



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:40 AM UTC

PDB ID : 9OT6 / pdb\_00009ot6  
EMDB ID : EMD-70826  
Title : Cryo-EM structure of the PI4KA complex bound to an EFR3 interfering nanobody (F3IN)  
Authors : Shaw, A.L.; Suresh, S.; Yip, C.K.; Burke, J.E.  
Deposited on : 2025-05-26  
Resolution : 3.54 Å (reported)  
Based on initial models : ., 9BAX

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : **NOT EXECUTED**  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

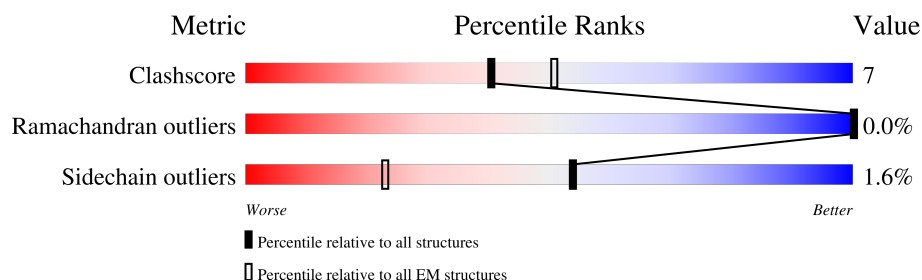
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.54 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            | 229148                      | 23984                       |
| Ramachandran outliers | 224038                      | 23583                       |
| Sidechain outliers    | 223484                      | 23102                       |

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  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 2104   | 67% 14% 18%      |
| 1   | B     | 2104   | 67% 15% 18%      |
| 2   | C     | 165    | 48% 14% 37%      |
| 2   | H     | 165    | 50% 12% 37%      |
| 3   | D     | 843    | 58% 11% 30%      |
| 3   | F     | 843    | 58% 12% 30%      |
| 4   | E     | 308    | 67% 14% 18%      |
| 4   | G     | 308    | 67% 14% 18%      |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 42678 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 Phosphatidylinositol 4-kinase alpha.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 1724     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 13842 | 8951 | 2305 | 2489 | 97 |         |       |
| 1   | B     | 1724     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 13842 | 8951 | 2305 | 2489 | 97 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -1      | GLY      | -      | expression tag | UNP P42356 |
| A     | 0       | SER      | -      | expression tag | UNP P42356 |
| B     | -1      | GLY      | -      | expression tag | UNP P42356 |
| B     | 0       | SER      | -      | expression tag | UNP P42356 |

- Molecule 2 is a protein called EFR3 interfering Nanobody (F3IN).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | C     | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 811   | 511 | 141 | 154 | 5 |         |       |
| 2   | H     | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 811   | 511 | 141 | 154 | 5 |         |       |

- Molecule 3 is a protein called Tetratricopeptide repeat protein 7B.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | D     | 592      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4676  | 2983 | 811 | 855 | 27 |         |       |
| 3   | F     | 592      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4676  | 2983 | 811 | 855 | 27 |         |       |

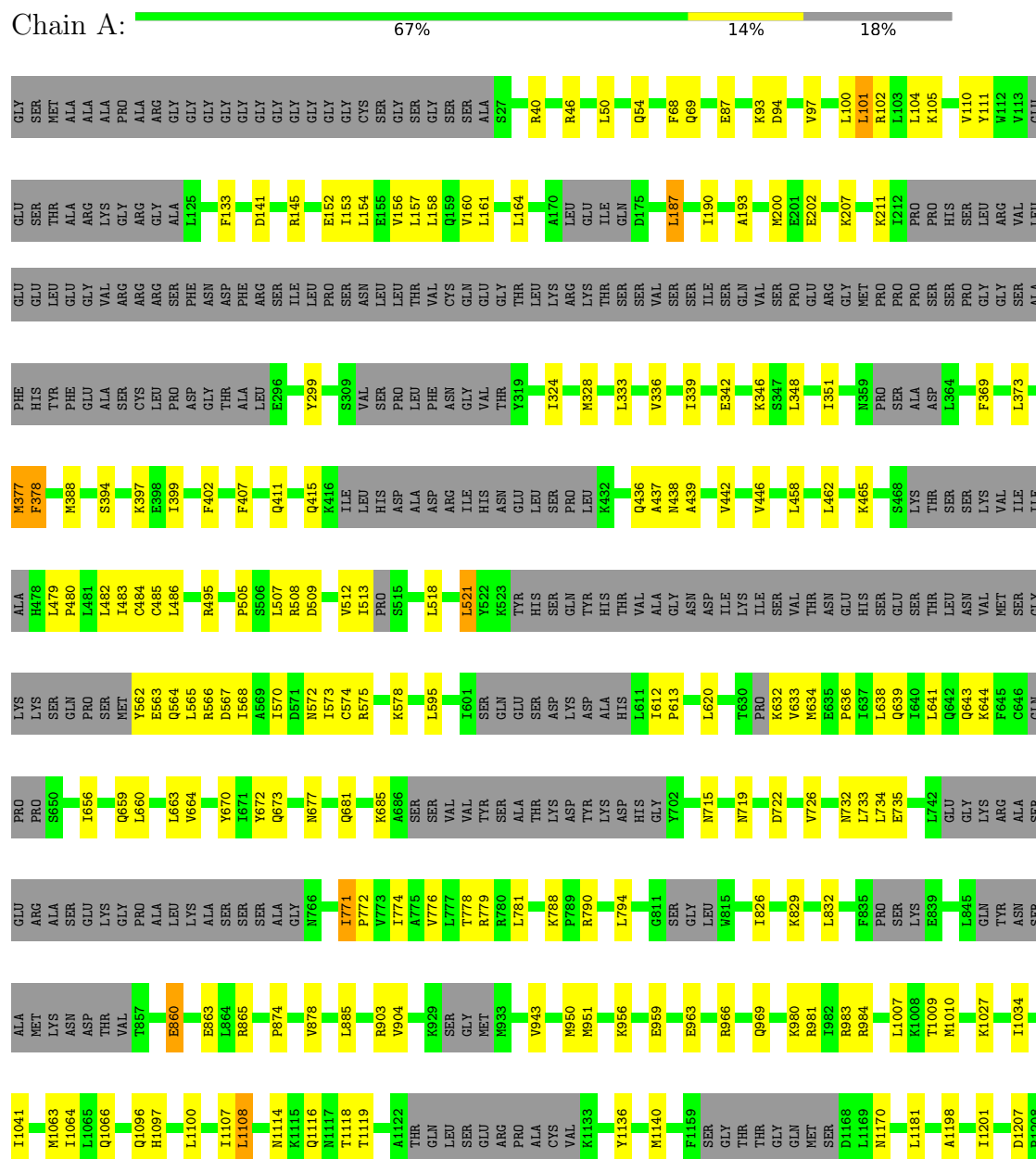
- Molecule 4 is a protein called Hyccin.

| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 4   | E     | 252      | Total<br>2010 | C<br>1309 | N<br>323 | O<br>366 | S<br>12 | 0       | 0     |
| 4   | G     | 252      | Total<br>2010 | C<br>1309 | N<br>323 | O<br>366 | S<br>12 | 0       | 0     |

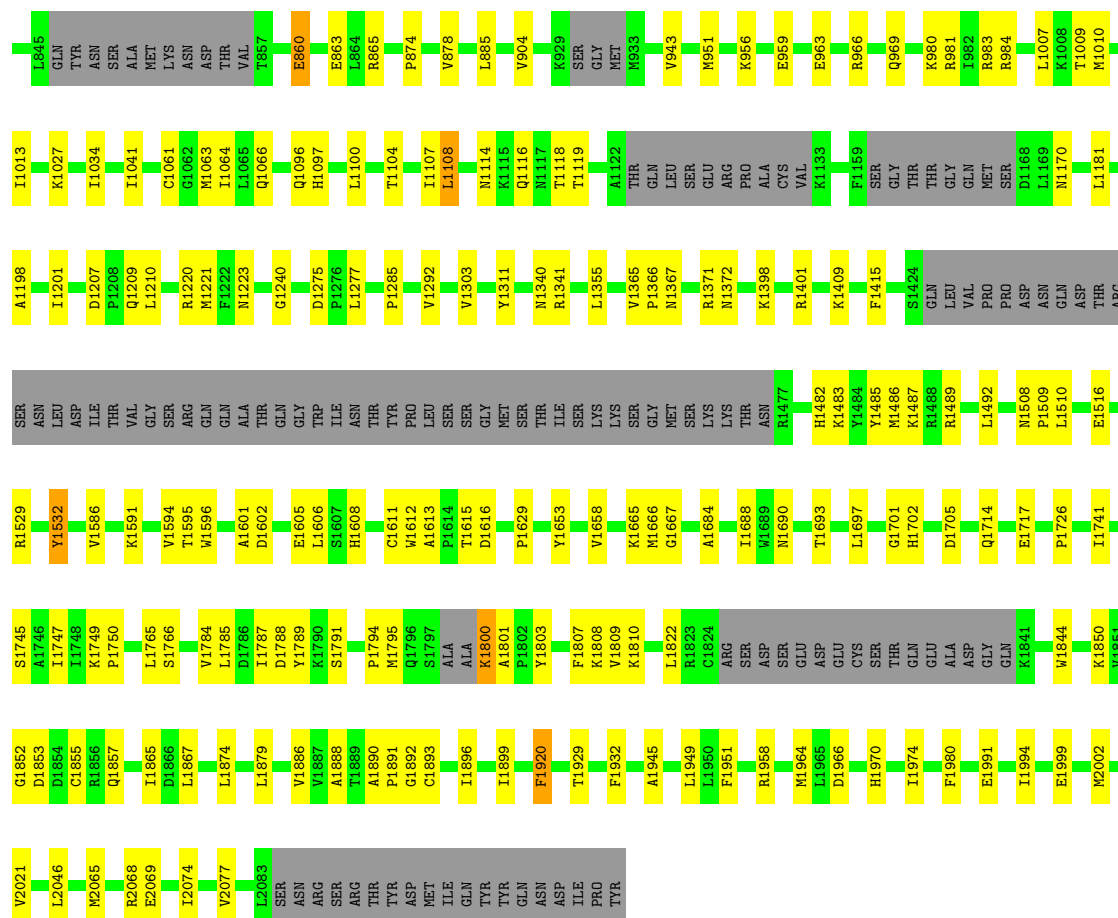
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Phosphatidylinositol 4-kinase alpha

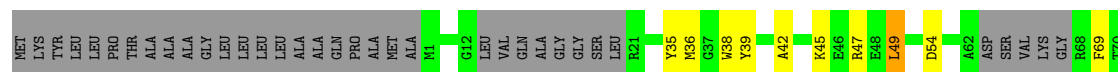






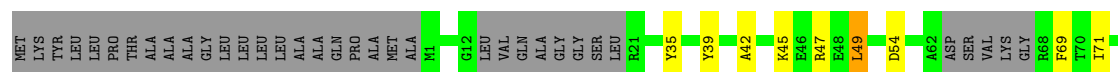
• Molecule 2: EFR3 interfering Nanobody (F3IN)

