALA:HB1   | 2:A:109:LEU:HB2  | 2.00                     | 0.42              |
| 2:D:351:LEU:CD1  | 2:D:391:ALA:HB1  | 2.49                     | 0.42              |
| 2:D:742:GLU:HB3  | 2:D:791:HIS:CE1  | 2.54                     | 0.42              |
| 2:E:166:LEU:HA   | 2:E:167:ALA:CB   | 2.49                     | 0.42              |
| 1:1:216:PHE:HA   | 2:A:440:ALA:HB2  | 2.00                     | 0.42              |
| 2:A:22:LEU:HD22  | 2:A:22:LEU:H     | 1.85                     | 0.42              |
| 2:A:743:LEU:HB3  | 2:A:747:ALA:HB3  | 2.02                     | 0.42              |
| 2:F:371:ILE:O    | 2:F:374:ALA:HB3  | 2.20                     | 0.42              |
| 1:6:142:LEU:HB2  | 1:6:185:TYR:CD2  | 2.55                     | 0.42              |
| 2:B:571:ARG:NH2  | 2:B:617:ASP:OD2  | 2.52                     | 0.42              |
| 2:D:6:PHE:HA     | 2:D:102:TYR:HA   | 2.01                     | 0.42              |
| 2:D:271:ALA:HA   | 2:D:274:ILE:HG22 | 2.02                     | 0.42              |
| 2:D:392:ILE:HA   | 2:D:395:ILE:HD12 | 2.01                     | 0.42              |
| 2:D:549:VAL:HG13 | 2:D:714:LEU:CD2  | 2.49                     | 0.42              |
| 2:E:581:HIS:CE1  | 2:E:585:ARG:CZ   | 3.02                     | 0.42              |
| 2:F:100:HIS:CE1  | 2:F:102:TYR:HB2  | 2.55                     | 0.42              |
| 2:F:374:ALA:HB1  | 2:F:391:ALA:HA   | 2.01                     | 0.42              |
| 1:2:154:LEU:HB2  | 1:2:208:ALA:HB1  | 2.01                     | 0.42              |
| 1:2:215:HIS:HB2  | 2:B:436:PHE:HB3  | 2.00                     | 0.42              |
| 1:5:216:PHE:CE2  | 2:E:439:ALA:HB3  | 2.55                     | 0.42              |
| 2:B:113:ILE:HG21 | 2:B:135:ARG:HB2  | 2.01                     | 0.42              |
| 2:C:281:LEU:HG   | 2:C:285:ILE:HD13 | 2.01                     | 0.42              |
| 2:E:483:TRP:CD1  | 2:F:335:GLN:HG3  | 2.55                     | 0.42              |
| 2:F:46:ALA:H     | 2:F:105:THR:HB   | 1.84                     | 0.42              |
| 2:A:403:ARG:HA   | 2:A:467:GLU:HG3  | 2.01                     | 0.42              |
| 2:B:26:HIS:CD2   | 2:B:33:HIS:NE2   | 2.86                     | 0.42              |
| 2:B:743:LEU:HA   | 2:B:794:LEU:HB2  | 2.02                     | 0.42              |
| 2:B:777:LEU:HD11 | 2:B:794:LEU:HD11 | 2.02                     | 0.42              |
| 2:D:361:HIS:CG   | 2:E:233:ILE:HG23 | 2.55                     | 0.42              |
| 2:D:682:HIS:CD2  | 2:D:712:HIS:CE1  | 3.07                     | 0.42              |
| 2:E:370:ALA:HB2  | 2:E:472:THR:HA   | 2.00                     | 0.42              |
| 2:F:374:ALA:HB2  | 2:F:476:ILE:HG12 | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:786:ILE:HD12 | 2:A:792:ILE:HD13 | 2.00                     | 0.42              |
| 2:B:398:ALA:HB1  | 2:B:475:ASP:HB3  | 2.01                     | 0.42              |
| 2:B:427:LYS:HD2  | 2:B:443:ARG:HA   | 2.02                     | 0.42              |
| 2:D:627:PHE:HB3  | 2:D:701:PHE:CD2  | 2.55                     | 0.42              |
| 1:1:128:GLN:HG3  | 1:1:166:ASP:HA   | 2.02                     | 0.42              |
| 1:1:133:PHE:CZ   | 1:1:163:LEU:HD12 | 2.55                     | 0.42              |
| 2:A:739:LEU:HD21 | 2:A:792:ILE:HD11 | 2.02                     | 0.42              |
| 2:B:355:ARG:HA   | 2:B:358:TYR:CZ   | 2.55                     | 0.42              |
| 2:C:373:ALA:HB2  | 2:C:473:VAL:HG13 | 2.02                     | 0.42              |
| 2:E:634:LEU:HD22 | 2:E:701:PHE:CE1  | 2.54                     | 0.42              |
| 2:F:502:MET:HA   | 2:F:505:ILE:HG12 | 2.02                     | 0.42              |
| 2:A:142:LEU:HG   | 2:A:144:SER:H    | 1.85                     | 0.41              |
| 2:A:383:SER:H    | 2:A:390:LYS:CD   | 2.31                     | 0.41              |
| 2:B:507:HIS:CD2  | 2:B:517:VAL:CG1  | 3.02                     | 0.41              |
| 2:C:413:LEU:HB2  | 2:C:460:TRP:CZ2  | 2.55                     | 0.41              |
| 2:D:631:LEU:HA   | 2:D:634:LEU:HD22 | 2.02                     | 0.41              |
| 2:E:743:LEU:HD21 | 2:E:773:VAL:HG22 | 2.02                     | 0.41              |
| 2:F:382:ILE:H    | 2:F:383:SER:HB2  | 1.84                     | 0.41              |
| 2:F:392:ILE:HA   | 2:F:395:ILE:HD12 | 2.02                     | 0.41              |
| 2:B:183:ILE:HD12 | 2:B:350:ILE:HA   | 2.01                     | 0.41              |
| 2:C:361:HIS:CE1  | 2:C:396:ASP:HA   | 2.55                     | 0.41              |
| 2:D:20:GLU:HB2   | 2:D:33:HIS:CG    | 2.55                     | 0.41              |
| 2:E:366:ILE:HB   | 2:E:367:THR:HA   | 2.02                     | 0.41              |
| 2:F:395:ILE:HA   | 2:F:476:ILE:HD11 | 2.02                     | 0.41              |
| 2:A:165:SER:HB2  | 2:A:166:LEU:HB2  | 2.02                     | 0.41              |
| 2:D:714:LEU:HD12 | 2:D:762:ALA:HB2  | 2.02                     | 0.41              |
| 2:F:427:LYS:HG3  | 2:F:443:ARG:CA   | 2.48                     | 0.41              |
| 2:F:507:HIS:CE1  | 2:F:518:VAL:HG22 | 2.56                     | 0.41              |
| 2:B:106:GLU:CG   | 2:B:142:LEU:HD11 | 2.50                     | 0.41              |
| 2:B:476:ILE:O    | 2:B:479:VAL:HG13 | 2.21                     | 0.41              |
| 2:C:357:ARG:C    | 2:C:359:GLU:H    | 2.24                     | 0.41              |
| 2:D:427:LYS:HD3  | 2:D:427:LYS:C    | 2.41                     | 0.41              |
| 2:D:507:HIS:CE1  | 2:D:518:VAL:HG22 | 2.56                     | 0.41              |
| 2:D:747:ALA:HB1  | 2:D:801:PHE:CZ   | 2.56                     | 0.41              |
| 2:E:9:ARG:HB2    | 2:E:105:THR:HB   | 2.03                     | 0.41              |
| 2:E:303:SER:HB3  | 2:E:309:LEU:HB2  | 2.02                     | 0.41              |
| 2:F:53:LEU:HD12  | 2:F:129:VAL:HG13 | 2.02                     | 0.41              |
| 2:F:484:THR:HG22 | 2:F:563:PHE:HA   | 2.02                     | 0.41              |
| 1:1:140:ILE:HG23 | 1:1:216:PHE:HB3  | 2.03                     | 0.41              |
| 2:B:364:VAL:HG11 | 2:B:471:VAL:HG13 | 2.03                     | 0.41              |
| 2:E:445:THR:O    | 2:E:449:LEU:HD23 | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:474:ASP:HA   | 2:F:493:GLN:H    | 1.85                     | 0.41              |
| 1:6:210:GLU:CD   | 1:6:210:GLU:H    | 2.23                     | 0.41              |
| 2:C:304:LEU:HD22 | 2:C:311:CYS:SG   | 2.60                     | 0.41              |
| 2:C:417:GLU:CD   | 2:C:417:GLU:H    | 2.24                     | 0.41              |
| 2:D:21:ALA:HB2   | 2:D:29:ILE:CD1   | 2.51                     | 0.41              |
| 2:D:70:ARG:H     | 2:D:70:ARG:HD2   | 1.85                     | 0.41              |
| 2:D:400:SER:HA   | 2:E:233:ILE:HD12 | 2.02                     | 0.41              |
| 2:F:579:GLU:HA   | 2:F:593:TYR:CD1  | 2.55                     | 0.41              |
| 1:4:203:ILE:HG21 | 2:D:434:GLN:HE21 | 1.85                     | 0.41              |
| 1:6:127:LEU:CB   | 1:6:175:VAL:HG21 | 2.50                     | 0.41              |
| 2:B:26:HIS:CB    | 2:B:33:HIS:HE1   | 2.33                     | 0.41              |
| 2:B:627:PHE:CE2  | 2:B:697:PHE:HA   | 2.55                     | 0.41              |
| 2:B:632:GLN:HB2  | 2:B:639:LEU:HD22 | 2.03                     | 0.41              |
| 2:C:437:GLU:HA   | 2:C:440:ALA:HB3  | 2.01                     | 0.41              |
| 1:1:194:HIS:CD2  | 2:B:141:LEU:HD22 | 2.55                     | 0.41              |
| 1:2:216:PHE:CZ   | 2:B:439:ALA:HB3  | 2.55                     | 0.41              |
| 1:3:171:THR:O    | 1:3:175:VAL:HG23 | 2.21                     | 0.41              |
| 1:4:128:GLN:HG3  | 1:4:166:ASP:HA   | 2.02                     | 0.41              |
| 2:A:324:ILE:HD13 | 2:F:385:ARG:HH12 | 1.86                     | 0.41              |
| 2:A:362:HIS:CE1  | 2:B:232:GLU:OE2  | 2.74                     | 0.41              |
| 2:C:5:ARG:HH22   | 2:C:357:ARG:HH21 | 1.69                     | 0.41              |
| 2:C:615:LEU:HD21 | 2:C:657:THR:HG23 | 2.03                     | 0.41              |
| 1:4:147:VAL:HG13 | 1:4:148:ASN:H    | 1.85                     | 0.41              |
| 2:B:109:LEU:HD23 | 2:B:138:VAL:HG22 | 2.02                     | 0.41              |
| 2:B:589:SER:H    | 2:C:584:SER:HA   | 1.86                     | 0.41              |
| 2:B:739:LEU:HD13 | 2:B:741:ILE:HG23 | 2.03                     | 0.41              |
| 2:C:545:GLY:N    | 2:C:661:GLY:HA3  | 2.36                     | 0.41              |
| 2:C:741:ILE:HA   | 2:C:792:ILE:HB   | 2.01                     | 0.41              |
| 2:D:59:LYS:HG2   | 2:D:127:LEU:HD22 | 2.02                     | 0.41              |
| 2:D:110:LEU:HD21 | 2:D:138:VAL:HB   | 2.03                     | 0.41              |
| 2:F:100:HIS:HD2  | 2:F:107:HIS:CE1  | 2.39                     | 0.41              |
| 2:F:201:LYS:C    | 2:F:203:ASN:H    | 2.24                     | 0.41              |
| 2:F:746:ALA:HB1  | 2:F:796:VAL:HB   | 2.03                     | 0.41              |
| 2:B:188:GLU:HG3  | 2:B:339:VAL:HA   | 2.02                     | 0.41              |
| 2:B:361:HIS:HB2  | 2:C:233:ILE:HG23 | 2.03                     | 0.41              |
| 2:B:395:ILE:HA   | 2:B:471:VAL:HG11 | 2.03                     | 0.41              |
| 2:B:719:LEU:HD12 | 2:B:752:ALA:HB1  | 2.02                     | 0.41              |
| 2:C:480:VAL:HG13 | 2:C:483:TRP:CZ3  | 2.56                     | 0.41              |
| 2:D:394:LEU:CD2  | 2:D:479:VAL:HG22 | 2.51                     | 0.41              |
| 2:D:665:LEU:HD11 | 2:D:710:VAL:HG13 | 2.02                     | 0.41              |
| 2:B:624:PRO:HA   | 2:B:627:PHE:CE2  | 2.56                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:20:GLU:HB3   | 2:D:33:HIS:CD2   | 2.56                     | 0.40              |
| 2:D:98:LEU:HD12  | 2:D:110:LEU:HD13 | 2.02                     | 0.40              |
| 2:E:741:ILE:HG22 | 2:E:792:ILE:HD12 | 2.04                     | 0.40              |
| 2:F:544:LEU:HD13 | 2:F:690:MET:CE   | 2.51                     | 0.40              |
| 1:6:127:LEU:HA   | 1:6:175:VAL:HG21 | 2.03                     | 0.40              |
| 2:B:387:LEU:H    | 2:B:387:LEU:HD22 | 1.86                     | 0.40              |
| 2:C:427:LYS:HG3  | 2:C:443:ARG:HA   | 2.03                     | 0.40              |
| 2:C:685:MET:HB2  | 2:C:712:HIS:CE1  | 2.56                     | 0.40              |
| 2:D:620:GLU:O    | 2:D:696:ALA:HB1  | 2.21                     | 0.40              |
| 2:E:29:ILE:HG23  | 2:E:33:HIS:HD1   | 1.86                     | 0.40              |
| 2:E:686:LYS:HB2  | 2:E:712:HIS:HE1  | 1.86                     | 0.40              |
| 2:F:94:GLU:O     | 2:F:107:HIS:CD2  | 2.74                     | 0.40              |
| 2:F:271:ALA:HB2  | 2:F:308:GLU:HA   | 2.03                     | 0.40              |
| 1:2:133:PHE:CD1  | 1:2:186:ALA:HB2  | 2.57                     | 0.40              |
| 1:3:139:VAL:HG11 | 1:3:212:ILE:HD13 | 2.03                     | 0.40              |
| 2:B:235:ARG:NE   | 2:B:236:ASP:H    | 2.19                     | 0.40              |
| 2:B:570:ILE:HG13 | 2:B:606:VAL:HG22 | 2.03                     | 0.40              |
| 2:B:742:GLU:O    | 2:B:794:LEU:HD12 | 2.22                     | 0.40              |
| 2:D:55:LEU:HD11  | 2:D:129:VAL:HG11 | 2.04                     | 0.40              |
| 2:E:710:VAL:CG1  | 2:E:712:HIS:CE1  | 3.04                     | 0.40              |
| 2:A:87:VAL:HG13  | 2:A:112:LEU:HA   | 2.02                     | 0.40              |
| 2:A:110:LEU:HD11 | 2:A:142:LEU:HD13 | 2.04                     | 0.40              |
| 2:A:370:ALA:CB   | 2:A:471:VAL:HG13 | 2.51                     | 0.40              |
| 2:C:363:ARG:HD3  | 2:C:399:GLY:HA2  | 2.02                     | 0.40              |
| 2:D:14:LEU:O     | 2:D:17:ALA:HB3   | 2.22                     | 0.40              |
| 2:D:506:LEU:HD21 | 2:D:558:LEU:HD23 | 2.04                     | 0.40              |
| 2:D:714:LEU:HD22 | 2:D:718:HIS:CD2  | 2.56                     | 0.40              |
| 2:D:727:SER:O    | 2:D:731:THR:HG23 | 2.22                     | 0.40              |
| 2:E:484:THR:HG23 | 2:E:611:TYR:CD2  | 2.57                     | 0.40              |
| 2:C:627:PHE:CD2  | 2:C:697:PHE:HA   | 2.57                     | 0.40              |
| 2:D:91:SER:HB2   | 2:D:108:ILE:HD13 | 2.03                     | 0.40              |
| 2:E:484:THR:HG23 | 2:E:611:TYR:CE2  | 2.57                     | 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   | 1     | 92/218 (42%)    | 78 (85%)   | 8 (9%)    | 6 (6%)   | 1           | 16 |
| 1   | 2     | 92/218 (42%)    | 78 (85%)   | 9 (10%)   | 5 (5%)   | 2           | 19 |
| 1   | 3     | 92/218 (42%)    | 74 (80%)   | 12 (13%)  | 6 (6%)   | 1           | 16 |
| 1   | 4     | 92/218 (42%)    | 79 (86%)   | 8 (9%)    | 5 (5%)   | 2           | 19 |
| 1   | 5     | 92/218 (42%)    | 76 (83%)   | 12 (13%)  | 4 (4%)   | 2           | 22 |
| 1   | 6     | 92/218 (42%)    | 76 (83%)   | 13 (14%)  | 3 (3%)   | 4           | 26 |
| 2   | A     | 794/810 (98%)   | 627 (79%)  | 109 (14%) | 58 (7%)  | 1           | 14 |
| 2   | B     | 794/810 (98%)   | 625 (79%)  | 117 (15%) | 52 (6%)  | 1           | 16 |
| 2   | C     | 794/810 (98%)   | 623 (78%)  | 118 (15%) | 53 (7%)  | 1           | 15 |
| 2   | D     | 794/810 (98%)   | 614 (77%)  | 125 (16%) | 55 (7%)  | 1           | 15 |
| 2   | E     | 794/810 (98%)   | 629 (79%)  | 107 (14%) | 58 (7%)  | 1           | 14 |
| 2   | F     | 794/810 (98%)   | 628 (79%)  | 112 (14%) | 54 (7%)  | 1           | 15 |
| All | All   | 5316/6168 (86%) | 4207 (79%) | 750 (14%) | 359 (7%) | 2           | 15 |

