



## Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 02:53 PM UTC

PDB ID : 7L6N / pdb\_00007l6n  
EMDB ID : EMD-23206  
Title : The Mycobacterium tuberculosis ClpB disaggregase hexamer structure with three locally refined ClpB middle domains and three DnaK nucleotide binding domains  
Authors : Yin, Y.Y.; Feng, X.; Li, H.  
Deposited on : 2020-12-23  
Resolution : 7.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

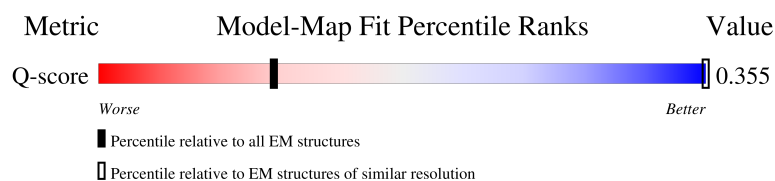
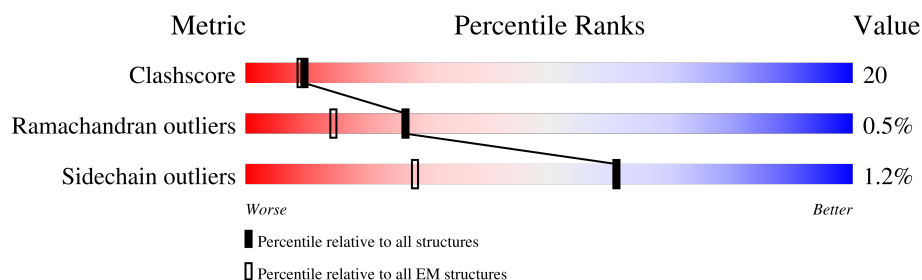
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.00 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.



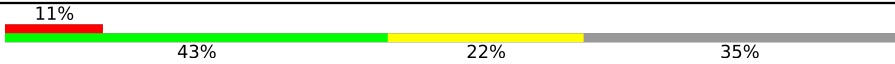
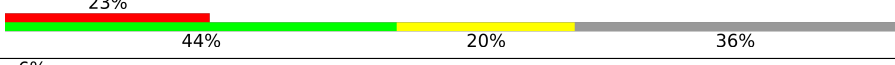
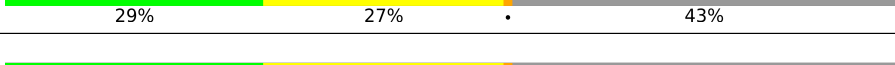
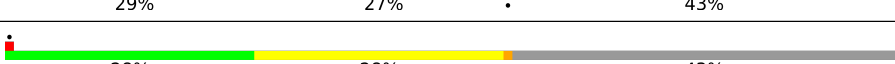
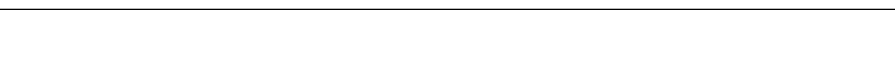
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 483 ( 6.50 - 7.50 )                                      |

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

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 848    |  |
| 1   | B     | 848    |  |
| 1   | C     | 848    |  |
| 1   | D     | 848    |  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 1   | E     | 848    |  |
| 1   | F     | 848    |  |
| 2   | N     | 33     |  |
| 3   | I     | 625    |  |
| 3   | J     | 625    |  |
| 3   | K     | 625    |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4   | AGS  | D     | 902 | -         | -        | X       | -                |
| 4   | AGS  | E     | 901 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 36999 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 Chaperone protein ClpB.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 1   | A     | 674      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5222  | 3253 | 954 | 1004 | 11 |         |       |
| 1   | B     | 672      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5207  | 3241 | 952 | 1004 | 10 |         |       |
| 1   | C     | 675      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5224  | 3251 | 955 | 1008 | 10 |         |       |
| 1   | D     | 562      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 4321  | 2701 | 790 | 821  | 9  |         |       |
| 1   | E     | 548      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 4230  | 2647 | 772 | 802  | 9  |         |       |
| 1   | F     | 546      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 4219  | 2641 | 770 | 799  | 9  |         |       |

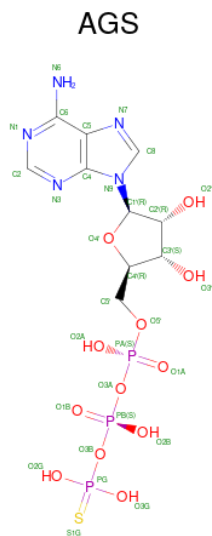
- Molecule 2 is a protein called Substrate.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 2   | N     | 26       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 130   | 78 | 26 | 26 |         |       |

- Molecule 3 is a protein called Chaperone protein DnaK.