Chain C: 48% 14% 37%

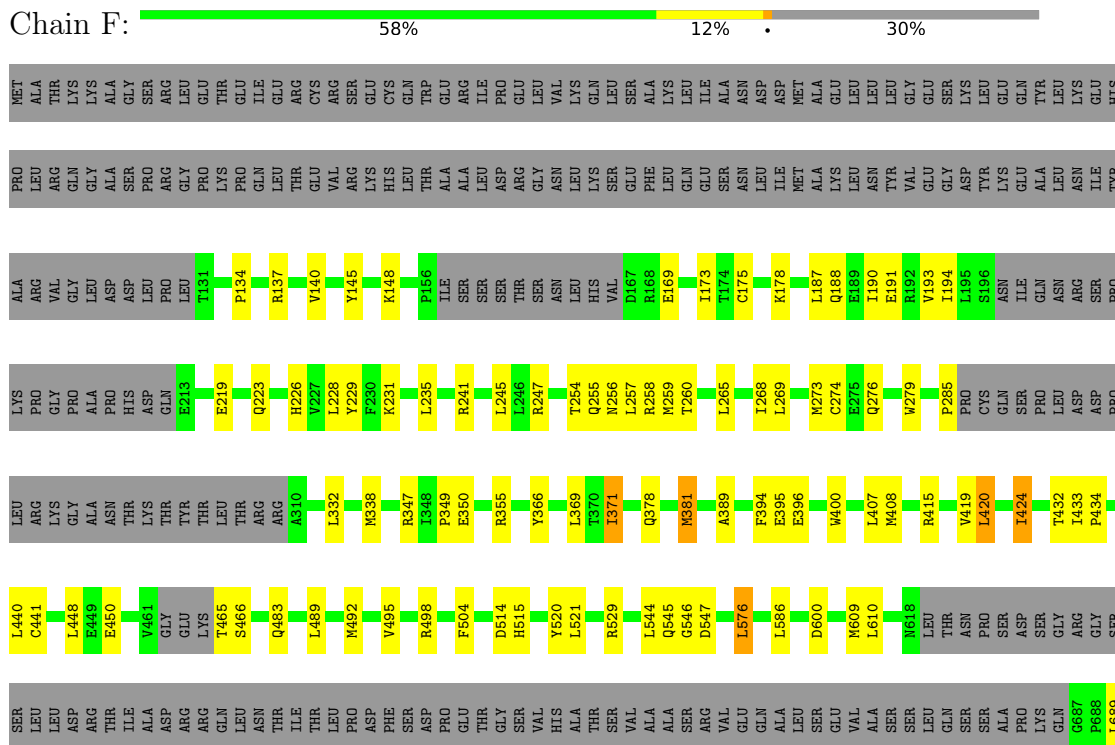


• Molecule 2: EFR3 interfering Nanobody (F3IN)

Chain H: 50% 12% 37%

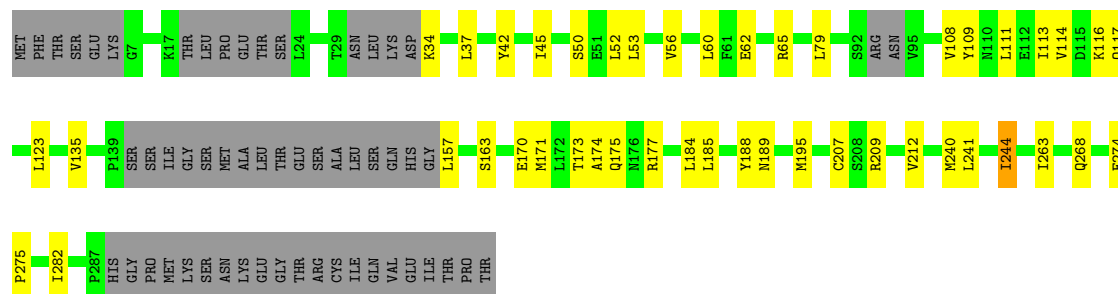


• Molecule 3: Tetratricopeptide repeat protein 7B

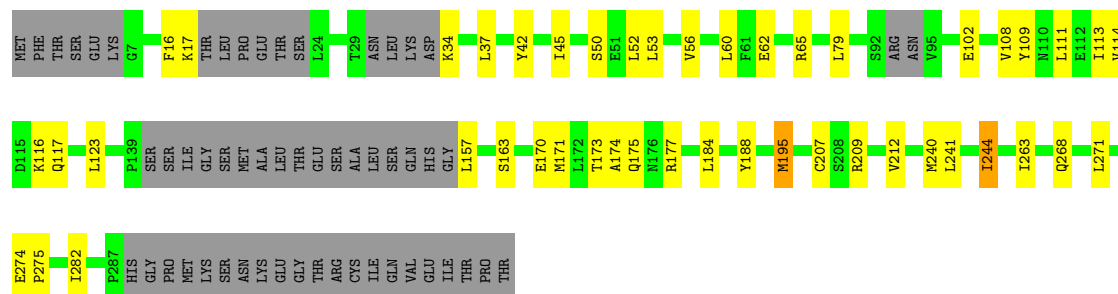




• Molecule 4: Hyccin



• Molecule 4: Hyccin



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C2                               | Depositor |
| Number of particles used             | 282982                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | 165000                                  | Depositor |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |

## 5 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | A     | 0.10         | 0/14149 | 0.26        | 0/19141 |
| 1   | B     | 0.10         | 0/14149 | 0.26        | 0/19141 |
| 2   | C     | 0.11         | 0/826   | 0.33        | 0/1116  |
| 2   | H     | 0.11         | 0/826   | 0.33        | 0/1116  |
| 3   | D     | 0.09         | 0/4762  | 0.25        | 0/6443  |
| 3   | F     | 0.09         | 0/4762  | 0.25        | 0/6443  |
| 4   | E     | 0.10         | 0/2058  | 0.28        | 0/2793  |
| 4   | G     | 0.10         | 0/2058  | 0.28        | 0/2793  |
| All | All   | 0.10         | 0/43590 | 0.26        | 0/58986 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 13842 | 0        | 13974    | 193     | 0            |
| 1   | B     | 13842 | 0        | 13974    | 197     | 0            |
| 2   | C     | 811   | 0        | 771      | 20      | 0            |
| 2   | H     | 811   | 0        | 771      | 15      | 0            |
| 3   | D     | 4676  | 0        | 4734     | 66      | 0            |
| 3   | F     | 4676  | 0        | 4734     | 68      | 0            |
| 4   | E     | 2010  | 0        | 2017     | 27      | 0            |
| 4   | G     | 2010  | 0        | 2017     | 28      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All   | 42678 | 0        | 42992    | 598     | 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 7.