All (359) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 207 | HIS  |
| 1   | 2     | 145 | LEU  |
| 1   | 2     | 147 | VAL  |
| 1   | 3     | 145 | LEU  |
| 1   | 3     | 146 | ASN  |
| 1   | 5     | 148 | ASN  |
| 2   | A     | 100 | HIS  |
| 2   | A     | 271 | ALA  |
| 2   | A     | 294 | ILE  |
| 2   | A     | 366 | ILE  |
| 2   | A     | 412 | ASN  |
| 2   | A     | 468 | ASN  |
| 2   | A     | 472 | THR  |
| 2   | A     | 493 | GLN  |
| 2   | A     | 579 | GLU  |
| 2   | A     | 650 | ARG  |
| 2   | A     | 669 | LYS  |
| 2   | B     | 100 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 150 | SER  |
| 2   | B     | 151 | ALA  |
| 2   | B     | 343 | SER  |
| 2   | B     | 365 | SER  |
| 2   | B     | 366 | ILE  |
| 2   | B     | 410 | PRO  |
| 2   | B     | 468 | ASN  |
| 2   | B     | 470 | GLU  |
| 2   | B     | 493 | GLN  |
| 2   | B     | 531 | LEU  |
| 2   | B     | 652 | THR  |
| 2   | B     | 667 | ARG  |
| 2   | C     | 78  | ILE  |
| 2   | C     | 271 | ALA  |
| 2   | C     | 294 | ILE  |
| 2   | C     | 363 | ARG  |
| 2   | C     | 365 | SER  |
| 2   | C     | 366 | ILE  |
| 2   | C     | 434 | GLN  |
| 2   | C     | 468 | ASN  |
| 2   | C     | 472 | THR  |
| 2   | C     | 493 | GLN  |
| 2   | C     | 547 | THR  |
| 2   | C     | 589 | SER  |
| 2   | C     | 590 | PRO  |
| 2   | C     | 642 | SER  |
| 2   | C     | 713 | SER  |
| 2   | D     | 293 | ALA  |
| 2   | D     | 333 | ARG  |
| 2   | D     | 339 | VAL  |
| 2   | D     | 365 | SER  |
| 2   | D     | 410 | PRO  |
| 2   | D     | 412 | ASN  |
| 2   | D     | 468 | ASN  |
| 2   | D     | 471 | VAL  |
| 2   | D     | 473 | VAL  |
| 2   | D     | 535 | LYS  |
| 2   | D     | 591 | PRO  |
| 2   | D     | 669 | LYS  |
| 2   | D     | 762 | ALA  |
| 2   | E     | 150 | SER  |
| 2   | E     | 167 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 183 | ILE  |
| 2   | E     | 293 | ALA  |
| 2   | E     | 363 | ARG  |
| 2   | E     | 366 | ILE  |
| 2   | E     | 412 | ASN  |
| 2   | E     | 468 | ASN  |
| 2   | E     | 473 | VAL  |
| 2   | E     | 493 | GLN  |
| 2   | E     | 585 | ARG  |
| 2   | E     | 674 | ASN  |
| 2   | F     | 7   | THR  |
| 2   | F     | 78  | ILE  |
| 2   | F     | 117 | GLU  |
| 2   | F     | 183 | ILE  |
| 2   | F     | 294 | ILE  |
| 2   | F     | 410 | PRO  |
| 2   | F     | 412 | ASN  |
| 2   | F     | 434 | GLN  |
| 2   | F     | 468 | ASN  |
| 2   | F     | 472 | THR  |
| 2   | F     | 493 | GLN  |
| 2   | F     | 547 | THR  |
| 2   | F     | 668 | ASN  |
| 2   | F     | 670 | TYR  |
| 1   | 1     | 147 | VAL  |
| 1   | 4     | 145 | LEU  |
| 1   | 4     | 147 | VAL  |
| 1   | 5     | 147 | VAL  |
| 1   | 6     | 145 | LEU  |
| 2   | A     | 68  | ILE  |
| 2   | A     | 144 | SER  |
| 2   | A     | 157 | ASN  |
| 2   | A     | 165 | SER  |
| 2   | A     | 183 | ILE  |
| 2   | A     | 391 | ALA  |
| 2   | A     | 471 | VAL  |
| 2   | A     | 473 | VAL  |
| 2   | A     | 652 | THR  |
| 2   | A     | 662 | ALA  |
| 2   | A     | 675 | VAL  |
| 2   | B     | 99  | GLY  |
| 2   | B     | 163 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 165 | SER  |
| 2   | B     | 177 | ASP  |
| 2   | B     | 212 | VAL  |
| 2   | B     | 271 | ALA  |
| 2   | B     | 291 | GLU  |
| 2   | B     | 294 | ILE  |
| 2   | B     | 383 | SER  |
| 2   | B     | 547 | THR  |
| 2   | B     | 579 | GLU  |
| 2   | B     | 642 | SER  |
| 2   | B     | 659 | ASN  |
| 2   | B     | 662 | ALA  |
| 2   | B     | 674 | ASN  |
| 2   | B     | 716 | LYS  |
| 2   | B     | 757 | ASP  |
| 2   | C     | 99  | GLY  |
| 2   | C     | 150 | SER  |
| 2   | C     | 165 | SER  |
| 2   | C     | 212 | VAL  |
| 2   | C     | 293 | ALA  |
| 2   | C     | 362 | HIS  |
| 2   | C     | 412 | ASN  |
| 2   | C     | 568 | SER  |
| 2   | C     | 662 | ALA  |
| 2   | D     | 72  | GLN  |
| 2   | D     | 99  | GLY  |
| 2   | D     | 100 | HIS  |
| 2   | D     | 165 | SER  |
| 2   | D     | 166 | LEU  |
| 2   | D     | 178 | SER  |
| 2   | D     | 183 | ILE  |
| 2   | D     | 362 | HIS  |
| 2   | D     | 363 | ARG  |
| 2   | D     | 366 | ILE  |
| 2   | D     | 413 | LEU  |
| 2   | D     | 493 | GLN  |
| 2   | D     | 578 | MET  |
| 2   | D     | 662 | ALA  |
| 2   | D     | 738 | ASP  |
| 2   | E     | 100 | HIS  |
| 2   | E     | 152 | ALA  |
| 2   | E     | 165 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 177 | ASP  |
| 2   | E     | 271 | ALA  |
| 2   | E     | 365 | SER  |
| 2   | E     | 383 | SER  |
| 2   | E     | 384 | ASP  |
| 2   | E     | 410 | PRO  |
| 2   | E     | 434 | GLN  |
| 2   | E     | 618 | ALA  |
| 2   | E     | 642 | SER  |
| 2   | E     | 662 | ALA  |
| 2   | E     | 738 | ASP  |
| 2   | E     | 759 | GLU  |
| 2   | F     | 100 | HIS  |
| 2   | F     | 118 | GLY  |
| 2   | F     | 150 | SER  |
| 2   | F     | 165 | SER  |
| 2   | F     | 168 | ARG  |
| 2   | F     | 271 | ALA  |
| 2   | F     | 343 | SER  |
| 2   | F     | 366 | ILE  |
| 2   | F     | 662 | ALA  |
| 2   | F     | 673 | PHE  |
| 2   | F     | 717 | LYS  |
| 2   | F     | 757 | ASP  |
| 1   | 1     | 144 | LYS  |
| 1   | 1     | 177 | ASN  |
| 1   | 2     | 144 | LYS  |
| 1   | 2     | 177 | ASN  |
| 1   | 3     | 144 | LYS  |
| 1   | 3     | 177 | ASN  |
| 1   | 4     | 144 | LYS  |
| 1   | 4     | 177 | ASN  |
| 1   | 5     | 177 | ASN  |
| 1   | 6     | 177 | ASN  |
| 2   | A     | 99  | GLY  |
| 2   | A     | 151 | ALA  |
| 2   | A     | 162 | THR  |
| 2   | A     | 163 | LEU  |
| 2   | A     | 167 | ALA  |
| 2   | A     | 330 | LEU  |
| 2   | A     | 375 | VAL  |
| 2   | A     | 388 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 410 | PRO  |
| 2   | A     | 413 | LEU  |
| 2   | A     | 585 | ARG  |
| 2   | A     | 707 | GLU  |
| 2   | A     | 738 | ASP  |
| 2   | A     | 760 | TYR  |
| 2   | B     | 364 | VAL  |
| 2   | B     | 384 | ASP  |
| 2   | B     | 391 | ALA  |
| 2   | B     | 591 | PRO  |
| 2   | B     | 738 | ASP  |
| 2   | C     | 148 | GLY  |
| 2   | C     | 162 | THR  |
| 2   | C     | 163 | LEU  |
| 2   | C     | 364 | VAL  |
| 2   | C     | 375 | VAL  |
| 2   | C     | 391 | ALA  |
| 2   | C     | 410 | PRO  |
| 2   | C     | 413 | LEU  |
| 2   | C     | 550 | GLY  |
| 2   | C     | 580 | LYS  |
| 2   | C     | 757 | ASP  |
| 2   | C     | 761 | GLY  |
| 2   | C     | 788 | LYS  |
| 2   | D     | 143 | GLY  |
| 2   | D     | 150 | SER  |
| 2   | D     | 163 | LEU  |
| 2   | D     | 291 | GLU  |
| 2   | D     | 326 | LYS  |
| 2   | D     | 375 | VAL  |
| 2   | D     | 388 | PRO  |
| 2   | D     | 391 | ALA  |
| 2   | D     | 400 | SER  |
| 2   | D     | 472 | THR  |
| 2   | D     | 592 | GLY  |
| 2   | E     | 72  | GLN  |
| 2   | E     | 73  | GLU  |
| 2   | E     | 162 | THR  |
| 2   | E     | 163 | LEU  |
| 2   | E     | 210 | PRO  |
| 2   | E     | 391 | ALA  |
| 2   | E     | 413 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 472 | THR  |
| 2   | E     | 580 | LYS  |
| 2   | F     | 152 | ALA  |
| 2   | F     | 162 | THR  |
| 2   | F     | 163 | LEU  |
| 2   | F     | 177 | ASP  |
| 2   | F     | 185 | ARG  |
| 2   | F     | 384 | ASP  |
| 2   | F     | 388 | PRO  |
| 2   | F     | 391 | ALA  |
| 2   | F     | 413 | LEU  |
| 2   | F     | 568 | SER  |
| 2   | F     | 738 | ASP  |
| 1   | 1     | 145 | LEU  |
| 1   | 4     | 217 | ALA  |
| 1   | 6     | 144 | LYS  |
| 2   | A     | 150 | SER  |
| 2   | A     | 152 | ALA  |
| 2   | A     | 210 | PRO  |
| 2   | A     | 293 | ALA  |
| 2   | A     | 343 | SER  |
| 2   | A     | 550 | GLY  |
| 2   | A     | 690 | MET  |
| 2   | B     | 152 | ALA  |
| 2   | B     | 162 | THR  |
| 2   | B     | 226 | ILE  |
| 2   | B     | 388 | PRO  |
| 2   | B     | 400 | SER  |
| 2   | B     | 413 | LEU  |
| 2   | B     | 550 | GLY  |
| 2   | C     | 226 | ILE  |
| 2   | C     | 384 | ASP  |
| 2   | C     | 388 | PRO  |
| 2   | C     | 471 | VAL  |
| 2   | C     | 661 | GLY  |
| 2   | C     | 686 | LYS  |
| 2   | D     | 145 | ASN  |
| 2   | D     | 162 | THR  |
| 2   | D     | 197 | SER  |
| 2   | D     | 364 | VAL  |
| 2   | D     | 550 | GLY  |
| 2   | D     | 686 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 143 | GLY  |
| 2   | E     | 231 | PRO  |
| 2   | E     | 375 | VAL  |
| 2   | E     | 388 | PRO  |
| 2   | E     | 400 | SER  |
| 2   | E     | 550 | GLY  |
| 2   | E     | 586 | LEU  |
| 2   | E     | 686 | LYS  |
| 2   | F     | 166 | LEU  |
| 2   | F     | 293 | ALA  |
| 2   | F     | 375 | VAL  |
| 2   | F     | 531 | LEU  |
| 2   | F     | 550 | GLY  |
| 2   | F     | 642 | SER  |
| 2   | F     | 671 | VAL  |
| 1   | 1     | 191 | ILE  |
| 1   | 5     | 144 | LYS  |
| 2   | A     | 70  | ARG  |
| 2   | A     | 198 | ARG  |
| 2   | A     | 202 | ASN  |
| 2   | A     | 226 | ILE  |
| 2   | A     | 228 | ASN  |
| 2   | A     | 400 | SER  |
| 2   | A     | 469 | SER  |
| 2   | A     | 642 | SER  |
| 2   | B     | 375 | VAL  |
| 2   | B     | 434 | GLN  |
| 2   | B     | 472 | THR  |
| 2   | B     | 717 | LYS  |
| 2   | C     | 147 | THR  |
| 2   | C     | 400 | SER  |
| 2   | C     | 579 | GLU  |
| 2   | D     | 167 | ALA  |
| 2   | D     | 226 | ILE  |
| 2   | D     | 674 | ASN  |
| 2   | E     | 209 | GLU  |
| 2   | E     | 226 | ILE  |
| 2   | E     | 469 | SER  |
| 2   | E     | 534 | PRO  |
| 2   | E     | 690 | MET  |
| 2   | E     | 698 | ARG  |
| 2   | E     | 713 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 226 | ILE  |
| 2   | F     | 400 | SER  |
| 1   | 3     | 216 | PHE  |
| 2   | A     | 434 | GLN  |
| 2   | A     | 600 | GLY  |
| 2   | B     | 166 | LEU  |
| 2   | C     | 118 | GLY  |
| 2   | C     | 152 | ALA  |
| 2   | C     | 323 | TYR  |
| 2   | D     | 228 | ASN  |
| 2   | D     | 251 | THR  |
| 2   | D     | 343 | SER  |
| 2   | D     | 531 | LEU  |
| 2   | D     | 760 | TYR  |
| 2   | E     | 5   | ARG  |
| 2   | E     | 103 | VAL  |
| 2   | E     | 323 | TYR  |
| 2   | E     | 600 | GLY  |
| 2   | E     | 757 | ASP  |
| 2   | F     | 99  | GLY  |
| 2   | F     | 686 | LYS  |
| 2   | F     | 758 | LEU  |
| 1   | 3     | 191 | ILE  |
| 2   | C     | 210 | PRO  |
| 2   | C     | 512 | GLY  |
| 2   | E     | 661 | GLY  |
| 2   | F     | 212 | VAL  |
| 2   | F     | 382 | ILE  |
| 2   | F     | 610 | PRO  |
| 2   | A     | 212 | VAL  |
| 2   | A     | 382 | ILE  |
| 2   | B     | 600 | GLY  |
| 2   | C     | 588 | GLY  |
| 2   | D     | 68  | ILE  |
| 2   | E     | 212 | VAL  |
| 2   | F     | 471 | VAL  |
| 1   | 2     | 191 | ILE  |
| 2   | A     | 761 | GLY  |
| 2   | B     | 182 | VAL  |
| 2   | B     | 660 | VAL  |
| 2   | D     | 382 | ILE  |
| 2   | F     | 210 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 364 | VAL  |
| 2   | B     | 382 | ILE  |
| 2   | B     | 534 | PRO  |
| 2   | C     | 392 | ILE  |
| 2   | A     | 160 | THR  |