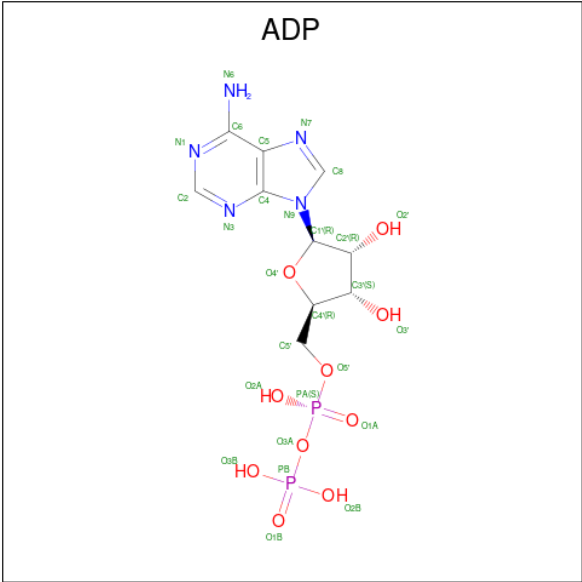
| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | I     | 357      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2694  | 1675 | 474 | 539 | 6 |         |       |
| 3   | J     | 357      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2694  | 1675 | 474 | 539 | 6 |         |       |
| 3   | K     | 357      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2694  | 1675 | 474 | 539 | 6 |         |       |

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



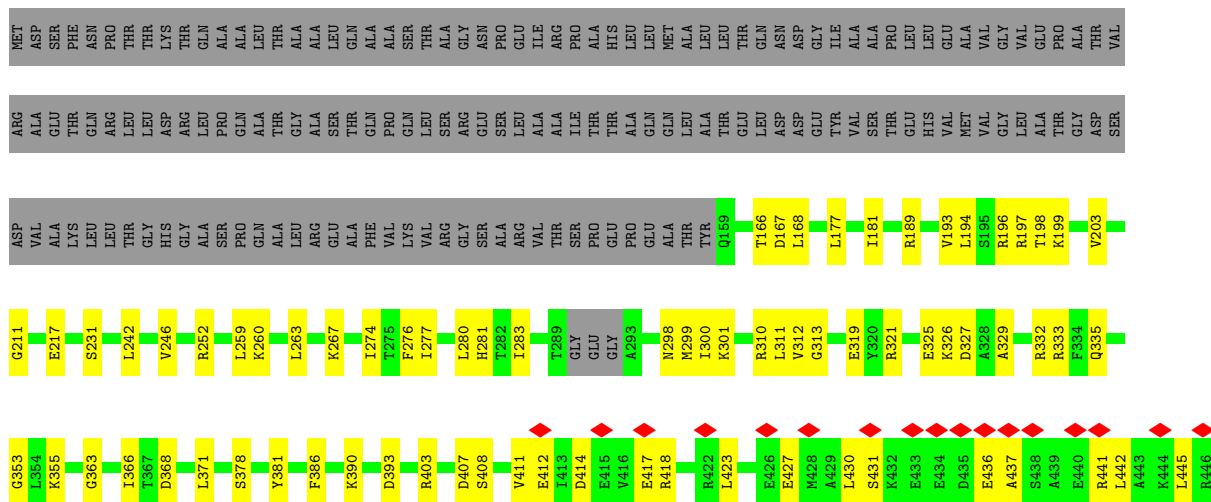
| Mol | Chain | Residues | Atoms       |         |        |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|--------|---------|
| 4   | A     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 4   | A     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 4   | B     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 4   | B     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 4   | C     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 4   | C     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 4   | D     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 4   | D     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 4   | E     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |
| 4   | F     | 1        | Total<br>31 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | S<br>1 | 0       |

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).