All (598) 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:H:92:THR:HA     | 2:H:120:VAL:O     | 1.73                     | 0.88              |
| 2:C:92:THR:HA     | 2:C:120:VAL:O     | 1.73                     | 0.88              |
| 3:F:378:GLN:HB3   | 3:F:381:MET:HE1   | 1.56                     | 0.88              |
| 3:D:378:GLN:HB3   | 3:D:381:MET:HE1   | 1.56                     | 0.87              |
| 3:D:347:ARG:HG3   | 3:D:349:PRO:HD3   | 1.66                     | 0.76              |
| 3:F:347:ARG:HG3   | 3:F:349:PRO:HD3   | 1.66                     | 0.75              |
| 1:A:1666:MET:HE3  | 1:A:1667:GLY:H    | 1.53                     | 0.74              |
| 1:B:1666:MET:HE3  | 1:B:1667:GLY:H    | 1.53                     | 0.73              |
| 3:D:424:ILE:HD11  | 3:D:434:PRO:HD3   | 1.72                     | 0.72              |
| 3:F:424:ILE:HD11  | 3:F:434:PRO:HD3   | 1.72                     | 0.70              |
| 3:D:371:ILE:HG13  | 4:G:282:ILE:HD11  | 1.70                     | 0.70              |
| 4:E:113:ILE:HG23  | 4:E:114:VAL:HG23  | 1.74                     | 0.70              |
| 4:G:113:ILE:HG23  | 4:G:114:VAL:HG23  | 1.74                     | 0.69              |
| 1:B:1201:ILE:HD11 | 1:B:1240:GLY:HA3  | 1.75                     | 0.69              |
| 1:B:1865:ILE:HG12 | 1:B:1949:LEU:HD11 | 1.76                     | 0.68              |
| 1:A:46:ARG:NH2    | 1:A:87:GLU:O      | 2.27                     | 0.67              |
| 1:B:46:ARG:NH2    | 1:B:87:GLU:O      | 2.27                     | 0.67              |
| 1:A:1201:ILE:HD11 | 1:A:1240:GLY:HA3  | 1.75                     | 0.67              |
| 1:A:1865:ILE:HG12 | 1:A:1949:LEU:HD11 | 1.76                     | 0.67              |
| 1:B:1596:TRP:HE1  | 1:B:1602:ASP:H    | 1.43                     | 0.66              |
| 1:A:339:ILE:HD12  | 1:A:377:MET:HG3   | 1.78                     | 0.65              |
| 1:B:980:LYS:HD2   | 1:B:983:ARG:HH21  | 1.62                     | 0.65              |
| 4:E:135:VAL:O     | 3:F:247:ARG:NH2   | 2.29                     | 0.65              |
| 1:A:1596:TRP:HE1  | 1:A:1602:ASP:H    | 1.43                     | 0.65              |
| 1:B:1034:ILE:HD11 | 1:B:1041:ILE:HG12 | 1.79                     | 0.65              |
| 3:F:274:CYS:SG    | 3:F:276:GLN:NE2   | 2.70                     | 0.65              |
| 1:A:568:ILE:O     | 1:A:572:ASN:ND2   | 2.30                     | 0.65              |
| 1:A:771:ILE:HG13  | 1:A:772:PRO:HD3   | 1.78                     | 0.65              |
| 2:H:95:TYR:O      | 2:H:117:GLY:HA2   | 1.97                     | 0.65              |
| 1:A:980:LYS:HD2   | 1:A:983:ARG:HH21  | 1.62                     | 0.65              |
| 3:D:274:CYS:SG    | 3:D:276:GLN:NE2   | 2.70                     | 0.65              |
| 1:B:339:ILE:HD12  | 1:B:377:MET:HG3   | 1.78                     | 0.64              |
| 1:A:507:LEU:HD13  | 1:A:573:ILE:HG12  | 1.78                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1034:ILE:HD11 | 1:A:1041:ILE:HG12 | 1.79                     | 0.64              |
| 1:A:1221:MET:O    | 1:A:1223:ASN:ND2  | 2.30                     | 0.64              |
| 1:B:507:LEU:HD13  | 1:B:573:ILE:HG12  | 1.79                     | 0.64              |
| 1:B:1221:MET:O    | 1:B:1223:ASN:ND2  | 2.30                     | 0.64              |
| 2:C:95:TYR:O      | 2:C:117:GLY:HA2   | 1.97                     | 0.64              |
| 1:B:771:ILE:HG13  | 1:B:772:PRO:HD3   | 1.79                     | 0.63              |
| 1:B:568:ILE:O     | 1:B:572:ASN:ND2   | 2.30                     | 0.63              |
| 1:B:378:PHE:HD2   | 1:B:437:ALA:HB1   | 1.63                     | 0.63              |
| 1:A:378:PHE:HD2   | 1:A:437:ALA:HB1   | 1.64                     | 0.63              |
| 1:A:735:GLU:OE2   | 1:A:790:ARG:NH2   | 2.30                     | 0.63              |
| 4:E:79:LEU:HD21   | 4:E:188:TYR:HB2   | 1.81                     | 0.62              |
| 1:A:673:GLN:O     | 1:A:677:ASN:ND2   | 2.28                     | 0.62              |
| 3:D:259:MET:HG2   | 3:D:338:MET:HE1   | 1.82                     | 0.62              |
| 2:C:42:ALA:H      | 2:C:45:LYS:HG2    | 1.65                     | 0.62              |
| 3:F:259:MET:HG2   | 3:F:338:MET:HE1   | 1.82                     | 0.62              |
| 1:B:1850:LYS:NZ   | 1:B:1855:CYS:SG   | 2.65                     | 0.62              |
| 1:B:865:ARG:NH2   | 1:B:885:LEU:O     | 2.32                     | 0.61              |
| 2:H:42:ALA:H      | 2:H:45:LYS:HG2    | 1.64                     | 0.61              |
| 1:A:164:LEU:HD22  | 1:A:187:LEU:HD11  | 1.82                     | 0.61              |
| 1:A:1207:ASP:OD1  | 1:A:1209:GLN:NE2  | 2.34                     | 0.61              |
| 1:A:1114:ASN:OD1  | 1:B:1096:GLN:NE2  | 2.34                     | 0.60              |
| 1:A:1890:ALA:HB3  | 1:A:1893:CYS:HB2  | 1.83                     | 0.60              |
| 1:B:164:LEU:HD22  | 1:B:187:LEU:HD11  | 1.82                     | 0.60              |
| 1:B:1749:LYS:HE2  | 1:B:1801:ALA:HB2  | 1.83                     | 0.60              |
| 4:G:79:LEU:HD21   | 4:G:188:TYR:HB2   | 1.81                     | 0.60              |
| 1:B:673:GLN:O     | 1:B:677:ASN:ND2   | 2.28                     | 0.60              |
| 1:B:1207:ASP:OD1  | 1:B:1209:GLN:NE2  | 2.34                     | 0.60              |
| 1:B:480:PRO:HA    | 1:B:483:ILE:HG12  | 1.83                     | 0.60              |
| 1:B:1890:ALA:HB3  | 1:B:1893:CYS:HB2  | 1.83                     | 0.60              |
| 1:A:1749:LYS:HE2  | 1:A:1801:ALA:HB2  | 1.83                     | 0.60              |
| 1:A:865:ARG:NH2   | 1:A:885:LEU:O     | 2.32                     | 0.59              |
| 1:A:1277:LEU:HD23 | 1:A:1867:LEU:HD11 | 1.84                     | 0.59              |
| 1:B:1665:LYS:O    | 3:D:347:ARG:NH1   | 2.26                     | 0.59              |
| 4:E:62:GLU:O      | 4:E:65:ARG:NE     | 2.34                     | 0.59              |
| 3:D:576:LEU:HD21  | 3:D:586:LEU:HD12  | 1.85                     | 0.58              |
| 1:A:480:PRO:HA    | 1:A:483:ILE:HG12  | 1.83                     | 0.58              |
| 1:A:634:MET:SD    | 1:A:634:MET:N     | 2.76                     | 0.58              |
| 1:A:595:LEU:HD13  | 1:A:620:LEU:HD21  | 1.84                     | 0.58              |
| 1:B:634:MET:SD    | 1:B:634:MET:N     | 2.76                     | 0.58              |
| 1:A:512:VAL:HG23  | 1:A:513:ILE:HG13  | 1.85                     | 0.58              |
| 1:A:788:LYS:HG3   | 1:A:790:ARG:H     | 1.67                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:595:LEU:HD13  | 1:B:620:LEU:HD21  | 1.84                     | 0.58              |
| 1:A:1850:LYS:NZ   | 1:A:1855:CYS:SG   | 2.65                     | 0.58              |
| 3:F:257:LEU:O     | 3:F:260:THR:OG1   | 2.18                     | 0.58              |
| 3:F:586:LEU:HB3   | 3:F:609:MET:HE2   | 1.86                     | 0.58              |
| 3:D:545:GLN:HE21  | 3:D:547:ASP:HB2   | 1.68                     | 0.58              |
| 1:A:572:ASN:OD1   | 1:A:575:ARG:NH2   | 2.37                     | 0.58              |
| 3:F:576:LEU:HD21  | 3:F:586:LEU:HD12  | 1.84                     | 0.58              |
| 4:G:62:GLU:O      | 4:G:65:ARG:NE     | 2.34                     | 0.58              |
| 1:A:1852:GLY:N    | 1:A:1892:GLY:O    | 2.37                     | 0.58              |
| 1:B:788:LYS:HG3   | 1:B:790:ARG:H     | 1.67                     | 0.58              |
| 1:B:1277:LEU:HD23 | 1:B:1867:LEU:HD11 | 1.84                     | 0.58              |
| 1:A:446:VAL:HG12  | 1:A:458:LEU:HD11  | 1.86                     | 0.57              |
| 1:B:512:VAL:HG23  | 1:B:513:ILE:HG13  | 1.85                     | 0.57              |
| 3:F:545:GLN:HE21  | 3:F:547:ASP:HB2   | 1.68                     | 0.57              |
| 1:B:735:GLU:OE2   | 1:B:790:ARG:NH2   | 2.30                     | 0.57              |
| 1:B:1372:ASN:OD1  | 1:B:1485:TYR:OH   | 2.22                     | 0.57              |
| 1:B:1852:GLY:N    | 1:B:1892:GLY:O    | 2.37                     | 0.57              |
| 3:D:586:LEU:HB3   | 3:D:609:MET:HE2   | 1.85                     | 0.57              |
| 2:H:39:TYR:CZ     | 2:H:49:LEU:HD13   | 2.40                     | 0.57              |
| 1:B:446:VAL:HG12  | 1:B:458:LEU:HD11  | 1.87                     | 0.57              |
| 1:A:1372:ASN:OD1  | 1:A:1485:TYR:OH   | 2.22                     | 0.57              |
| 1:B:1303:VAL:HG22 | 1:B:1355:LEU:HD13 | 1.87                     | 0.57              |
| 2:C:39:TYR:CZ     | 2:C:49:LEU:HD13   | 2.40                     | 0.57              |
| 3:D:515:HIS:HB3   | 3:D:544:LEU:HD22  | 1.85                     | 0.57              |
| 1:B:1483:LYS:HG2  | 1:B:1487:LYS:HE2  | 1.87                     | 0.57              |
| 1:B:1596:TRP:NE1  | 1:B:1602:ASP:O    | 2.38                     | 0.57              |
| 1:A:154:LEU:O     | 1:A:157:LEU:HB2   | 2.05                     | 0.57              |
| 1:A:981:ARG:HG2   | 1:A:984:ARG:HH21  | 1.70                     | 0.57              |
| 1:B:572:ASN:OD1   | 1:B:575:ARG:NH2   | 2.37                     | 0.57              |
| 1:A:1483:LYS:HG2  | 1:A:1487:LYS:HE2  | 1.87                     | 0.56              |
| 1:A:1303:VAL:HG22 | 1:A:1355:LEU:HD13 | 1.87                     | 0.56              |
| 1:A:1787:ILE:HG22 | 1:A:1807:PHE:HD2  | 1.70                     | 0.56              |
| 1:B:154:LEU:O     | 1:B:157:LEU:HB2   | 2.05                     | 0.56              |
| 1:B:1787:ILE:HG22 | 1:B:1807:PHE:HD2  | 1.70                     | 0.56              |
| 3:F:235:LEU:HD11  | 3:F:268:ILE:HD11  | 1.87                     | 0.56              |
| 3:F:515:HIS:HB3   | 3:F:544:LEU:HD22  | 1.85                     | 0.56              |
| 4:G:116:LYS:HG3   | 4:G:117:GLN:H     | 1.70                     | 0.56              |
| 1:B:1726:PRO:HB2  | 1:B:1822:LEU:HD12 | 1.87                     | 0.56              |
| 3:D:235:LEU:HD11  | 3:D:268:ILE:HD11  | 1.86                     | 0.56              |
| 3:D:741:GLU:HG2   | 3:D:746:MET:HE1   | 1.88                     | 0.56              |
| 3:F:741:GLU:HG2   | 3:F:746:MET:HE1   | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1285:PRO:HB2  | 1:A:1874:LEU:HD13 | 1.88                     | 0.56              |
| 1:B:981:ARG:HG2   | 1:B:984:ARG:HH21  | 1.70                     | 0.56              |
| 1:B:369:PHE:O     | 1:B:373:LEU:HB2   | 2.06                     | 0.56              |
| 1:B:963:GLU:OE1   | 1:B:966:ARG:NH1   | 2.30                     | 0.56              |
| 1:A:1596:TRP:NE1  | 1:A:1602:ASP:O    | 2.38                     | 0.56              |
| 1:B:521:LEU:HD21  | 1:B:562:TYR:HA    | 1.87                     | 0.56              |
| 1:B:1285:PRO:HB2  | 1:B:1874:LEU:HD13 | 1.88                     | 0.56              |
| 1:A:521:LEU:HD21  | 1:A:562:TYR:HA    | 1.87                     | 0.56              |
| 1:B:565:LEU:HD23  | 1:B:565:LEU:H     | 1.71                     | 0.56              |
| 4:E:116:LYS:HG3   | 4:E:117:GLN:H     | 1.70                     | 0.55              |
| 1:B:1784:VAL:HA   | 1:B:1809:VAL:HG23 | 1.89                     | 0.55              |
| 1:A:369:PHE:O     | 1:A:373:LEU:HB2   | 2.05                     | 0.55              |
| 4:E:50:SER:HB2    | 4:E:53:LEU:HG     | 1.88                     | 0.55              |
| 3:F:720:GLN:HG2   | 3:F:736:ARG:HH22  | 1.72                     | 0.55              |
| 1:A:1784:VAL:HA   | 1:A:1809:VAL:HG23 | 1.89                     | 0.55              |
| 1:A:565:LEU:HD23  | 1:A:565:LEU:H     | 1.71                     | 0.55              |
| 1:B:505:PRO:HA    | 1:B:508:ARG:HG2   | 1.89                     | 0.55              |
| 1:B:1586:VAL:HG12 | 1:B:1612:TRP:HE3  | 1.72                     | 0.55              |
| 4:G:50:SER:HB2    | 4:G:53:LEU:HG     | 1.88                     | 0.55              |
| 1:B:2065:MET:HE2  | 1:B:2069:GLU:HB3  | 1.89                     | 0.54              |
| 1:B:161:LEU:HD13  | 1:B:164:LEU:HD12  | 1.89                     | 0.54              |
| 1:A:161:LEU:HD13  | 1:A:164:LEU:HD12  | 1.89                     | 0.54              |
| 1:A:1726:PRO:HB2  | 1:A:1822:LEU:HD12 | 1.87                     | 0.54              |
| 1:A:505:PRO:HA    | 1:A:508:ARG:HG2   | 1.89                     | 0.54              |
| 1:A:1586:VAL:HG12 | 1:A:1612:TRP:HE3  | 1.72                     | 0.54              |
| 1:A:1794:PRO:HA   | 1:A:1803:TYR:HA   | 1.89                     | 0.54              |
| 1:A:2065:MET:HE2  | 1:A:2069:GLU:HB3  | 1.89                     | 0.54              |
| 1:A:436:GLN:N     | 1:A:436:GLN:OE1   | 2.40                     | 0.54              |
| 1:A:101:LEU:HD13  | 1:A:104:LEU:HD21  | 1.90                     | 0.54              |
| 1:A:1608:HIS:O    | 1:A:1608:HIS:ND1  | 2.41                     | 0.54              |
| 1:B:101:LEU:HD13  | 1:B:104:LEU:HD21  | 1.90                     | 0.54              |
| 3:D:720:GLN:HG2   | 3:D:736:ARG:HH22  | 1.72                     | 0.54              |
| 3:F:169:GLU:O     | 3:F:173:ILE:HG12  | 2.08                     | 0.54              |
| 1:B:639:GLN:O     | 1:B:643:GLN:NE2   | 2.41                     | 0.53              |