### 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   | 1     | 88/201 (44%)    | 80 (91%)   | 8 (9%)    | 9           | 29 |
| 1   | 2     | 88/201 (44%)    | 79 (90%)   | 9 (10%)   | 7           | 25 |
| 1   | 3     | 88/201 (44%)    | 79 (90%)   | 9 (10%)   | 7           | 25 |
| 1   | 4     | 88/201 (44%)    | 81 (92%)   | 7 (8%)    | 12          | 35 |
| 1   | 5     | 88/201 (44%)    | 80 (91%)   | 8 (9%)    | 9           | 29 |
| 1   | 6     | 88/201 (44%)    | 81 (92%)   | 7 (8%)    | 12          | 35 |
| 2   | A     | 667/686 (97%)   | 584 (88%)  | 83 (12%)  | 4           | 19 |
| 2   | B     | 667/686 (97%)   | 585 (88%)  | 82 (12%)  | 4           | 19 |
| 2   | C     | 667/686 (97%)   | 591 (89%)  | 76 (11%)  | 5           | 21 |
| 2   | D     | 667/686 (97%)   | 589 (88%)  | 78 (12%)  | 5           | 21 |
| 2   | E     | 667/686 (97%)   | 597 (90%)  | 70 (10%)  | 7           | 24 |
| 2   | F     | 667/686 (97%)   | 597 (90%)  | 70 (10%)  | 7           | 24 |
| All | All   | 4530/5322 (85%) | 4023 (89%) | 507 (11%) | 9           | 22 |