| 1:B:1794:PRO:HA   | 1:B:1803:TYR:HA   | 1.89                     | 0.53              |
| 1:B:1899:ILE:HD11 | 1:B:1964:MET:HG2  | 1.89                     | 0.53              |
| 1:A:438:ASN:O     | 1:A:442:VAL:HG23  | 2.09                     | 0.53              |
| 1:B:388:MET:SD    | 1:B:388:MET:N     | 2.80                     | 0.53              |
| 1:B:438:ASN:O     | 1:B:442:VAL:HG23  | 2.09                     | 0.53              |
| 1:B:1529:ARG:HA   | 1:B:1532:TYR:HD1  | 1.73                     | 0.53              |
| 3:D:257:LEU:O     | 3:D:260:THR:OG1   | 2.18                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:639:GLN:O     | 1:A:643:GLN:NE2   | 2.41                     | 0.53              |
| 3:D:256:ASN:HA    | 3:D:259:MET:HE3   | 1.91                     | 0.53              |
| 1:B:1608:HIS:O    | 1:B:1608:HIS:ND1  | 2.41                     | 0.53              |
| 1:A:715:ASN:O     | 1:A:719:ASN:ND2   | 2.38                     | 0.53              |
| 1:A:963:GLU:OE1   | 1:A:966:ARG:NH1   | 2.30                     | 0.53              |
| 1:A:1899:ILE:HD11 | 1:A:1964:MET:HG2  | 1.89                     | 0.53              |
| 3:F:256:ASN:HA    | 3:F:259:MET:HE3   | 1.91                     | 0.53              |
| 1:A:388:MET:SD    | 1:A:388:MET:N     | 2.80                     | 0.53              |
| 1:B:612:ILE:N     | 1:B:613:PRO:HD2   | 2.24                     | 0.53              |
| 1:A:1529:ARG:HA   | 1:A:1532:TYR:HD1  | 1.73                     | 0.52              |
| 1:B:1951:PHE:HB2  | 1:B:1994:ILE:HD11 | 1.92                     | 0.52              |
| 1:B:202:GLU:OE2   | 1:B:207:LYS:NZ    | 2.32                     | 0.52              |
| 1:B:1401:ARG:NH2  | 1:B:1516:GLU:O    | 2.43                     | 0.52              |
| 3:D:169:GLU:O     | 3:D:173:ILE:HG12  | 2.08                     | 0.52              |
| 3:F:600:ASP:OD1   | 3:F:600:ASP:N     | 2.41                     | 0.52              |
| 2:H:95:TYR:O      | 2:H:117:GLY:CA    | 2.57                     | 0.52              |
| 1:A:612:ILE:N     | 1:A:613:PRO:HD2   | 2.24                     | 0.52              |
| 1:A:1401:ARG:NH2  | 1:A:1516:GLU:O    | 2.43                     | 0.52              |
| 1:B:68:PHE:HB2    | 1:B:110:VAL:HG22  | 1.91                     | 0.52              |
| 1:B:1929:THR:HG23 | 1:B:1932:PHE:H    | 1.75                     | 0.52              |
| 1:B:715:ASN:O     | 1:B:719:ASN:ND2   | 2.38                     | 0.52              |
| 3:D:273:MET:SD    | 3:D:273:MET:N     | 2.83                     | 0.52              |
| 2:C:95:TYR:O      | 2:C:117:GLY:CA    | 2.57                     | 0.52              |
| 3:D:255:GLN:O     | 3:D:258:ARG:HB2   | 2.10                     | 0.52              |
| 3:D:751:ARG:NH1   | 3:D:755:GLU:OE2   | 2.43                     | 0.52              |
| 1:A:1951:PHE:HB2  | 1:A:1994:ILE:HD11 | 1.92                     | 0.51              |
| 1:A:1701:GLY:O    | 1:A:1702:HIS:ND1  | 2.44                     | 0.51              |
| 3:F:273:MET:SD    | 3:F:273:MET:N     | 2.83                     | 0.51              |
| 1:B:436:GLN:OE1   | 1:B:436:GLN:N     | 2.40                     | 0.51              |
| 1:A:160:VAL:O     | 1:A:164:LEU:HG    | 2.11                     | 0.51              |
| 4:E:268:GLN:NE2   | 3:F:432:THR:OG1   | 2.36                     | 0.51              |
| 1:A:68:PHE:HB2    | 1:A:110:VAL:HG22  | 1.91                     | 0.51              |
| 1:A:1136:TYR:HB2  | 1:B:1104:THR:HG21 | 1.93                     | 0.51              |
| 1:B:61:PRO:O      | 1:B:99:TYR:OH     | 2.25                     | 0.51              |
| 1:B:160:VAL:O     | 1:B:164:LEU:HG    | 2.11                     | 0.51              |
| 1:B:1701:GLY:O    | 1:B:1702:HIS:ND1  | 2.44                     | 0.51              |
| 3:D:366:TYR:CZ    | 3:D:389:ALA:HB2   | 2.46                     | 0.51              |
| 3:F:366:TYR:CZ    | 3:F:389:ALA:HB2   | 2.46                     | 0.51              |
| 3:F:751:ARG:NH1   | 3:F:755:GLU:OE2   | 2.43                     | 0.51              |
| 1:A:1170:ASN:HD22 | 1:A:1210:LEU:HD11 | 1.75                     | 0.51              |
| 1:A:1929:THR:HG23 | 1:A:1932:PHE:H    | 1.75                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:255:GLN:O     | 3:F:258:ARG:HB2   | 2.11                     | 0.51              |
| 1:B:1785:LEU:HD11 | 1:B:1810:LYS:HB2  | 1.93                     | 0.51              |
| 3:D:492:MET:SD    | 3:D:492:MET:N     | 2.84                     | 0.51              |
| 2:H:69:PHE:CD1    | 2:H:84:MET:HG2    | 2.46                     | 0.51              |
| 1:A:1785:LEU:HD11 | 1:A:1810:LYS:HB2  | 1.93                     | 0.51              |
| 1:B:1170:ASN:HD22 | 1:B:1210:LEU:HD11 | 1.75                     | 0.50              |
| 1:A:672:TYR:OH    | 1:A:732:ASN:OD1   | 2.28                     | 0.50              |
| 1:A:781:LEU:O     | 1:A:829:LYS:NZ    | 2.37                     | 0.50              |
| 1:B:1509:PRO:O    | 1:B:2068:ARG:NH1  | 2.44                     | 0.50              |
| 1:B:1063:MET:O    | 1:B:1066:GLN:HG3  | 2.11                     | 0.50              |
| 1:B:1367:ASN:O    | 1:B:1371:ARG:NH1  | 2.44                     | 0.50              |
| 1:B:904:VAL:HG11  | 1:B:943:VAL:HG23  | 1.93                     | 0.50              |
| 1:B:1482:HIS:O    | 1:B:1486:MET:HG2  | 2.12                     | 0.50              |
| 3:D:432:THR:OG1   | 4:G:268:GLN:NE2   | 2.34                     | 0.50              |
| 2:H:71:ILE:HG22   | 2:H:82:LEU:HG     | 1.93                     | 0.50              |
| 4:E:282:ILE:HD11  | 3:F:371:ILE:HG13  | 1.94                     | 0.50              |
| 1:A:904:VAL:HG11  | 1:A:943:VAL:HG23  | 1.93                     | 0.50              |
| 1:A:1850:LYS:HZ3  | 1:A:1853:ASP:HB3  | 1.77                     | 0.50              |
| 1:A:1063:MET:O    | 1:A:1066:GLN:HG3  | 2.11                     | 0.49              |
| 2:C:105:ARG:NH2   | 3:F:546:GLY:H     | 2.10                     | 0.49              |
| 1:A:1665:LYS:O    | 3:F:347:ARG:NH1   | 2.33                     | 0.49              |
| 1:B:781:LEU:O     | 1:B:829:LYS:NZ    | 2.37                     | 0.49              |
| 2:C:69:PHE:CD1    | 2:C:84:MET:HG2    | 2.46                     | 0.49              |
| 3:D:187:LEU:HA    | 3:D:190:ILE:HG12  | 1.95                     | 0.49              |
| 1:A:1367:ASN:O    | 1:A:1371:ARG:NH1  | 2.44                     | 0.49              |
| 1:B:956:LYS:NZ    | 1:B:1311:TYR:O    | 2.46                     | 0.49              |
| 3:F:254:THR:O     | 3:F:257:LEU:HG    | 2.13                     | 0.49              |
| 2:C:71:ILE:HG22   | 2:C:82:LEU:HG     | 1.93                     | 0.49              |
| 1:A:1509:PRO:O    | 1:A:2068:ARG:NH1  | 2.44                     | 0.49              |
| 3:D:254:THR:O     | 3:D:257:LEU:HG    | 2.13                     | 0.49              |
| 4:E:135:VAL:HG22  | 3:F:247:ARG:NH2   | 2.27                     | 0.49              |
| 1:A:1482:HIS:O    | 1:A:1486:MET:HG2  | 2.12                     | 0.49              |
| 1:B:672:TYR:OH    | 1:B:732:ASN:OD1   | 2.28                     | 0.49              |
| 1:A:202:GLU:OE2   | 1:A:207:LYS:NZ    | 2.32                     | 0.49              |
| 1:B:153:ILE:O     | 1:B:156:VAL:HG22  | 2.12                     | 0.48              |
| 1:A:153:ILE:O     | 1:A:156:VAL:HG22  | 2.12                     | 0.48              |
| 1:A:377:MET:SD    | 1:A:377:MET:N     | 2.85                     | 0.48              |
| 2:H:39:TYR:CE1    | 2:H:49:LEU:HD13   | 2.48                     | 0.48              |
| 1:A:518:LEU:HD12  | 1:A:521:LEU:HD22  | 1.95                     | 0.48              |
| 1:A:1596:TRP:HE1  | 1:A:1602:ASP:N    | 2.11                     | 0.48              |
| 4:E:241:LEU:HA    | 4:E:244:ILE:HG22  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:324:ILE:HD11  | 1:A:328:MET:HB2   | 1.96                     | 0.48              |
| 1:B:479:LEU:HD12  | 1:B:479:LEU:H     | 1.78                     | 0.48              |
| 1:B:1415:PHE:O    | 1:B:1489:ARG:NH2  | 2.43                     | 0.48              |
| 2:C:39:TYR:CE1    | 2:C:49:LEU:HD13   | 2.48                     | 0.48              |
| 3:F:504:PHE:CE2   | 3:F:520:TYR:HB3   | 2.48                     | 0.48              |
| 3:D:495:VAL:HG22  | 3:D:498:ARG:HH21  | 1.78                     | 0.48              |
| 4:E:56:VAL:O      | 4:E:60:LEU:HG     | 2.13                     | 0.48              |
| 3:F:495:VAL:HG22  | 3:F:498:ARG:HH21  | 1.78                     | 0.48              |
| 2:H:75:ASN:OD1    | 2:H:75:ASN:N      | 2.47                     | 0.48              |
| 1:A:1096:GLN:NE2  | 1:B:1114:ASN:OD1  | 2.47                     | 0.48              |
| 1:A:956:LYS:NZ    | 1:A:1311:TYR:O    | 2.46                     | 0.48              |
| 1:B:377:MET:SD    | 1:B:377:MET:N     | 2.85                     | 0.48              |
| 3:F:492:MET:SD    | 3:F:492:MET:N     | 2.84                     | 0.48              |
| 1:A:483:ILE:HG13  | 1:A:484:CYS:N     | 2.29                     | 0.48              |
| 1:B:483:ILE:HG13  | 1:B:484:CYS:N     | 2.29                     | 0.48              |
| 3:D:529:ARG:NH1   | 3:D:830:SER:O     | 2.47                     | 0.48              |
| 3:F:187:LEU:HA    | 3:F:190:ILE:HG12  | 1.94                     | 0.48              |
| 1:A:394:SER:HA    | 1:A:397:LYS:HZ2   | 1.78                     | 0.47              |
| 1:A:479:LEU:HD12  | 1:A:479:LEU:H     | 1.78                     | 0.47              |
| 1:B:1601:ALA:HB2  | 1:B:1629:PRO:HG2  | 1.96                     | 0.47              |
| 3:D:600:ASP:OD1   | 3:D:600:ASP:N     | 2.41                     | 0.47              |
| 1:B:1658:VAL:HG21 | 1:B:1690:ASN:ND2  | 2.29                     | 0.47              |
| 3:D:504:PHE:CE2   | 3:D:520:TYR:HB3   | 2.48                     | 0.47              |
| 3:F:529:ARG:NH1   | 3:F:830:SER:O     | 2.47                     | 0.47              |
| 4:G:56:VAL:O      | 4:G:60:LEU:HG     | 2.13                     | 0.47              |
| 1:A:1658:VAL:HG21 | 1:A:1690:ASN:ND2  | 2.30                     | 0.47              |
| 4:G:123:LEU:HD12  | 4:G:163:SER:HB3   | 1.97                     | 0.47              |
| 1:A:638:LEU:HD21  | 1:A:670:TYR:HE2   | 1.79                     | 0.47              |
| 1:B:93:LYS:HE2    | 1:B:97:VAL:HG21   | 1.97                     | 0.47              |
| 1:B:638:LEU:HD21  | 1:B:670:TYR:HE2   | 1.79                     | 0.47              |
| 3:F:420:LEU:HD13  | 3:F:433:ILE:HG23  | 1.96                     | 0.47              |
| 1:A:399:ILE:HA    | 1:A:402:PHE:CD2   | 2.50                     | 0.47              |
| 1:B:1596:TRP:HE1  | 1:B:1602:ASP:N    | 2.11                     | 0.47              |
| 3:D:256:ASN:OD1   | 3:D:257:LEU:N     | 2.47                     | 0.47              |
| 1:A:1857:GLN:HG3  | 1:A:2046:LEU:HD13 | 1.97                     | 0.47              |
| 1:B:324:ILE:HD11  | 1:B:328:MET:HB2   | 1.96                     | 0.47              |
| 1:B:518:LEU:HD12  | 1:B:521:LEU:HD22  | 1.95                     | 0.47              |
| 1:B:1966:ASP:OD1  | 1:B:1970:HIS:N    | 2.47                     | 0.47              |
| 3:D:279:TRP:CE2   | 3:D:285:PRO:HG3   | 2.50                     | 0.47              |
| 3:F:332:LEU:HD13  | 3:F:369:LEU:HA    | 1.97                     | 0.47              |
| 1:A:93:LYS:HE2    | 1:A:97:VAL:HG21   | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1601:ALA:HB2  | 1:A:1629:PRO:HG2  | 1.96                     | 0.47              |
| 1:B:1107:ILE:HG23 | 1:B:1108:LEU:HG   | 1.97                     | 0.47              |
| 1:B:1958:ARG:NH1  | 1:B:1974:ILE:O    | 2.39                     | 0.47              |
| 3:D:420:LEU:HD13  | 3:D:433:ILE:HG23  | 1.96                     | 0.47              |
| 4:E:116:LYS:HG3   | 4:E:117:GLN:N     | 2.30                     | 0.47              |
| 1:B:1857:GLN:HG3  | 1:B:2046:LEU:HD13 | 1.97                     | 0.47              |
| 3:F:689:LEU:HA    | 3:F:692:TRP:HD1   | 1.80                     | 0.47              |
| 1:A:1107:ILE:HG23 | 1:A:1108:LEU:HG   | 1.97                     | 0.47              |
| 1:A:1966:ASP:OD1  | 1:A:1970:HIS:N    | 2.47                     | 0.47              |
| 2:C:47:ARG:HA     | 2:C:47:ARG:HH11   | 1.80                     | 0.47              |
| 3:D:190:ILE:HA    | 3:D:193:VAL:HG22  | 1.97                     | 0.47              |
| 2:H:47:ARG:HA     | 2:H:47:ARG:HH11   | 1.80                     | 0.47              |
| 2:H:99:VAL:HB     | 2:H:113:TYR:HB2   | 1.97                     | 0.46              |
| 1:A:1415:PHE:O    | 1:A:1489:ARG:NH2  | 2.43                     | 0.46              |
| 1:B:399:ILE:HA    | 1:B:402:PHE:CD2   | 2.50                     | 0.46              |
| 4:G:116:LYS:HG3   | 4:G:117:GLN:N     | 2.30                     | 0.46              |
| 4:G:171:MET:HE2   | 4:G:171:MET:HB2   | 1.84                     | 0.46              |
| 1:A:1596:TRP:HZ2  | 1:A:1601:ALA:HA   | 1.81                     | 0.46              |
| 3:D:226:HIS:HA    | 3:D:229:TYR:CD2   | 2.50                     | 0.46              |
| 4:G:241:LEU:HA    | 4:G:244:ILE:HG22  | 1.95                     | 0.46              |
| 2:H:84:MET:SD     | 2:H:85:ASN:N      | 2.88                     | 0.46              |
| 2:C:75:ASN:OD1    | 2:C:75:ASN:N      | 2.47                     | 0.46              |
| 2:C:84:MET:SD     | 2:C:85:ASN:N      | 2.88                     | 0.46              |
| 3:D:332:LEU:HD13  | 3:D:369:LEU:HA    | 1.97                     | 0.46              |
| 1:A:154:LEU:HA    | 1:A:157:LEU:HD12  | 1.98                     | 0.46              |
| 1:A:659:GLN:O     | 1:A:663:LEU:HG    | 2.16                     | 0.46              |
| 1:A:1027:LYS:HB3  | 1:A:1027:LYS:HE3  | 1.78                     | 0.46              |
| 1:A:1795:MET:SD   | 1:A:1795:MET:N    | 2.87                     | 0.46              |
| 1:B:411:GLN:O     | 1:B:415:GLN:NE2   | 2.39                     | 0.46              |
| 3:D:748:GLU:H     | 3:D:748:GLU:CD    | 2.23                     | 0.46              |
| 3:F:256:ASN:OD1   | 3:F:257:LEU:N     | 2.47                     | 0.46              |
| 3:F:279:TRP:CE2   | 3:F:285:PRO:HG3   | 2.50                     | 0.46              |
| 1:B:133:PHE:CE2   | 1:B:193:ALA:HB2   | 2.51                     | 0.46              |
| 3:F:226:HIS:HA    | 3:F:229:TYR:CD2   | 2.51                     | 0.46              |
| 1:A:1010:MET:HE3  | 1:A:1010:MET:HB2  | 1.71                     | 0.46              |
| 1:B:187:LEU:HD12  | 1:B:190:ILE:HD11  | 1.98                     | 0.46              |
| 1:B:1795:MET:SD   | 1:B:1795:MET:N    | 2.87                     | 0.46              |
| 3:D:689:LEU:HA    | 3:D:692:TRP:HD1   | 1.80                     | 0.46              |
| 4:E:123:LEU:HD12  | 4:E:163:SER:HB3   | 1.97                     | 0.46              |
| 1:B:659:GLN:O     | 1:B:663:LEU:HG    | 2.16                     | 0.45              |
| 2:C:99:VAL:HB     | 2:C:113:TYR:HB2   | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:187:LEU:HD12  | 1:A:190:ILE:HD11  | 1.98                     | 0.45              |
| 1:A:1615:THR:OG1  | 1:A:1616:ASP:N    | 2.49                     | 0.45              |
| 1:A:1999:GLU:O    | 1:A:2002:MET:HG3  | 2.17                     | 0.45              |
| 1:A:681:GLN:O     | 1:A:685:LYS:HG2   | 2.16                     | 0.45              |
| 1:B:333:LEU:HA    | 1:B:336:VAL:HG22  | 1.99                     | 0.45              |
| 3:F:190:ILE:HA    | 3:F:193:VAL:HG22  | 1.97                     | 0.45              |
| 3:F:338:MET:HE3   | 3:F:338:MET:HB3   | 1.68                     | 0.45              |
| 2:H:116:GLN:OE1   | 2:H:116:GLN:N     | 2.46                     | 0.45              |
| 1:A:1508:ASN:ND2  | 1:A:1510:LEU:O    | 2.48                     | 0.45              |
| 1:B:154:LEU:HA    | 1:B:157:LEU:HD12  | 1.98                     | 0.45              |
| 1:B:1275:ASP:N    | 1:B:1275:ASP:OD1  | 2.48                     | 0.45              |
| 1:B:1850:LYS:HZ3  | 1:B:1853:ASP:HB3  | 1.82                     | 0.45              |
| 1:B:1999:GLU:O    | 1:B:2002:MET:HG3  | 2.16                     | 0.45              |
| 2:C:116:GLN:OE1   | 2:C:116:GLN:N     | 2.46                     | 0.45              |
| 1:A:567:ASP:HA    | 1:A:570:ILE:HG12  | 1.98                     | 0.45              |
| 3:D:714:GLU:OE1   | 3:D:714:GLU:N     | 2.44                     | 0.45              |
| 4:E:42:TYR:HA     | 4:E:45:ILE:HG22   | 1.99                     | 0.45              |
| 3:F:514:ASP:OD1   | 3:F:514:ASP:N     | 2.50                     | 0.45              |
| 4:G:42:TYR:HA     | 4:G:45:ILE:HG22   | 1.99                     | 0.45              |
| 1:A:342:GLU:O     | 1:A:346:LYS:HG2   | 2.17                     | 0.45              |
| 1:B:508:ARG:HG3   | 1:B:509:ASP:N     | 2.32                     | 0.45              |
| 1:B:1714:GLN:O    | 1:B:1717:GLU:HG2  | 2.17                     | 0.45              |
| 4:G:207:CYS:HB3   | 4:G:240:MET:HE3   | 1.99                     | 0.45              |
| 1:A:133:PHE:CE2   | 1:A:193:ALA:HB2   | 2.51                     | 0.45              |
| 1:B:969:GLN:NE2   | 1:B:1009:THR:OG1  | 2.50                     | 0.45              |
| 1:B:1596:TRP:HZ2  | 1:B:1601:ALA:HA   | 1.81                     | 0.45              |
| 4:G:102:GLU:OE1   | 4:G:102:GLU:N     | 2.44                     | 0.45              |
| 1:A:1693:THR:HG23 | 1:A:1891:PRO:HA   | 1.99                     | 0.45              |
| 1:B:681:GLN:O     | 1:B:685:LYS:HG2   | 2.17                     | 0.45              |
| 2:C:39:TYR:OH     | 2:C:100:ASP:OD2   | 2.33                     | 0.45              |
| 1:A:333:LEU:HA    | 1:A:336:VAL:HG22  | 1.99                     | 0.44              |
| 1:A:1591:LYS:HA   | 1:A:1594:VAL:HG12 | 1.99                     | 0.44              |
| 1:B:1277:LEU:O    | 1:B:1653:TYR:OH   | 2.33                     | 0.44              |
| 4:E:171:MET:HE2   | 4:E:171:MET:HB2   | 1.84                     | 0.44              |
| 4:E:174:ALA:HA    | 4:E:177:ARG:HD2   | 2.00                     | 0.44              |
| 4:E:185:LEU:O     | 4:E:189:ASN:ND2   | 2.30                     | 0.44              |
| 3:F:714:GLU:OE1   | 3:F:714:GLU:N     | 2.44                     | 0.44              |
| 3:D:448:LEU:HD13  | 3:D:483:GLN:HG2   | 1.99                     | 0.44              |
| 3:F:441:CYS:SG    | 3:F:450:GLU:HB2   | 2.57                     | 0.44              |
| 4:G:109:TYR:HB2   | 4:G:184:LEU:HD21  | 2.00                     | 0.44              |
| 1:A:660:LEU:O     | 1:A:664:VAL:HG23  | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:462:LEU:HA    | 1:B:465:LYS:HG2   | 2.00                     | 0.44              |
| 1:B:660:LEU:O     | 1:B:664:VAL:HG23  | 2.17                     | 0.44              |
| 4:E:109:TYR:HB2   | 4:E:184:LEU:HD21  | 2.00                     | 0.44              |
| 1:A:1114:ASN:ND2  | 1:A:1116:GLN:H    | 2.14                     | 0.44              |
| 3:F:145:TYR:HA    | 3:F:148:LYS:HZ3   | 1.82                     | 0.44              |
| 4:G:174:ALA:HA    | 4:G:177:ARG:HD2   | 2.00                     | 0.44              |
| 1:A:462:LEU:HA    | 1:A:465:LYS:HG2   | 2.00                     | 0.44              |
| 1:B:93:LYS:HG2    | 1:B:97:VAL:HG21   | 2.00                     | 0.44              |
| 1:B:342:GLU:O     | 1:B:346:LYS:HG2   | 2.17                     | 0.44              |
| 1:B:394:SER:HA    | 1:B:397:LYS:HZ2   | 1.82                     | 0.44              |
| 1:B:1114:ASN:ND2  | 1:B:1116:GLN:H    | 2.14                     | 0.44              |
| 1:A:508:ARG:HG3   | 1:A:509:ASP:N     | 2.32                     | 0.44              |
| 3:D:441:CYS:SG    | 3:D:450:GLU:HB2   | 2.57                     | 0.44              |
| 3:D:504:PHE:HE2   | 3:D:520:TYR:HB3   | 1.83                     | 0.44              |
| 4:E:207:CYS:HB3   | 4:E:240:MET:HE3   | 1.99                     | 0.44              |
| 4:E:240:MET:HE2   | 4:E:263:ILE:HD11  | 2.00                     | 0.44              |
| 4:G:195:MET:HE2   | 4:G:195:MET:HB2   | 1.91                     | 0.44              |
| 1:A:632:LYS:HG3   | 1:A:633:VAL:HG23  | 2.00                     | 0.44              |
| 1:A:1007:LEU:HA   | 1:A:1010:MET:HG2  | 2.00                     | 0.44              |
| 1:B:1508:ASN:ND2  | 1:B:1510:LEU:O    | 2.48                     | 0.44              |
| 1:B:1787:ILE:HG22 | 1:B:1807:PHE:CD2  | 2.51                     | 0.44              |
| 1:B:567:ASP:HA    | 1:B:570:ILE:HG12  | 1.98                     | 0.44              |
| 1:B:633:VAL:C     | 1:B:636:PRO:HD2   | 2.43                     | 0.44              |
| 1:B:1010:MET:SD   | 1:B:1064:ILE:HD11 | 2.58                     | 0.44              |
| 1:B:1693:THR:HG23 | 1:B:1891:PRO:HA   | 1.99                     | 0.44              |
| 4:E:170:GLU:HG2   | 4:E:171:MET:SD    | 2.58                     | 0.44              |
| 3:F:748:GLU:H     | 3:F:748:GLU:CD    | 2.23                     | 0.44              |
| 4:G:240:MET:HE2   | 4:G:263:ILE:HD11  | 2.00                     | 0.44              |
| 1:A:93:LYS:HG2    | 1:A:97:VAL:HG21   | 2.00                     | 0.44              |
| 1:A:1714:GLN:O    | 1:A:1717:GLU:HG2  | 2.17                     | 0.44              |
| 1:B:1529:ARG:HA   | 1:B:1532:TYR:CD1  | 2.52                     | 0.44              |
| 1:A:141:ASP:O     | 1:A:145:ARG:HG2   | 2.19                     | 0.43              |
| 1:B:860:GLU:O     | 1:B:863:GLU:HG3   | 2.18                     | 0.43              |
| 1:B:1027:LYS:HB3  | 1:B:1027:LYS:HE3  | 1.78                     | 0.43              |
| 1:B:1684:ALA:O    | 1:B:1688:ILE:HG22 | 2.18                     | 0.43              |
| 4:E:209:ARG:HA    | 4:E:212:VAL:HG12  | 2.00                     | 0.43              |
| 1:A:969:GLN:NE2   | 1:A:1009:THR:OG1  | 2.50                     | 0.43              |
| 1:A:1787:ILE:HG22 | 1:A:1807:PHE:CD2  | 2.51                     | 0.43              |
| 1:B:495:ARG:O     | 1:B:495:ARG:NE    | 2.51                     | 0.43              |
| 1:B:632:LYS:HG3   | 1:B:633:VAL:HG23  | 2.00                     | 0.43              |
| 1:B:1118:THR:HG23 | 1:B:1119:THR:HG23 | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1591:LYS:HA   | 1:B:1594:VAL:HG12 | 1.99                     | 0.43              |
| 1:B:1596:TRP:CZ2  | 1:B:1601:ALA:HA   | 2.53                     | 0.43              |
| 1:B:1615:THR:OG1  | 1:B:1616:ASP:N    | 2.49                     | 0.43              |
| 1:A:633:VAL:C     | 1:A:636:PRO:HD2   | 2.43                     | 0.43              |
| 1:A:638:LEU:O     | 1:A:641:LEU:HG    | 2.18                     | 0.43              |
| 1:A:1181:LEU:HD13 | 1:A:1220:ARG:HD2  | 2.00                     | 0.43              |
| 1:A:1529:ARG:HA   | 1:A:1532:TYR:CD1  | 2.52                     | 0.43              |
| 3:D:514:ASP:N     | 3:D:514:ASP:OD1   | 2.50                     | 0.43              |
| 4:G:108:VAL:HA    | 4:G:111:LEU:HG    | 2.00                     | 0.43              |
| 1:A:94:ASP:OD1    | 1:A:94:ASP:N      | 2.52                     | 0.43              |
| 1:A:1010:MET:SD   | 1:A:1064:ILE:HD11 | 2.58                     | 0.43              |
| 3:D:137:ARG:HA    | 3:D:140:VAL:HG22  | 2.01                     | 0.43              |
| 1:A:874:PRO:HB2   | 1:A:878:VAL:HB    | 2.01                     | 0.43              |
| 1:A:111:TYR:HD1   | 2:C:116:GLN:HG3   | 1.83                     | 0.43              |
| 1:B:102:ARG:HA    | 1:B:105:LYS:HG2   | 2.00                     | 0.43              |
| 1:B:1007:LEU:HA   | 1:B:1010:MET:HG2  | 2.00                     | 0.43              |
| 2:C:36:MET:HE3    | 2:C:36:MET:HB2    | 1.94                     | 0.43              |
| 3:D:424:ILE:HA    | 3:D:424:ILE:HD13  | 1.86                     | 0.43              |
| 3:D:489:LEU:HB2   | 3:D:492:MET:SD    | 2.58                     | 0.43              |
| 3:D:504:PHE:HD2   | 3:D:521:LEU:HA    | 1.83                     | 0.43              |
| 1:A:495:ARG:O     | 1:A:495:ARG:NE    | 2.51                     | 0.43              |
| 1:A:1684:ALA:O    | 1:A:1688:ILE:HG22 | 2.18                     | 0.43              |
| 1:B:1788:ASP:OD2  | 1:B:1791:SER:OG   | 2.37                     | 0.43              |
| 3:D:258:ARG:O     | 3:D:259:MET:C     | 2.62                     | 0.43              |
| 1:A:564:GLN:H     | 1:A:564:GLN:CD    | 2.27                     | 0.43              |
| 1:A:1596:TRP:CZ2  | 1:A:1601:ALA:HA   | 2.53                     | 0.43              |
| 3:F:381:MET:HE2   | 3:F:381:MET:HB2   | 1.75                     | 0.43              |
| 3:F:504:PHE:HD2   | 3:F:521:LEU:HA    | 1.83                     | 0.43              |
| 4:G:209:ARG:HA    | 4:G:212:VAL:HG12  | 2.00                     | 0.43              |
| 1:B:1181:LEU:HD13 | 1:B:1220:ARG:HD2  | 2.00                     | 0.43              |
| 1:B:1586:VAL:HG11 | 1:B:1613:ALA:O    | 2.19                     | 0.43              |
| 1:B:1800:LYS:HE2  | 1:B:1800:LYS:HB2  | 1.85                     | 0.43              |
| 3:F:448:LEU:HD13  | 3:F:483:GLN:HG2   | 1.99                     | 0.43              |
| 3:F:489:LEU:HB2   | 3:F:492:MET:SD    | 2.58                     | 0.43              |
| 1:B:575:ARG:HA    | 1:B:578:LYS:HG2   | 2.01                     | 0.43              |
| 1:B:874:PRO:HB2   | 1:B:878:VAL:HB    | 2.01                     | 0.43              |
| 1:B:1010:MET:HE3  | 1:B:1010:MET:HB2  | 1.71                     | 0.43              |
| 1:A:102:ARG:HA    | 1:A:105:LYS:HG2   | 2.00                     | 0.42              |
| 1:A:1991:GLU:CD   | 1:A:1991:GLU:H    | 2.27                     | 0.42              |
| 1:B:141:ASP:O     | 1:B:145:ARG:HG2   | 2.19                     | 0.42              |
| 3:F:223:GLN:HA    | 3:F:226:HIS:NE2   | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1275:ASP:OD1  | 1:A:1275:ASP:N    | 2.48                     | 0.42              |
| 1:B:776:VAL:O     | 1:B:779:ARG:HG2   | 2.20                     | 0.42              |
| 1:B:1850:LYS:NZ   | 1:B:1853:ASP:HB3  | 2.33                     | 0.42              |
| 3:D:435:LEU:HG    | 4:G:271:LEU:HD21  | 2.00                     | 0.42              |
| 3:F:694:THR:O     | 3:F:698:ILE:HG13  | 2.19                     | 0.42              |