All (507) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 136 | PHE  |
| 1   | 1     | 137 | GLU  |
| 1   | 1     | 145 | LEU  |
| 1   | 1     | 147 | VAL  |
| 1   | 1     | 151 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 175 | VAL  |
| 1   | 1     | 204 | ILE  |
| 1   | 1     | 216 | PHE  |
| 1   | 2     | 140 | ILE  |
| 1   | 2     | 142 | LEU  |
| 1   | 2     | 145 | LEU  |
| 1   | 2     | 147 | VAL  |
| 1   | 2     | 151 | LYS  |
| 1   | 2     | 170 | MET  |
| 1   | 2     | 214 | LYS  |
| 1   | 2     | 215 | HIS  |
| 1   | 2     | 216 | PHE  |
| 1   | 3     | 145 | LEU  |
| 1   | 3     | 151 | LYS  |
| 1   | 3     | 152 | THR  |
| 1   | 3     | 165 | VAL  |
| 1   | 3     | 195 | ARG  |
| 1   | 3     | 204 | ILE  |
| 1   | 3     | 210 | GLU  |
| 1   | 3     | 214 | LYS  |
| 1   | 3     | 216 | PHE  |
| 1   | 4     | 136 | PHE  |
| 1   | 4     | 145 | LEU  |
| 1   | 4     | 147 | VAL  |
| 1   | 4     | 151 | LYS  |
| 1   | 4     | 170 | MET  |
| 1   | 4     | 195 | ARG  |
| 1   | 4     | 204 | ILE  |
| 1   | 5     | 137 | GLU  |
| 1   | 5     | 142 | LEU  |
| 1   | 5     | 144 | LYS  |
| 1   | 5     | 151 | LYS  |
| 1   | 5     | 170 | MET  |
| 1   | 5     | 176 | GLU  |
| 1   | 5     | 204 | ILE  |
| 1   | 5     | 216 | PHE  |
| 1   | 6     | 130 | VAL  |
| 1   | 6     | 136 | PHE  |
| 1   | 6     | 142 | LEU  |
| 1   | 6     | 145 | LEU  |
| 1   | 6     | 151 | LYS  |
| 1   | 6     | 170 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 6     | 215 | HIS  |
| 2   | A     | 3   | PHE  |
| 2   | A     | 5   | ARG  |
| 2   | A     | 8   | GLU  |
| 2   | A     | 9   | ARG  |
| 2   | A     | 19  | GLU  |
| 2   | A     | 22  | LEU  |
| 2   | A     | 41  | GLU  |
| 2   | A     | 43  | GLU  |
| 2   | A     | 53  | LEU  |
| 2   | A     | 62  | LYS  |
| 2   | A     | 74  | MET  |
| 2   | A     | 76  | GLN  |
| 2   | A     | 78  | ILE  |
| 2   | A     | 92  | MET  |
| 2   | A     | 94  | GLU  |
| 2   | A     | 105 | THR  |
| 2   | A     | 106 | GLU  |
| 2   | A     | 117 | GLU  |
| 2   | A     | 138 | VAL  |
| 2   | A     | 139 | LEU  |
| 2   | A     | 142 | LEU  |
| 2   | A     | 155 | ASN  |
| 2   | A     | 170 | LEU  |
| 2   | A     | 185 | ARG  |
| 2   | A     | 187 | LYS  |
| 2   | A     | 194 | GLU  |
| 2   | A     | 209 | GLU  |
| 2   | A     | 224 | GLN  |
| 2   | A     | 238 | ARG  |
| 2   | A     | 262 | LYS  |
| 2   | A     | 268 | ILE  |
| 2   | A     | 269 | ARG  |
| 2   | A     | 294 | ILE  |
| 2   | A     | 303 | SER  |
| 2   | A     | 315 | THR  |
| 2   | A     | 335 | GLN  |
| 2   | A     | 337 | ILE  |
| 2   | A     | 341 | GLN  |
| 2   | A     | 354 | LEU  |
| 2   | A     | 355 | ARG  |
| 2   | A     | 364 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 379 | ASP  |
| 2   | A     | 380 | ARG  |
| 2   | A     | 392 | ILE  |
| 2   | A     | 415 | GLU  |
| 2   | A     | 423 | VAL  |
| 2   | A     | 424 | ARG  |
| 2   | A     | 443 | ARG  |
| 2   | A     | 449 | LEU  |
| 2   | A     | 452 | GLN  |
| 2   | A     | 457 | LYS  |
| 2   | A     | 461 | LYS  |
| 2   | A     | 463 | LYS  |
| 2   | A     | 470 | GLU  |
| 2   | A     | 471 | VAL  |
| 2   | A     | 475 | ASP  |
| 2   | A     | 497 | ASP  |
| 2   | A     | 503 | GLU  |
| 2   | A     | 509 | ARG  |
| 2   | A     | 511 | ILE  |
| 2   | A     | 563 | PHE  |
| 2   | A     | 578 | MET  |
| 2   | A     | 597 | ASP  |
| 2   | A     | 624 | PRO  |
| 2   | A     | 626 | VAL  |
| 2   | A     | 632 | GLN  |
| 2   | A     | 634 | LEU  |
| 2   | A     | 641 | ASP  |
| 2   | A     | 647 | VAL  |
| 2   | A     | 673 | PHE  |
| 2   | A     | 674 | ASN  |
| 2   | A     | 675 | VAL  |
| 2   | A     | 676 | GLN  |
| 2   | A     | 687 | ASP  |
| 2   | A     | 690 | MET  |
| 2   | A     | 694 | LYS  |
| 2   | A     | 700 | GLU  |
| 2   | A     | 713 | SER  |
| 2   | A     | 729 | GLN  |
| 2   | A     | 730 | LEU  |
| 2   | A     | 741 | ILE  |
| 2   | A     | 763 | ARG  |
| 2   | A     | 795 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 3   | PHE  |
| 2   | B     | 5   | ARG  |
| 2   | B     | 11  | GLN  |
| 2   | B     | 18  | GLN  |
| 2   | B     | 20  | GLU  |
| 2   | B     | 27  | ASN  |
| 2   | B     | 41  | GLU  |
| 2   | B     | 62  | LYS  |
| 2   | B     | 72  | GLN  |
| 2   | B     | 74  | MET  |
| 2   | B     | 78  | ILE  |
| 2   | B     | 83  | ARG  |
| 2   | B     | 96  | ARG  |
| 2   | B     | 100 | HIS  |
| 2   | B     | 105 | THR  |
| 2   | B     | 115 | GLU  |
| 2   | B     | 117 | GLU  |
| 2   | B     | 137 | GLN  |
| 2   | B     | 138 | VAL  |
| 2   | B     | 139 | LEU  |
| 2   | B     | 166 | LEU  |
| 2   | B     | 170 | LEU  |
| 2   | B     | 185 | ARG  |
| 2   | B     | 194 | GLU  |
| 2   | B     | 214 | LYS  |
| 2   | B     | 230 | VAL  |
| 2   | B     | 232 | GLU  |
| 2   | B     | 235 | ARG  |
| 2   | B     | 265 | MET  |
| 2   | B     | 268 | ILE  |
| 2   | B     | 269 | ARG  |
| 2   | B     | 308 | GLU  |
| 2   | B     | 309 | LEU  |
| 2   | B     | 355 | ARG  |
| 2   | B     | 358 | TYR  |
| 2   | B     | 359 | GLU  |
| 2   | B     | 361 | HIS  |
| 2   | B     | 363 | ARG  |
| 2   | B     | 364 | VAL  |
| 2   | B     | 380 | ARG  |
| 2   | B     | 385 | ARG  |
| 2   | B     | 387 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 392 | ILE  |
| 2   | B     | 415 | GLU  |
| 2   | B     | 423 | VAL  |
| 2   | B     | 424 | ARG  |
| 2   | B     | 425 | LYS  |
| 2   | B     | 443 | ARG  |
| 2   | B     | 451 | GLU  |
| 2   | B     | 452 | GLN  |
| 2   | B     | 457 | LYS  |
| 2   | B     | 472 | THR  |
| 2   | B     | 478 | MET  |
| 2   | B     | 479 | VAL  |
| 2   | B     | 480 | VAL  |
| 2   | B     | 481 | SER  |
| 2   | B     | 483 | TRP  |
| 2   | B     | 503 | GLU  |
| 2   | B     | 509 | ARG  |
| 2   | B     | 511 | ILE  |
| 2   | B     | 531 | LEU  |
| 2   | B     | 567 | GLU  |
| 2   | B     | 578 | MET  |
| 2   | B     | 586 | LEU  |
| 2   | B     | 597 | ASP  |
| 2   | B     | 609 | LYS  |
| 2   | B     | 620 | GLU  |
| 2   | B     | 624 | PRO  |
| 2   | B     | 639 | LEU  |
| 2   | B     | 641 | ASP  |
| 2   | B     | 643 | LYS  |
| 2   | B     | 682 | HIS  |
| 2   | B     | 693 | LEU  |
| 2   | B     | 695 | ARG  |
| 2   | B     | 716 | LYS  |
| 2   | B     | 719 | LEU  |
| 2   | B     | 729 | GLN  |
| 2   | B     | 730 | LEU  |
| 2   | B     | 739 | LEU  |
| 2   | B     | 742 | GLU  |
| 2   | B     | 790 | GLN  |
| 2   | B     | 795 | ASP  |
| 2   | C     | 5   | ARG  |
| 2   | C     | 11  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 18  | GLN  |
| 2   | C     | 19  | GLU  |
| 2   | C     | 20  | GLU  |
| 2   | C     | 27  | ASN  |
| 2   | C     | 31  | THR  |
| 2   | C     | 32  | GLU  |
| 2   | C     | 45  | ILE  |
| 2   | C     | 53  | LEU  |
| 2   | C     | 62  | LYS  |
| 2   | C     | 72  | GLN  |
| 2   | C     | 74  | MET  |
| 2   | C     | 83  | ARG  |
| 2   | C     | 105 | THR  |
| 2   | C     | 106 | GLU  |
| 2   | C     | 135 | ARG  |
| 2   | C     | 138 | VAL  |
| 2   | C     | 139 | LEU  |
| 2   | C     | 202 | ASN  |
| 2   | C     | 254 | ARG  |
| 2   | C     | 269 | ARG  |
| 2   | C     | 285 | ILE  |
| 2   | C     | 308 | GLU  |
| 2   | C     | 323 | TYR  |
| 2   | C     | 342 | PRO  |
| 2   | C     | 346 | GLU  |
| 2   | C     | 357 | ARG  |
| 2   | C     | 362 | HIS  |
| 2   | C     | 363 | ARG  |
| 2   | C     | 379 | ASP  |
| 2   | C     | 380 | ARG  |
| 2   | C     | 385 | ARG  |
| 2   | C     | 392 | ILE  |
| 2   | C     | 397 | GLU  |
| 2   | C     | 410 | PRO  |
| 2   | C     | 415 | GLU  |
| 2   | C     | 423 | VAL  |
| 2   | C     | 424 | ARG  |
| 2   | C     | 427 | LYS  |
| 2   | C     | 431 | VAL  |
| 2   | C     | 434 | GLN  |
| 2   | C     | 443 | ARG  |
| 2   | C     | 449 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 452 | GLN  |
| 2   | C     | 460 | TRP  |
| 2   | C     | 463 | LYS  |
| 2   | C     | 478 | MET  |
| 2   | C     | 495 | GLU  |
| 2   | C     | 503 | GLU  |
| 2   | C     | 549 | VAL  |
| 2   | C     | 565 | ASP  |
| 2   | C     | 586 | LEU  |
| 2   | C     | 603 | THR  |
| 2   | C     | 609 | LYS  |
| 2   | C     | 611 | TYR  |
| 2   | C     | 624 | PRO  |
| 2   | C     | 634 | LEU  |
| 2   | C     | 639 | LEU  |
| 2   | C     | 647 | VAL  |
| 2   | C     | 648 | ASP  |
| 2   | C     | 665 | LEU  |
| 2   | C     | 667 | ARG  |
| 2   | C     | 669 | LYS  |
| 2   | C     | 679 | THR  |
| 2   | C     | 680 | GLN  |
| 2   | C     | 688 | LYS  |
| 2   | C     | 690 | MET  |
| 2   | C     | 695 | ARG  |
| 2   | C     | 713 | SER  |
| 2   | C     | 729 | GLN  |
| 2   | C     | 730 | LEU  |
| 2   | C     | 741 | ILE  |
| 2   | C     | 742 | GLU  |
| 2   | C     | 767 | ARG  |
| 2   | C     | 795 | ASP  |
| 2   | D     | 11  | GLN  |
| 2   | D     | 19  | GLU  |
| 2   | D     | 22  | LEU  |