| 1:A:950:MET:HE3   | 1:A:950:MET:HB3   | 1.94                     | 0.42              |
| 1:A:1277:LEU:O    | 1:A:1653:TYR:OH   | 2.33                     | 0.42              |
| 1:A:1766:SER:HA   | 1:A:1789:TYR:CD1  | 2.55                     | 0.42              |
| 1:B:94:ASP:N      | 1:B:94:ASP:OD1    | 2.52                     | 0.42              |
| 1:B:1879:LEU:HD12 | 1:B:1945:ALA:HB2  | 2.01                     | 0.42              |
| 3:D:223:GLN:HA    | 3:D:226:HIS:NE2   | 2.34                     | 0.42              |
| 4:E:108:VAL:HA    | 4:E:111:LEU:HG    | 2.00                     | 0.42              |
| 1:B:1097:HIS:HD2  | 1:B:1100:LEU:HD22 | 1.84                     | 0.42              |
| 4:G:170:GLU:HG2   | 4:G:171:MET:SD    | 2.58                     | 0.42              |
| 1:A:439:ALA:HB1   | 1:A:484:CYS:SG    | 2.60                     | 0.42              |
| 1:A:734:LEU:HD23  | 1:A:794:LEU:HB3   | 2.01                     | 0.42              |
| 1:A:860:GLU:O     | 1:A:863:GLU:HG3   | 2.18                     | 0.42              |
| 1:A:1118:THR:HG23 | 1:A:1119:THR:HG23 | 2.00                     | 0.42              |
| 1:B:734:LEU:HD23  | 1:B:794:LEU:HB3   | 2.00                     | 0.42              |
| 3:D:134:PRO:HG2   | 3:D:137:ARG:HG3   | 2.02                     | 0.42              |
| 4:E:34:LYS:HB3    | 4:E:37:LEU:HB2    | 2.02                     | 0.42              |
| 3:F:188:GLN:O     | 3:F:191:GLU:HG3   | 2.19                     | 0.42              |
| 1:B:638:LEU:O     | 1:B:641:LEU:HG    | 2.18                     | 0.42              |
| 1:B:778:THR:HG21  | 1:B:826:ILE:HD13  | 2.01                     | 0.42              |
| 1:B:1611:CYS:HB3  | 3:D:418:LYS:HD3   | 2.01                     | 0.42              |
| 3:D:241:ARG:O     | 3:D:245:LEU:HG    | 2.19                     | 0.42              |
| 3:F:134:PRO:HG2   | 3:F:137:ARG:HG3   | 2.02                     | 0.42              |
| 3:F:137:ARG:HA    | 3:F:140:VAL:HG22  | 2.01                     | 0.42              |
| 3:F:415:ARG:O     | 3:F:419:VAL:HG23  | 2.20                     | 0.42              |
| 1:A:776:VAL:O     | 1:A:779:ARG:HG2   | 2.20                     | 0.42              |
| 1:B:1766:SER:HA   | 1:B:1789:TYR:CD1  | 2.55                     | 0.42              |
| 3:F:241:ARG:O     | 3:F:245:LEU:HG    | 2.19                     | 0.42              |
| 3:F:265:LEU:HD12  | 3:F:265:LEU:HA    | 1.82                     | 0.42              |
| 3:F:394:PHE:CD2   | 3:F:395:GLU:HG2   | 2.55                     | 0.42              |
| 3:F:407:LEU:HD23  | 3:F:407:LEU:HA    | 1.90                     | 0.42              |
| 1:A:1586:VAL:HG11 | 1:A:1613:ALA:O    | 2.19                     | 0.42              |
| 1:A:1850:LYS:NZ   | 1:A:1853:ASP:HB3  | 2.33                     | 0.42              |
| 1:B:564:GLN:CD    | 1:B:564:GLN:H     | 2.27                     | 0.42              |
| 4:E:52:LEU:HD23   | 4:E:52:LEU:H      | 1.84                     | 0.42              |
| 3:F:228:LEU:HD13  | 3:F:231:LYS:HD2   | 2.01                     | 0.42              |
| 3:F:396:GLU:O     | 3:F:400:TRP:HD1   | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:641:LEU:HA    | 1:A:644:LYS:HG2   | 2.01                     | 0.42              |
| 1:A:959:GLU:O     | 1:A:963:GLU:HG2   | 2.20                     | 0.42              |
| 1:B:439:ALA:HB1   | 1:B:484:CYS:SG    | 2.60                     | 0.42              |
| 1:B:641:LEU:HA    | 1:B:644:LYS:HG2   | 2.02                     | 0.42              |
| 1:B:1991:GLU:CD   | 1:B:1991:GLU:H    | 2.27                     | 0.42              |
| 2:C:35:TYR:CZ     | 2:C:54:ASP:HB3    | 2.55                     | 0.42              |
| 3:D:228:LEU:HD13  | 3:D:231:LYS:HD2   | 2.01                     | 0.42              |
| 3:D:415:ARG:O     | 3:D:419:VAL:HG23  | 2.20                     | 0.42              |
| 4:G:52:LEU:HD23   | 4:G:52:LEU:H      | 1.84                     | 0.42              |
| 1:A:2074:ILE:HA   | 1:A:2077:VAL:HG12 | 2.02                     | 0.42              |
| 1:B:40:ARG:HG2    | 1:B:211:LYS:NZ    | 2.35                     | 0.42              |
| 1:B:407:PHE:CE2   | 1:B:442:VAL:HG22  | 2.55                     | 0.42              |
| 1:B:959:GLU:O     | 1:B:963:GLU:HG2   | 2.20                     | 0.42              |
| 3:D:396:GLU:O     | 3:D:400:TRP:HD1   | 2.02                     | 0.42              |
| 3:D:694:THR:O     | 3:D:698:ILE:HG13  | 2.19                     | 0.42              |
| 1:A:407:PHE:CE2   | 1:A:442:VAL:HG22  | 2.55                     | 0.41              |
| 1:A:575:ARG:HA    | 1:A:578:LYS:HG2   | 2.01                     | 0.41              |
| 1:A:1097:HIS:HD2  | 1:A:1100:LEU:HD22 | 1.84                     | 0.41              |
| 1:B:1765:LEU:HD22 | 1:B:1789:TYR:HA   | 2.02                     | 0.41              |
| 1:A:101:LEU:HD13  | 1:A:101:LEU:HA    | 1.89                     | 0.41              |
| 1:B:636:PRO:O     | 1:B:639:GLN:HG2   | 2.20                     | 0.41              |
| 1:B:1605:GLU:O    | 1:B:1606:LEU:HG   | 2.20                     | 0.41              |
| 1:B:1886:VAL:HG23 | 1:B:1896:ILE:HG12 | 2.02                     | 0.41              |
| 3:D:188:GLN:O     | 3:D:191:GLU:HG3   | 2.19                     | 0.41              |
| 3:D:191:GLU:HA    | 3:D:194:ILE:HG12  | 2.03                     | 0.41              |
| 4:E:274:GLU:HB2   | 4:E:275:PRO:HD3   | 2.02                     | 0.41              |
| 2:H:35:TYR:CZ     | 2:H:54:ASP:HB3    | 2.55                     | 0.41              |
| 1:A:778:THR:HG21  | 1:A:826:ILE:HD13  | 2.01                     | 0.41              |
| 1:A:1710:ASP:OD1  | 1:A:1710:ASP:N    | 2.52                     | 0.41              |
| 1:A:564:GLN:HA    | 1:A:567:ASP:OD2   | 2.21                     | 0.41              |
| 1:A:1788:ASP:OD2  | 1:A:1791:SER:OG   | 2.37                     | 0.41              |
| 1:B:1010:MET:HA   | 1:B:1013:ILE:HG12 | 2.02                     | 0.41              |
| 1:B:1745:SER:OG   | 1:B:1801:ALA:O    | 2.27                     | 0.41              |
| 1:A:1879:LEU:HD12 | 1:A:1945:ALA:HB2  | 2.01                     | 0.41              |
| 1:B:157:LEU:O     | 1:B:158:LEU:C     | 2.63                     | 0.41              |
| 1:B:2074:ILE:HA   | 1:B:2077:VAL:HG12 | 2.02                     | 0.41              |
| 3:F:355:ARG:HB3   | 3:F:355:ARG:NH1   | 2.36                     | 0.41              |
| 4:G:173:THR:HG23  | 4:G:175:GLN:H     | 1.86                     | 0.41              |
| 1:A:1340:ASN:OD1  | 1:A:1341:ARG:N    | 2.54                     | 0.41              |
| 1:A:1509:PRO:HB3  | 1:A:2021:VAL:HG11 | 2.03                     | 0.41              |
| 1:B:722:ASP:O     | 1:B:726:VAL:HG23  | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1409:LYS:HB2  | 1:B:1409:LYS:HE3  | 1.88                     | 0.41              |
| 3:D:338:MET:HE3   | 3:D:338:MET:HB3   | 1.68                     | 0.41              |
| 3:F:465:THR:OG1   | 3:F:466:SER:N     | 2.53                     | 0.41              |
| 4:G:274:GLU:HB2   | 4:G:275:PRO:HD3   | 2.02                     | 0.41              |
| 2:H:39:TYR:OH     | 2:H:100:ASP:OD2   | 2.33                     | 0.41              |
| 1:A:40:ARG:HG2    | 1:A:211:LYS:NZ    | 2.35                     | 0.41              |
| 1:A:152:GLU:O     | 1:A:156:VAL:HG13  | 2.21                     | 0.41              |
| 1:A:348:LEU:HA    | 1:A:351:ILE:HG12  | 2.03                     | 0.41              |
| 1:B:50:LEU:O      | 1:B:54:GLN:HG2    | 2.21                     | 0.41              |
| 1:B:564:GLN:HA    | 1:B:567:ASP:OD2   | 2.21                     | 0.41              |
| 1:B:1198:ALA:O    | 1:B:1201:ILE:HG22 | 2.21                     | 0.41              |
| 1:B:1340:ASN:OD1  | 1:B:1341:ARG:N    | 2.54                     | 0.41              |
| 1:A:69:GLN:OE1    | 1:A:111:TYR:HB2   | 2.21                     | 0.41              |
| 1:A:157:LEU:O     | 1:A:158:LEU:C     | 2.64                     | 0.41              |
| 1:A:1605:GLU:O    | 1:A:1606:LEU:HG   | 2.20                     | 0.41              |
| 1:B:99:TYR:O      | 1:B:103:LEU:HG    | 2.21                     | 0.41              |
| 1:B:1697:LEU:HD21 | 1:B:1705:ASP:HB3  | 2.03                     | 0.41              |
| 1:B:1741:ILE:HD12 | 1:B:1741:ILE:HA   | 1.96                     | 0.41              |
| 3:D:355:ARG:HB3   | 3:D:355:ARG:NH1   | 2.36                     | 0.41              |
| 1:A:111:TYR:CD1   | 2:C:116:GLN:HG3   | 2.56                     | 0.41              |
| 1:A:636:PRO:O     | 1:A:639:GLN:HG2   | 2.20                     | 0.41              |
| 1:A:656:ILE:O     | 1:A:660:LEU:HG    | 2.21                     | 0.41              |
| 1:A:832:LEU:HD23  | 1:A:903:ARG:HH22  | 1.86                     | 0.41              |
| 1:A:1747:ILE:O    | 1:A:1750:PRO:HD2  | 2.21                     | 0.41              |
| 1:A:1952:LEU:HD12 | 1:A:1952:LEU:HA   | 1.93                     | 0.41              |
| 1:B:1747:ILE:O    | 1:B:1750:PRO:HD2  | 2.21                     | 0.41              |
| 1:B:1808:LYS:HB2  | 1:B:1844:TRP:CZ3  | 2.56                     | 0.41              |
| 3:D:219:GLU:OE1   | 3:D:219:GLU:N     | 2.48                     | 0.41              |
| 3:D:265:LEU:HD12  | 3:D:265:LEU:HA    | 1.82                     | 0.41              |
| 3:D:394:PHE:CD2   | 3:D:395:GLU:HG2   | 2.55                     | 0.41              |
| 1:A:733:LEU:HD13  | 1:A:774:ILE:HG12  | 2.02                     | 0.41              |
| 1:A:1855:CYS:HB2  | 1:A:1888:ALA:HB2  | 2.03                     | 0.41              |
| 1:A:1886:VAL:HG23 | 1:A:1896:ILE:HG12 | 2.02                     | 0.41              |
| 1:B:578:LYS:HA    | 1:B:581:LEU:HG    | 2.03                     | 0.41              |
| 1:B:733:LEU:HD13  | 1:B:774:ILE:HG12  | 2.02                     | 0.41              |
| 1:B:1010:MET:HE1  | 1:B:1061:CYS:HA   | 2.02                     | 0.41              |
| 1:B:1509:PRO:HB3  | 1:B:2021:VAL:HG11 | 2.03                     | 0.41              |
| 3:D:465:THR:OG1   | 3:D:466:SER:N     | 2.53                     | 0.41              |
| 4:G:34:LYS:HB3    | 4:G:37:LEU:HB2    | 2.02                     | 0.41              |
| 1:A:411:GLN:O     | 1:A:415:GLN:NE2   | 2.39                     | 0.40              |
| 1:A:722:ASP:O     | 1:A:726:VAL:HG23  | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:394:SER:HA    | 1:A:397:LYS:HG2   | 2.03                     | 0.40              |
| 1:A:1745:SER:OG   | 1:A:1801:ALA:O    | 2.27                     | 0.40              |
| 1:A:1765:LEU:HD22 | 1:A:1789:TYR:HA   | 2.02                     | 0.40              |
| 1:B:69:GLN:OE1    | 1:B:111:TYR:HB2   | 2.21                     | 0.40              |
| 1:B:1398:LYS:HD3  | 1:B:1398:LYS:HA   | 1.95                     | 0.40              |
| 1:B:1920:PHE:HD2  | 1:B:1920:PHE:HA   | 1.72                     | 0.40              |
| 3:D:260:THR:O     | 3:D:264:GLN:HG2   | 2.22                     | 0.40              |
| 3:F:175:CYS:HA    | 3:F:178:LYS:HE3   | 2.03                     | 0.40              |
| 3:F:258:ARG:O     | 3:F:259:MET:C     | 2.62                     | 0.40              |
| 3:F:408:MET:HE2   | 3:F:408:MET:HB3   | 1.87                     | 0.40              |
| 4:G:16:PHE:CD1    | 4:G:17:LYS:HG2    | 2.56                     | 0.40              |
| 1:A:378:PHE:HD1   | 1:A:378:PHE:HA    | 1.72                     | 0.40              |
| 1:A:1198:ALA:O    | 1:A:1201:ILE:HG22 | 2.21                     | 0.40              |
| 1:B:125:LEU:HA    | 1:B:126:PRO:HD3   | 1.98                     | 0.40              |
| 1:B:656:ILE:O     | 1:B:660:LEU:HG    | 2.21                     | 0.40              |
| 1:B:676:TRP:CE2   | 1:B:732:ASN:HB3   | 2.57                     | 0.40              |
| 2:C:38:TRP:HH2    | 2:C:80:VAL:HB     | 1.87                     | 0.40              |
| 3:D:400:TRP:CZ3   | 3:D:422:GLU:HG2   | 2.57                     | 0.40              |
| 3:F:191:GLU:HA    | 3:F:194:ILE:HG12  | 2.03                     | 0.40              |
| 1:A:50:LEU:O      | 1:A:54:GLN:HG2    | 2.21                     | 0.40              |
| 1:A:563:GLU:HB3   | 1:A:566:ARG:HH21  | 1.86                     | 0.40              |
| 1:A:1140:MET:N    | 1:A:1140:MET:SD   | 2.95                     | 0.40              |
| 1:A:1483:LYS:HE3  | 1:A:1483:LYS:HB2  | 1.90                     | 0.40              |
| 1:A:1808:LYS:HB2  | 1:A:1844:TRP:CZ3  | 2.56                     | 0.40              |
| 1:A:1974:ILE:HG12 | 1:A:1975:ASP:H    | 1.86                     | 0.40              |
| 1:B:378:PHE:HD1   | 1:B:378:PHE:HA    | 1.72                     | 0.40              |
| 3:F:219:GLU:OE1   | 3:F:219:GLU:N     | 2.48                     | 0.40              |
| 1:B:147:PRO:HA    | 1:B:150:ARG:HG3   | 2.03                     | 0.40              |
| 1:B:453:GLN:H     | 1:B:453:GLN:CD    | 2.29                     | 0.40              |
| 1:B:1365:VAL:HA   | 1:B:1366:PRO:HD3  | 1.97                     | 0.40              |
| 1:B:1855:CYS:HB2  | 1:B:1888:ALA:HB2  | 2.03                     | 0.40              |
| 4:E:173:THR:HG23  | 4:E:175:GLN:H     | 1.86                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

entries.

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 1676/2104 (80%) | 1605 (96%) | 70 (4%)  | 1 (0%)   | 48          | 79  |
| 1   | B     | 1676/2104 (80%) | 1605 (96%) | 70 (4%)  | 1 (0%)   | 48          | 79  |
| 2   | C     | 96/165 (58%)    | 91 (95%)   | 5 (5%)   | 0        | 100         | 100 |
| 2   | H     | 96/165 (58%)    | 91 (95%)   | 5 (5%)   | 0        | 100         | 100 |
| 3   | D     | 580/843 (69%)   | 571 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 3   | F     | 580/843 (69%)   | 571 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 4   | E     | 242/308 (79%)   | 232 (96%)  | 10 (4%)  | 0        | 100         | 100 |
| 4   | G     | 242/308 (79%)   | 233 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| All | All   | 5188/6840 (76%) | 4999 (96%) | 187 (4%) | 2 (0%)   | 100         | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1980 | PHE  |
| 1   | B     | 1980 | PHE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 1527/1842 (83%) | 1505 (99%) | 22 (1%)  | 59          | 71 |
| 1   | B     | 1527/1842 (83%) | 1506 (99%) | 21 (1%)  | 59          | 71 |
| 2   | C     | 82/129 (64%)    | 80 (98%)   | 2 (2%)   | 43          | 64 |
| 2   | H     | 82/129 (64%)    | 80 (98%)   | 2 (2%)   | 43          | 64 |
| 3   | D     | 494/712 (69%)   | 484 (98%)  | 10 (2%)  | 48          | 67 |
| 3   | F     | 494/712 (69%)   | 484 (98%)  | 10 (2%)  | 48          | 67 |
| 4   | E     | 227/277 (82%)   | 224 (99%)  | 3 (1%)   | 61          | 72 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 4   | G     | 227/277 (82%)   | 224 (99%)  | 3 (1%)   | 61          | 72 |
| All | All   | 4660/5920 (79%) | 4587 (98%) | 73 (2%)  | 54          | 70 |