| 2   | D     | 31  | THR  |
| 2   | D     | 32  | GLU  |
| 2   | D     | 41  | GLU  |
| 2   | D     | 53  | LEU  |
| 2   | D     | 62  | LYS  |
| 2   | D     | 74  | MET  |
| 2   | D     | 76  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 85  | LYS  |
| 2   | D     | 90  | LEU  |
| 2   | D     | 105 | THR  |
| 2   | D     | 106 | GLU  |
| 2   | D     | 115 | GLU  |
| 2   | D     | 117 | GLU  |
| 2   | D     | 136 | GLN  |
| 2   | D     | 138 | VAL  |
| 2   | D     | 139 | LEU  |
| 2   | D     | 185 | ARG  |
| 2   | D     | 194 | GLU  |
| 2   | D     | 224 | GLN  |
| 2   | D     | 229 | GLU  |
| 2   | D     | 234 | LEU  |
| 2   | D     | 235 | ARG  |
| 2   | D     | 237 | LYS  |
| 2   | D     | 265 | MET  |
| 2   | D     | 269 | ARG  |
| 2   | D     | 308 | GLU  |
| 2   | D     | 323 | TYR  |
| 2   | D     | 337 | ILE  |
| 2   | D     | 342 | PRO  |
| 2   | D     | 357 | ARG  |
| 2   | D     | 361 | HIS  |
| 2   | D     | 364 | VAL  |
| 2   | D     | 380 | ARG  |
| 2   | D     | 381 | TYR  |
| 2   | D     | 387 | LEU  |
| 2   | D     | 392 | ILE  |
| 2   | D     | 397 | GLU  |
| 2   | D     | 403 | ARG  |
| 2   | D     | 412 | ASN  |
| 2   | D     | 415 | GLU  |
| 2   | D     | 423 | VAL  |
| 2   | D     | 424 | ARG  |
| 2   | D     | 428 | ASP  |
| 2   | D     | 431 | VAL  |
| 2   | D     | 443 | ARG  |
| 2   | D     | 452 | GLN  |
| 2   | D     | 457 | LYS  |
| 2   | D     | 462 | GLU  |
| 2   | D     | 471 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 479 | VAL  |
| 2   | D     | 503 | GLU  |
| 2   | D     | 511 | ILE  |
| 2   | D     | 546 | PRO  |
| 2   | D     | 563 | PHE  |
| 2   | D     | 567 | GLU  |
| 2   | D     | 570 | ILE  |
| 2   | D     | 574 | MET  |
| 2   | D     | 578 | MET  |
| 2   | D     | 593 | TYR  |
| 2   | D     | 606 | VAL  |
| 2   | D     | 609 | LYS  |
| 2   | D     | 611 | TYR  |
| 2   | D     | 623 | HIS  |
| 2   | D     | 634 | LEU  |
| 2   | D     | 636 | ASP  |
| 2   | D     | 639 | LEU  |
| 2   | D     | 648 | ASP  |
| 2   | D     | 680 | GLN  |
| 2   | D     | 695 | ARG  |
| 2   | D     | 729 | GLN  |
| 2   | D     | 730 | LEU  |
| 2   | D     | 742 | GLU  |
| 2   | D     | 758 | LEU  |
| 2   | D     | 766 | ARG  |
| 2   | D     | 804 | LYS  |
| 2   | E     | 11  | GLN  |
| 2   | E     | 18  | GLN  |
| 2   | E     | 45  | ILE  |
| 2   | E     | 53  | LEU  |
| 2   | E     | 62  | LYS  |
| 2   | E     | 83  | ARG  |
| 2   | E     | 100 | HIS  |
| 2   | E     | 108 | ILE  |
| 2   | E     | 119 | VAL  |
| 2   | E     | 139 | LEU  |
| 2   | E     | 180 | ASP  |
| 2   | E     | 229 | GLU  |
| 2   | E     | 262 | LYS  |
| 2   | E     | 265 | MET  |
| 2   | E     | 269 | ARG  |
| 2   | E     | 270 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 299 | ILE  |
| 2   | E     | 337 | ILE  |
| 2   | E     | 342 | PRO  |
| 2   | E     | 355 | ARG  |
| 2   | E     | 359 | GLU  |
| 2   | E     | 363 | ARG  |
| 2   | E     | 378 | SER  |
| 2   | E     | 380 | ARG  |
| 2   | E     | 382 | ILE  |
| 2   | E     | 384 | ASP  |
| 2   | E     | 393 | ASP  |
| 2   | E     | 397 | GLU  |
| 2   | E     | 400 | SER  |
| 2   | E     | 401 | LYS  |
| 2   | E     | 410 | PRO  |
| 2   | E     | 415 | GLU  |
| 2   | E     | 421 | ASP  |
| 2   | E     | 423 | VAL  |
| 2   | E     | 424 | ARG  |
| 2   | E     | 427 | LYS  |
| 2   | E     | 428 | ASP  |
| 2   | E     | 435 | GLU  |
| 2   | E     | 443 | ARG  |
| 2   | E     | 452 | GLN  |
| 2   | E     | 457 | LYS  |
| 2   | E     | 461 | LYS  |
| 2   | E     | 462 | GLU  |
| 2   | E     | 480 | VAL  |
| 2   | E     | 503 | GLU  |
| 2   | E     | 509 | ARG  |
| 2   | E     | 511 | ILE  |
| 2   | E     | 544 | LEU  |
| 2   | E     | 593 | TYR  |
| 2   | E     | 597 | ASP  |
| 2   | E     | 611 | TYR  |
| 2   | E     | 624 | PRO  |
| 2   | E     | 626 | VAL  |
| 2   | E     | 639 | LEU  |
| 2   | E     | 641 | ASP  |
| 2   | E     | 647 | VAL  |
| 2   | E     | 665 | LEU  |
| 2   | E     | 667 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 685 | MET  |
| 2   | E     | 690 | MET  |
| 2   | E     | 697 | PHE  |
| 2   | E     | 711 | PHE  |
| 2   | E     | 719 | LEU  |
| 2   | E     | 730 | LEU  |
| 2   | E     | 741 | ILE  |
| 2   | E     | 759 | GLU  |
| 2   | E     | 760 | TYR  |
| 2   | E     | 790 | GLN  |
| 2   | E     | 791 | HIS  |
| 2   | E     | 795 | ASP  |
| 2   | F     | 11  | GLN  |
| 2   | F     | 19  | GLU  |
| 2   | F     | 20  | GLU  |
| 2   | F     | 32  | GLU  |
| 2   | F     | 62  | LYS  |
| 2   | F     | 72  | GLN  |
| 2   | F     | 74  | MET  |
| 2   | F     | 83  | ARG  |
| 2   | F     | 96  | ARG  |
| 2   | F     | 100 | HIS  |
| 2   | F     | 105 | THR  |
| 2   | F     | 119 | VAL  |
| 2   | F     | 137 | GLN  |
| 2   | F     | 138 | VAL  |
| 2   | F     | 170 | LEU  |
| 2   | F     | 185 | ARG  |
| 2   | F     | 209 | GLU  |
| 2   | F     | 262 | LYS  |
| 2   | F     | 269 | ARG  |
| 2   | F     | 303 | SER  |
| 2   | F     | 337 | ILE  |
| 2   | F     | 341 | GLN  |
| 2   | F     | 351 | LEU  |
| 2   | F     | 357 | ARG  |
| 2   | F     | 364 | VAL  |
| 2   | F     | 379 | ASP  |
| 2   | F     | 380 | ARG  |
| 2   | F     | 381 | TYR  |
| 2   | F     | 387 | LEU  |
| 2   | F     | 397 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 414 | LYS  |
| 2   | F     | 415 | GLU  |
| 2   | F     | 423 | VAL  |
| 2   | F     | 424 | ARG  |
| 2   | F     | 431 | VAL  |
| 2   | F     | 443 | ARG  |
| 2   | F     | 449 | LEU  |
| 2   | F     | 452 | GLN  |
| 2   | F     | 468 | ASN  |
| 2   | F     | 471 | VAL  |
| 2   | F     | 473 | VAL  |
| 2   | F     | 475 | ASP  |
| 2   | F     | 476 | ILE  |
| 2   | F     | 478 | MET  |
| 2   | F     | 479 | VAL  |
| 2   | F     | 503 | GLU  |
| 2   | F     | 509 | ARG  |
| 2   | F     | 579 | GLU  |
| 2   | F     | 586 | LEU  |
| 2   | F     | 589 | SER  |
| 2   | F     | 593 | TYR  |
| 2   | F     | 611 | TYR  |
| 2   | F     | 636 | ASP  |
| 2   | F     | 639 | LEU  |
| 2   | F     | 641 | ASP  |
| 2   | F     | 664 | GLU  |
| 2   | F     | 676 | GLN  |
| 2   | F     | 690 | MET  |
| 2   | F     | 692 | GLU  |
| 2   | F     | 697 | PHE  |
| 2   | F     | 704 | ARG  |
| 2   | F     | 710 | VAL  |
| 2   | F     | 719 | LEU  |
| 2   | F     | 729 | GLN  |
| 2   | F     | 730 | LEU  |
| 2   | F     | 741 | ILE  |
| 2   | F     | 742 | GLU  |
| 2   | F     | 760 | TYR  |
| 2   | F     | 766 | ARG  |
| 2   | F     | 790 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 194 | HIS  |
| 1   | 1     | 207 | HIS  |
| 1   | 3     | 207 | HIS  |
| 1   | 4     | 207 | HIS  |
| 1   | 5     | 146 | ASN  |
| 1   | 5     | 207 | HIS  |
| 2   | A     | 26  | HIS  |
| 2   | A     | 33  | HIS  |
| 2   | A     | 137 | GLN  |
| 2   | A     | 155 | ASN  |
| 2   | A     | 190 | GLN  |
| 2   | A     | 352 | GLN  |
| 2   | A     | 507 | HIS  |
| 2   | A     | 513 | GLN  |
| 2   | A     | 581 | HIS  |
| 2   | A     | 682 | HIS  |
| 2   | B     | 107 | HIS  |
| 2   | B     | 140 | GLN  |
| 2   | B     | 224 | GLN  |
| 2   | B     | 273 | ASN  |
| 2   | B     | 338 | GLN  |
| 2   | B     | 352 | GLN  |
| 2   | B     | 434 | GLN  |
| 2   | B     | 504 | ASN  |
| 2   | B     | 507 | HIS  |
| 2   | B     | 581 | HIS  |
| 2   | B     | 682 | HIS  |
| 2   | B     | 718 | HIS  |
| 2   | C     | 26  | HIS  |
| 2   | C     | 33  | HIS  |
| 2   | C     | 224 | GLN  |
| 2   | C     | 352 | GLN  |
| 2   | C     | 447 | GLN  |
| 2   | C     | 504 | ASN  |
| 2   | C     | 507 | HIS  |
| 2   | C     | 628 | ASN  |
| 2   | C     | 703 | ASN  |
| 2   | C     | 791 | HIS  |
| 2   | D     | 26  | HIS  |
| 2   | D     | 72  | GLN  |
| 2   | D     | 79  | HIS  |
| 2   | D     | 100 | HIS  |
| 2   | D     | 137 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 362 | HIS  |
| 2   | D     | 507 | HIS  |
| 2   | D     | 703 | ASN  |
| 2   | D     | 712 | HIS  |
| 2   | D     | 718 | HIS  |
| 2   | D     | 772 | HIS  |
| 2   | E     | 190 | GLN  |
| 2   | E     | 335 | GLN  |
| 2   | E     | 507 | HIS  |
| 2   | E     | 581 | HIS  |
| 2   | E     | 651 | ASN  |
| 2   | E     | 772 | HIS  |
| 2   | F     | 26  | HIS  |
| 2   | F     | 33  | HIS  |
| 2   | F     | 100 | HIS  |
| 2   | F     | 107 | HIS  |
| 2   | F     | 190 | GLN  |
| 2   | F     | 203 | ASN  |
| 2   | F     | 273 | ASN  |
| 2   | F     | 310 | GLN  |
| 2   | F     | 361 | HIS  |
| 2   | F     | 412 | ASN  |
| 2   | F     | 468 | ASN  |
| 2   | F     | 507 | HIS  |
| 2   | F     | 601 | GLN  |
| 2   | F     | 623 | HIS  |
| 2   | F     | 681 | ASN  |
| 2   | F     | 682 | HIS  |
| 2   | F     | 718 | HIS  |
| 2   | F     | 737 | GLN  |
| 2   | F     | 770 | GLN  |
| 2   | F     | 772 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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.

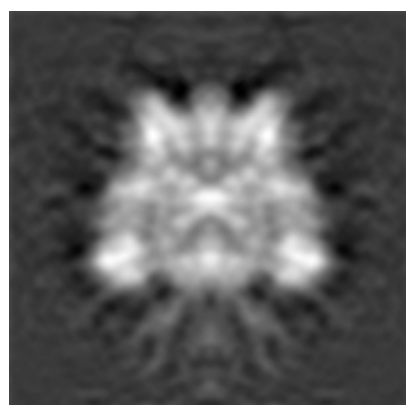
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5608. These allow visual inspection of the internal detail of the map and identification of artifacts.

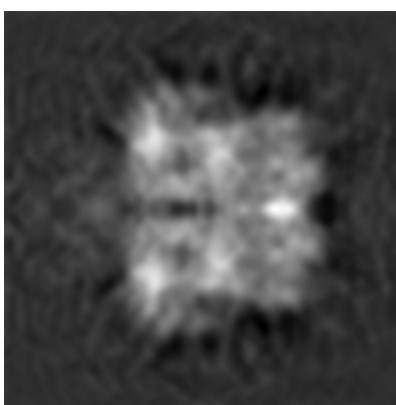
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

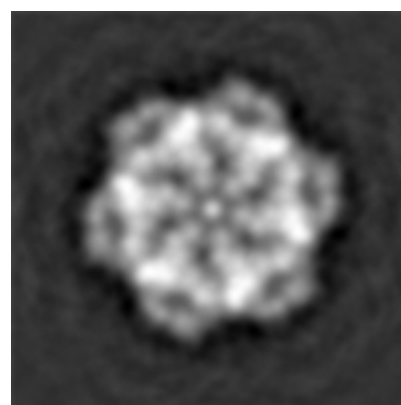
#### 6.1.1 Primary map



X



Y

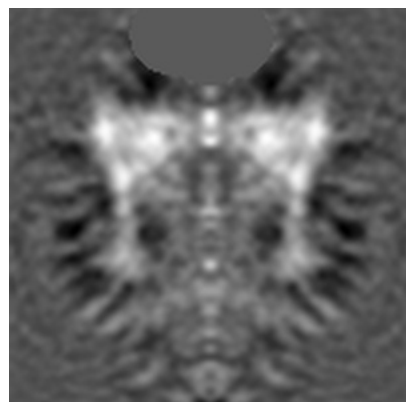


Z

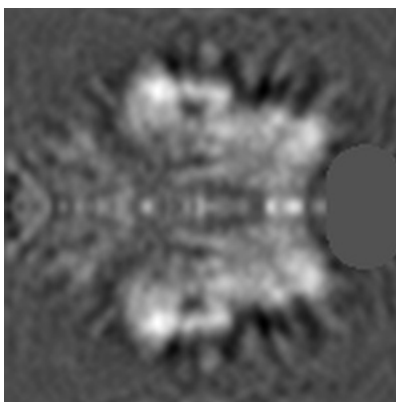
The images above show the map projected in three orthogonal directions.

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

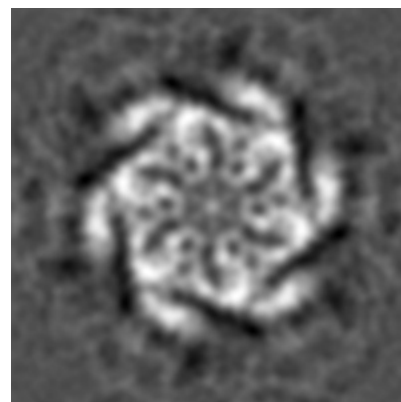
#### 6.2.1 Primary map



X Index: 75



Y Index: 75

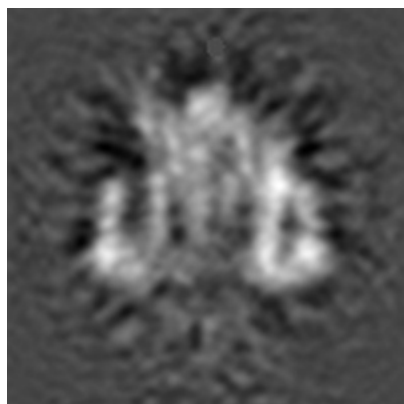


Z Index: 75

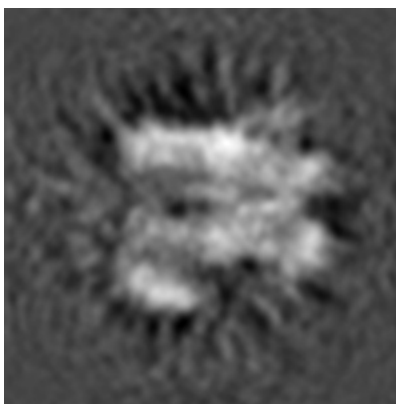
The images above show central slices of the map in three orthogonal directions.

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

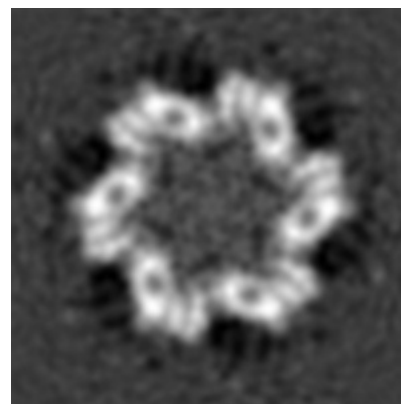
### 6.3.1 Primary map



X Index: 98



Y Index: 100

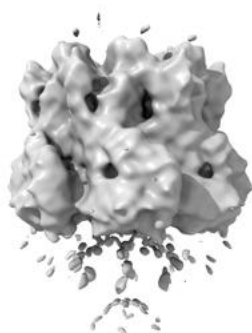


Z Index: 57

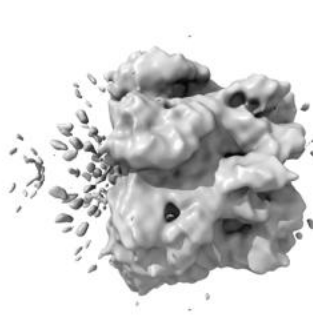
The images above show the largest variance slices of the map in three orthogonal directions.