All (73) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 100  | LEU  |
| 1   | A     | 101  | LEU  |
| 1   | A     | 187  | LEU  |
| 1   | A     | 200  | MET  |
| 1   | A     | 299  | TYR  |
| 1   | A     | 377  | MET  |
| 1   | A     | 378  | PHE  |
| 1   | A     | 482  | LEU  |
| 1   | A     | 485  | CYS  |
| 1   | A     | 486  | LEU  |
| 1   | A     | 521  | LEU  |
| 1   | A     | 574  | CYS  |
| 1   | A     | 771  | ILE  |
| 1   | A     | 860  | GLU  |
| 1   | A     | 951  | MET  |
| 1   | A     | 1108 | LEU  |
| 1   | A     | 1292 | VAL  |
| 1   | A     | 1492 | LEU  |
| 1   | A     | 1532 | TYR  |
| 1   | A     | 1595 | THR  |
| 1   | A     | 1800 | LYS  |
| 1   | A     | 1920 | PHE  |
| 1   | B     | 101  | LEU  |
| 1   | B     | 187  | LEU  |
| 1   | B     | 200  | MET  |
| 1   | B     | 299  | TYR  |
| 1   | B     | 377  | MET  |
| 1   | B     | 378  | PHE  |
| 1   | B     | 482  | LEU  |
| 1   | B     | 485  | CYS  |
| 1   | B     | 486  | LEU  |
| 1   | B     | 521  | LEU  |
| 1   | B     | 574  | CYS  |
| 1   | B     | 771  | ILE  |
| 1   | B     | 860  | GLU  |
| 1   | B     | 951  | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1108 | LEU  |
| 1   | B     | 1292 | VAL  |
| 1   | B     | 1492 | LEU  |
| 1   | B     | 1532 | TYR  |
| 1   | B     | 1595 | THR  |
| 1   | B     | 1800 | LYS  |
| 1   | B     | 1920 | PHE  |
| 2   | C     | 49   | LEU  |
| 2   | C     | 75   | ASN  |
| 3   | D     | 269  | LEU  |
| 3   | D     | 350  | GLU  |
| 3   | D     | 371  | ILE  |
| 3   | D     | 381  | MET  |
| 3   | D     | 420  | LEU  |
| 3   | D     | 424  | ILE  |
| 3   | D     | 440  | LEU  |
| 3   | D     | 576  | LEU  |
| 3   | D     | 610  | LEU  |
| 3   | D     | 706  | TYR  |
| 4   | E     | 157  | LEU  |
| 4   | E     | 195  | MET  |
| 4   | E     | 244  | ILE  |
| 3   | F     | 269  | LEU  |
| 3   | F     | 350  | GLU  |
| 3   | F     | 371  | ILE  |
| 3   | F     | 381  | MET  |
| 3   | F     | 420  | LEU  |
| 3   | F     | 424  | ILE  |
| 3   | F     | 440  | LEU  |
| 3   | F     | 576  | LEU  |
| 3   | F     | 610  | LEU  |
| 3   | F     | 706  | TYR  |
| 4   | G     | 157  | LEU  |
| 4   | G     | 195  | MET  |
| 4   | G     | 244  | ILE  |
| 2   | H     | 49   | LEU  |
| 2   | H     | 75   | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 91  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 438  | ASN  |
| 1   | A     | 457  | ASN  |
| 1   | A     | 501  | HIS  |
| 1   | A     | 643  | GLN  |
| 1   | A     | 766  | ASN  |
| 1   | A     | 969  | GLN  |
| 1   | A     | 976  | ASN  |
| 1   | A     | 1015 | GLN  |
| 1   | A     | 1029 | GLN  |
| 1   | A     | 1096 | GLN  |
| 1   | A     | 1097 | HIS  |
| 1   | A     | 1114 | ASN  |
| 1   | A     | 1170 | ASN  |
| 1   | A     | 1262 | GLN  |
| 1   | A     | 1304 | GLN  |
| 1   | A     | 1519 | GLN  |
| 1   | A     | 1539 | GLN  |
| 1   | A     | 1557 | GLN  |
| 1   | A     | 1570 | ASN  |
| 1   | A     | 1690 | ASN  |
| 1   | A     | 1694 | ASN  |
| 1   | A     | 2064 | ASN  |
| 1   | B     | 91   | GLN  |
| 1   | B     | 438  | ASN  |
| 1   | B     | 457  | ASN  |
| 1   | B     | 501  | HIS  |
| 1   | B     | 597  | ASN  |
| 1   | B     | 643  | GLN  |
| 1   | B     | 969  | GLN  |
| 1   | B     | 976  | ASN  |
| 1   | B     | 1015 | GLN  |
| 1   | B     | 1026 | HIS  |
| 1   | B     | 1029 | GLN  |
| 1   | B     | 1096 | GLN  |
| 1   | B     | 1097 | HIS  |
| 1   | B     | 1170 | ASN  |
| 1   | B     | 1304 | GLN  |
| 1   | B     | 1519 | GLN  |
| 1   | B     | 1539 | GLN  |
| 1   | B     | 1557 | GLN  |
| 1   | B     | 1690 | ASN  |
| 1   | B     | 1694 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 83  | GLN  |
| 2   | C     | 119 | GLN  |
| 3   | D     | 170 | GLN  |
| 3   | D     | 188 | GLN  |
| 3   | D     | 232 | ASN  |
| 3   | D     | 276 | GLN  |
| 3   | D     | 545 | GLN  |
| 3   | D     | 763 | HIS  |
| 3   | D     | 811 | GLN  |
| 4   | E     | 26  | ASN  |
| 4   | E     | 49  | GLN  |
| 4   | E     | 268 | GLN  |
| 3   | F     | 170 | GLN  |
| 3   | F     | 188 | GLN  |
| 3   | F     | 276 | GLN  |
| 3   | F     | 545 | GLN  |
| 3   | F     | 763 | HIS  |
| 3   | F     | 811 | GLN  |
| 4   | G     | 26  | ASN  |
| 4   | G     | 49  | GLN  |
| 4   | G     | 70  | GLN  |
| 2   | H     | 83  | GLN  |
| 2   | H     | 119 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70826. 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

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

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

## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit

This section was not generated.