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

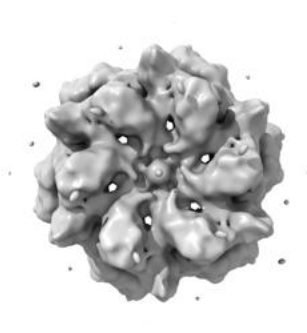
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

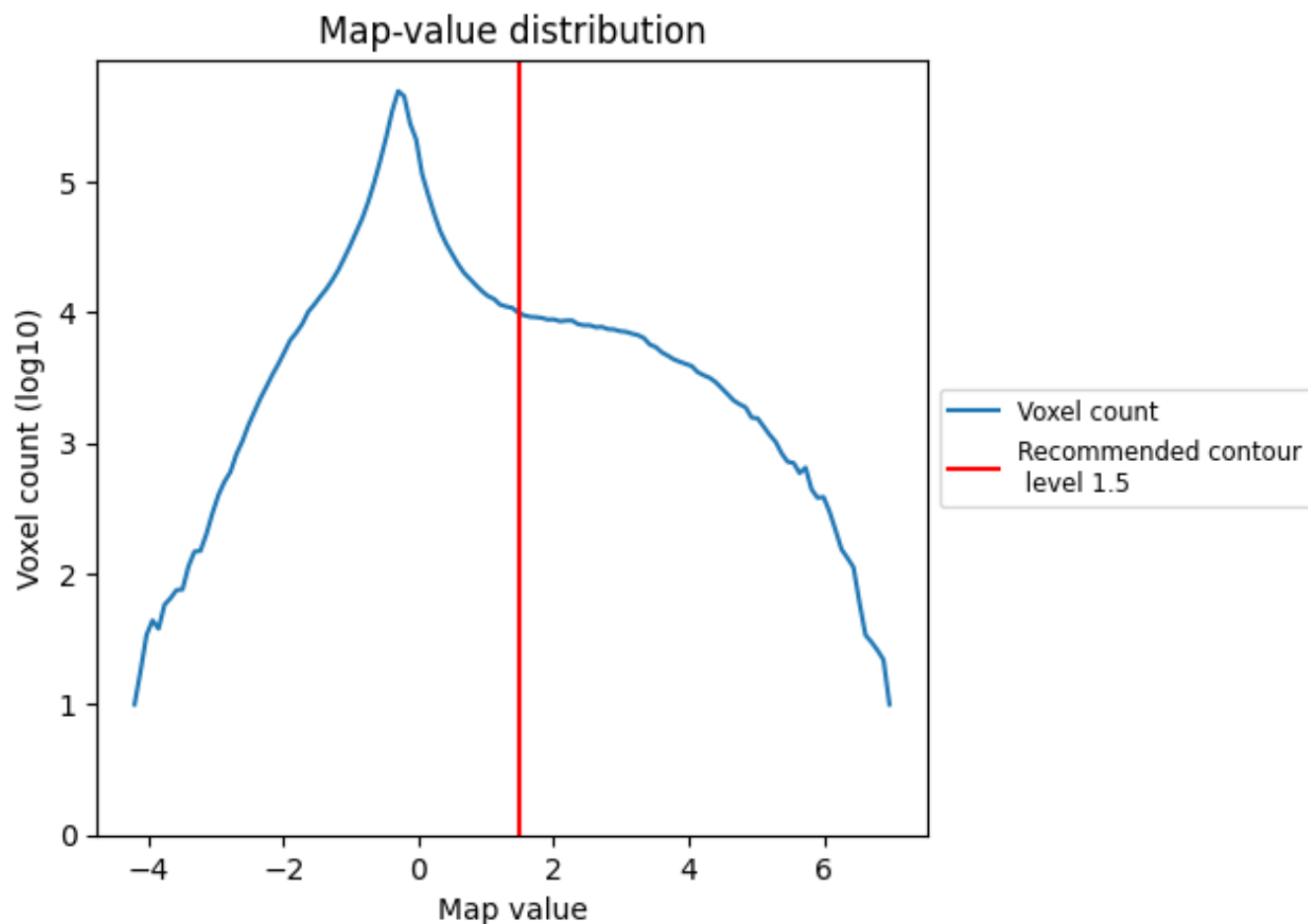
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

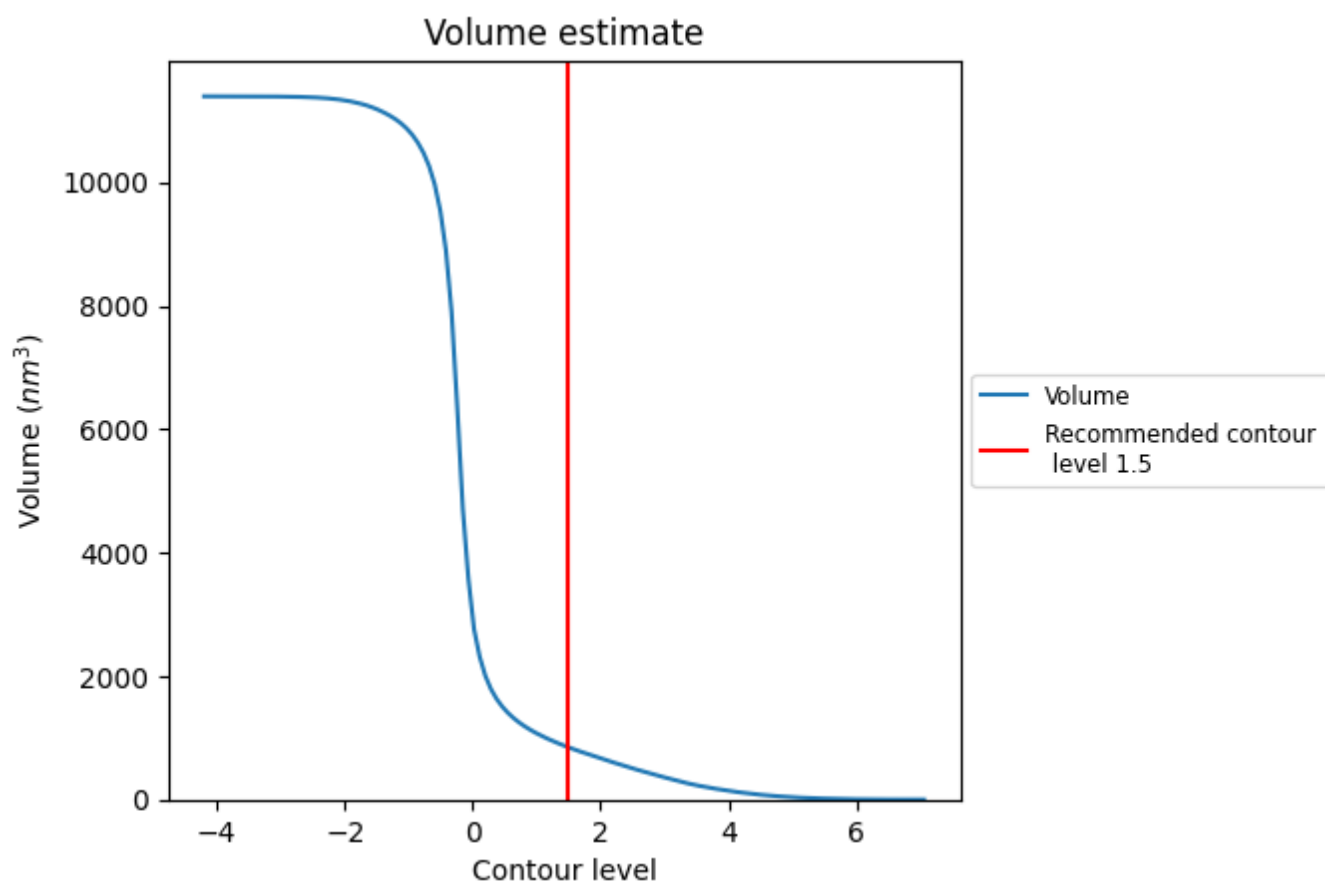
This section contains the results of statistical analysis of the map.

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



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

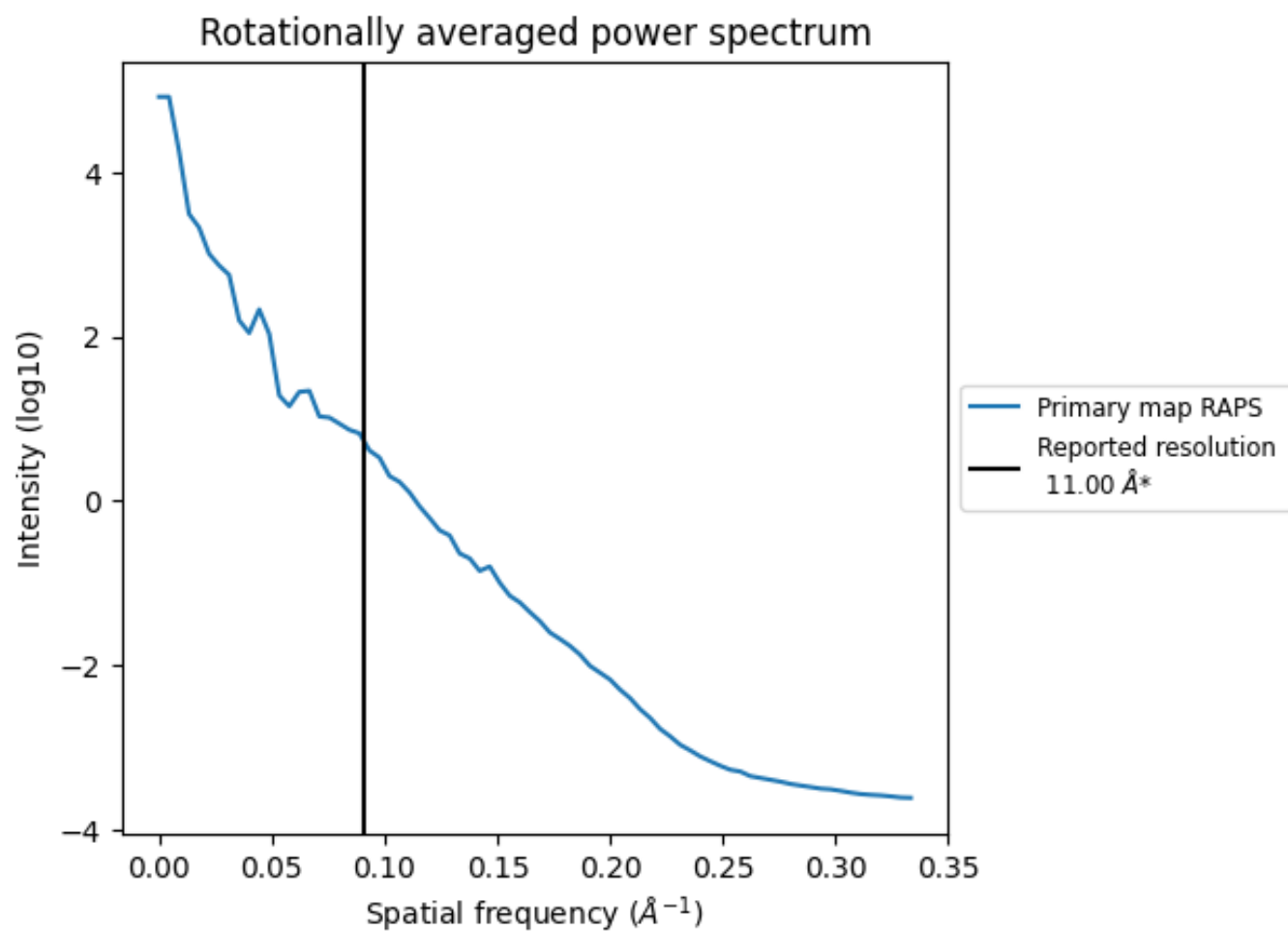
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 846 nm<sup>3</sup>; this corresponds to an approximate mass of 764 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 0.091 Å<sup>-1</sup>

## 8 Fourier-Shell correlation ⓘ

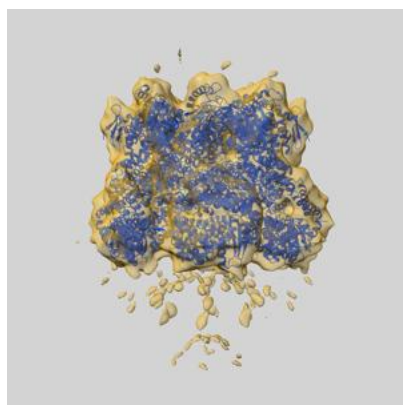
This section was not generated. No FSC curve or half-maps provided.



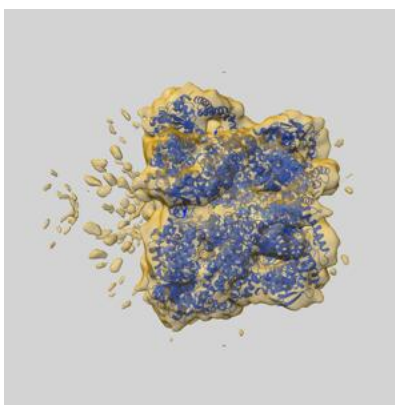
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5608 and PDB model 3J3S. Per-residue inclusion information can be found in section 3 on page 6.

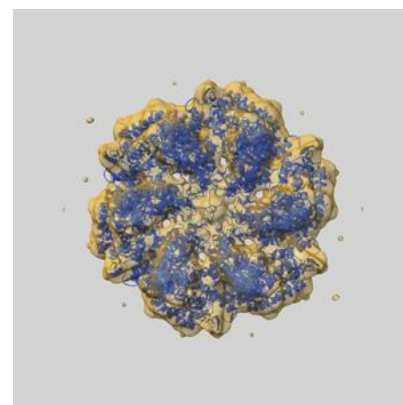
### 9.1 Map-model overlay [i](#)



X



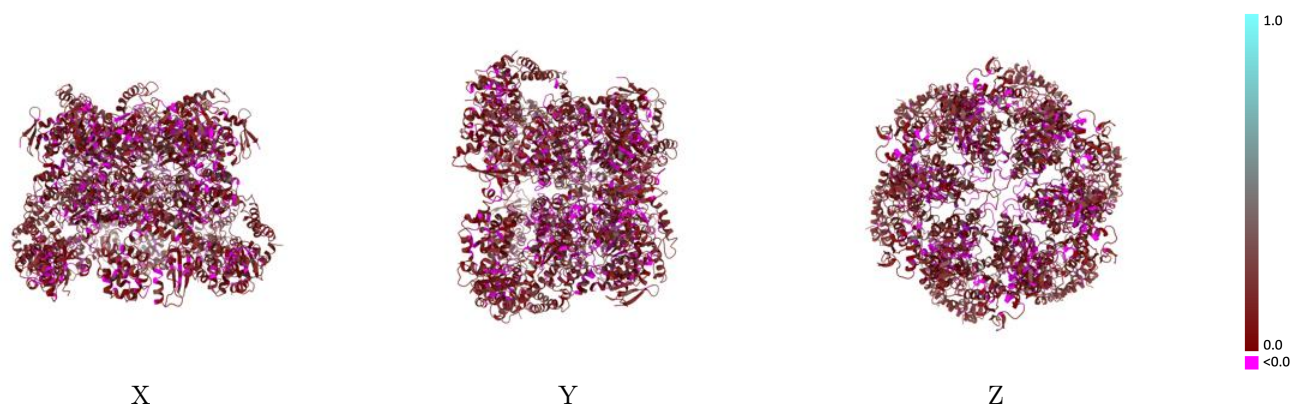
Y



Z

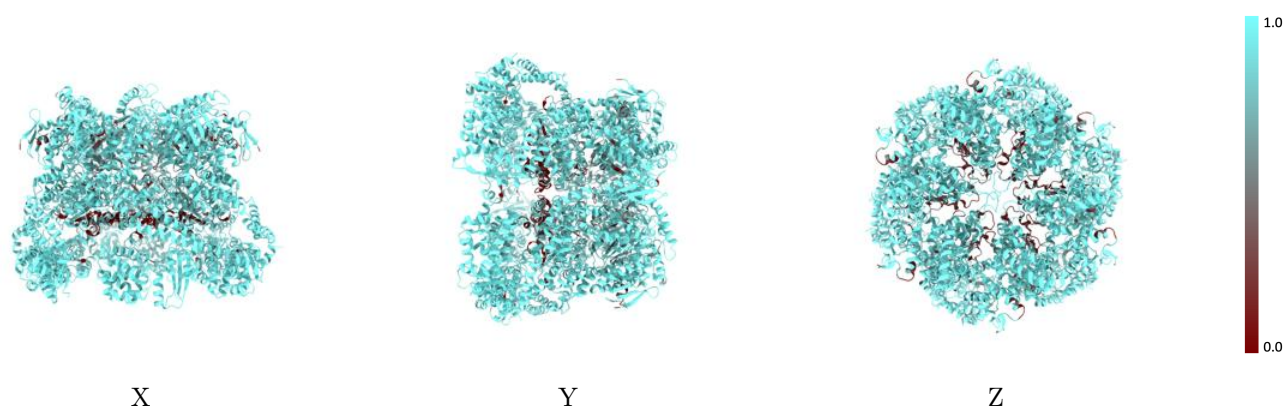
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



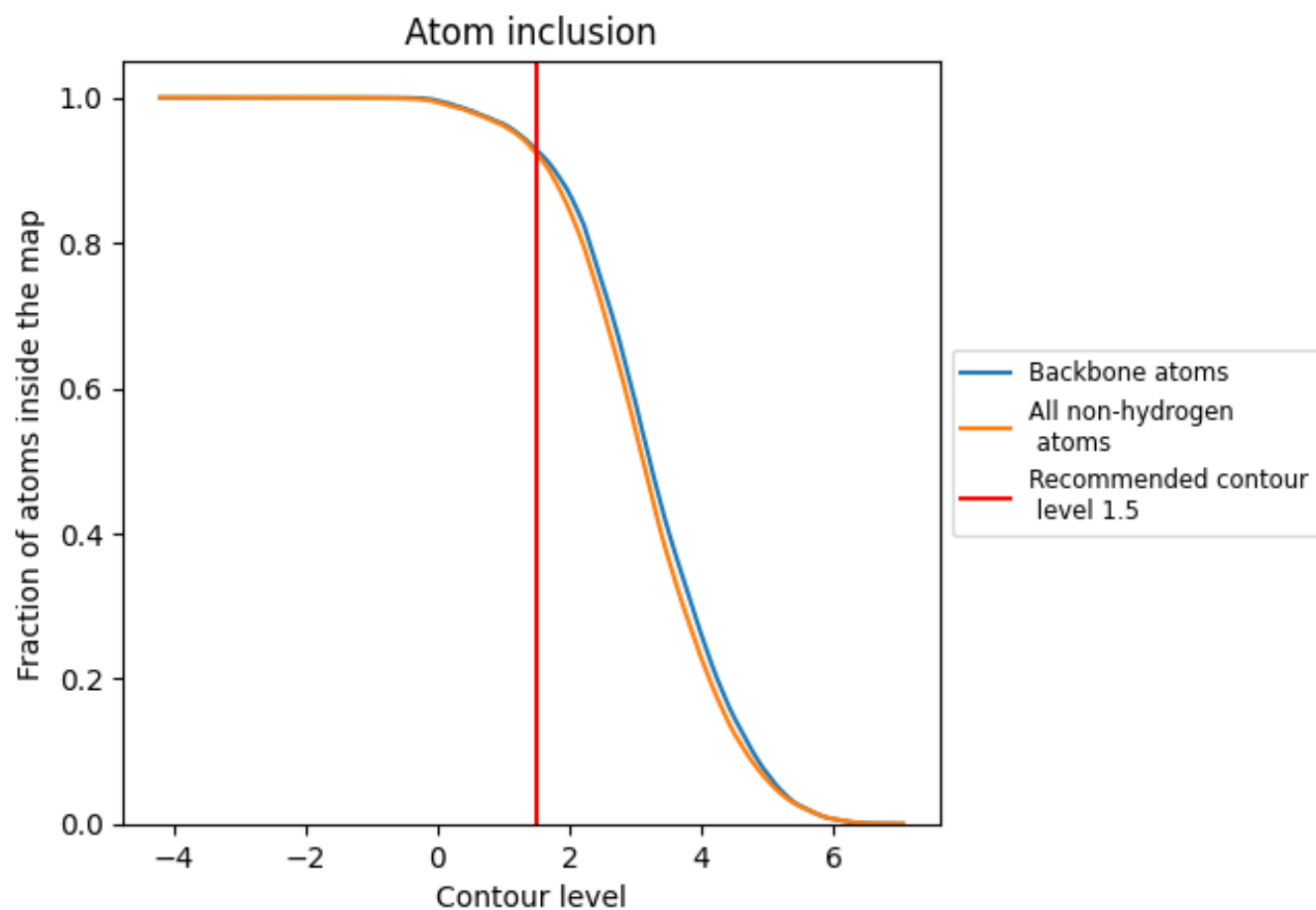
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (1.5) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion               | Q-score                      |
|-------|------------------------------|------------------------------|
| All   | <div><div></div>0.9231</div> | <div><div></div>0.1040</div> |
| 1     | <div><div></div>0.9569</div> | <div><div></div>0.0990</div> |
| 2     | <div><div></div>0.9621</div> | <div><div></div>0.0980</div> |
| 3     | <div><div></div>0.9647</div> | <div><div></div>0.1010</div> |
| 4     | <div><div></div>0.9765</div> | <div><div></div>0.0890</div> |
| 5     | <div><div></div>0.9739</div> | <div><div></div>0.0890</div> |
| 6     | <div><div></div>0.9621</div> | <div><div></div>0.1000</div> |
| A     | <div><div></div>0.9142</div> | <div><div></div>0.1050</div> |
| B     | <div><div></div>0.9137</div> | <div><div></div>0.1060</div> |
| C     | <div><div></div>0.9200</div> | <div><div></div>0.1050</div> |
| D     | <div><div></div>0.9215</div> | <div><div></div>0.1010</div> |
| E     | <div><div></div>0.9192</div> | <div><div></div>0.1030</div> |
| F     | <div><div></div>0.9175</div> | <div><div></div>0.1060</div> |

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