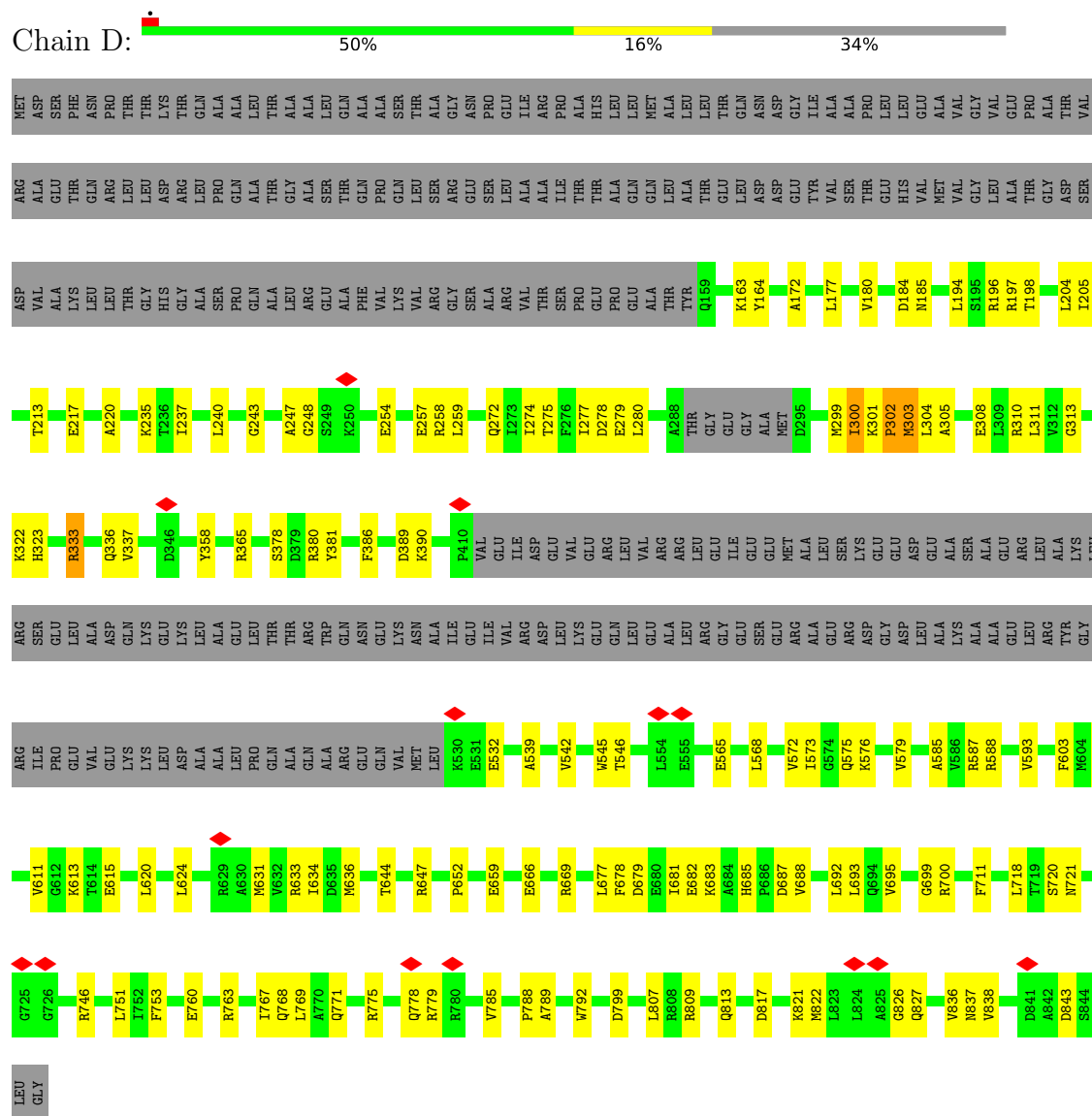
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 5   | E     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 5   | F     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |



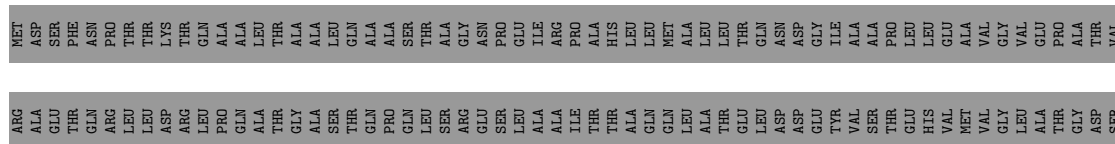




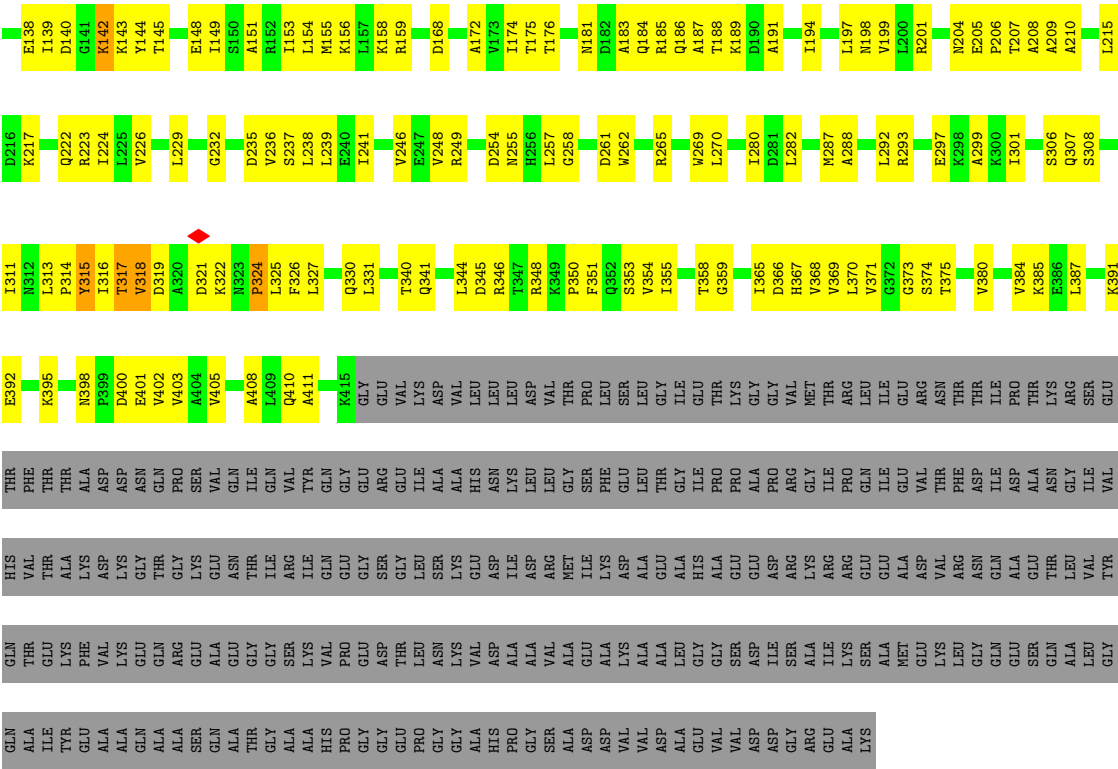
- Molecule 1: Chaperone protein ClpB



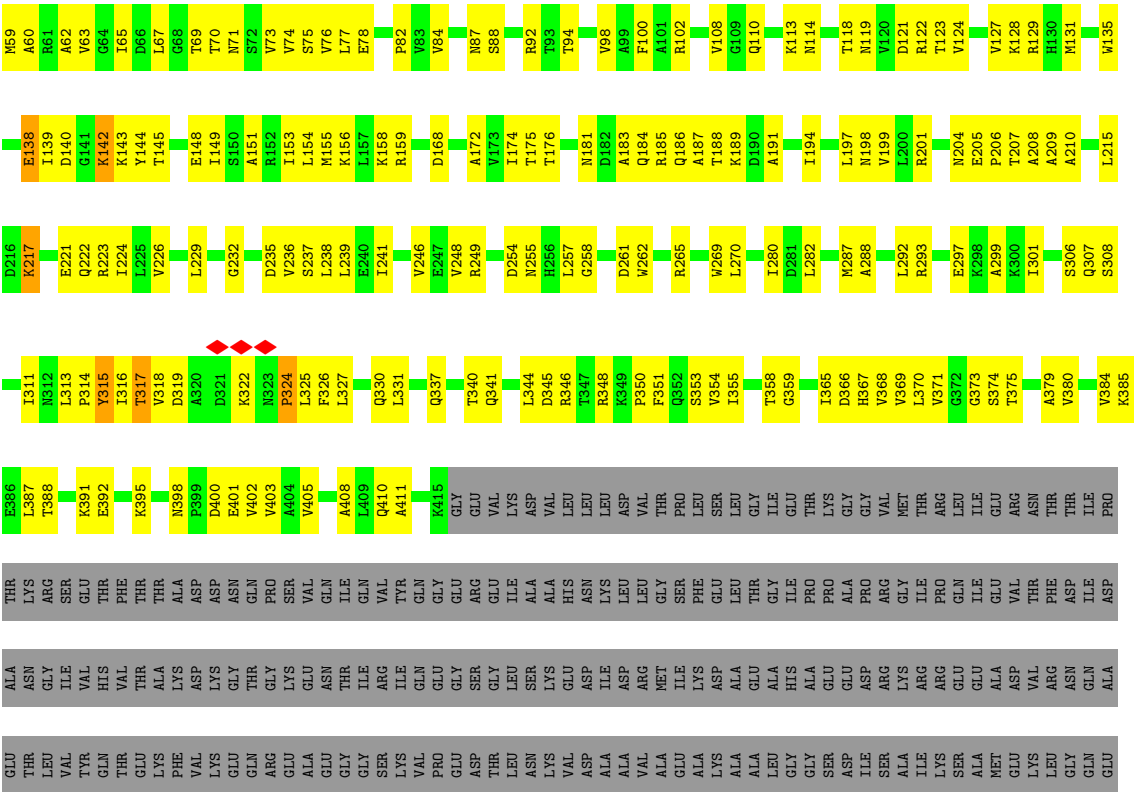
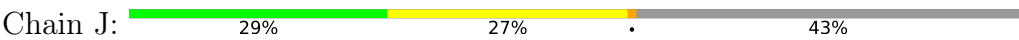
- Molecule 1: Chaperone protein ClpB



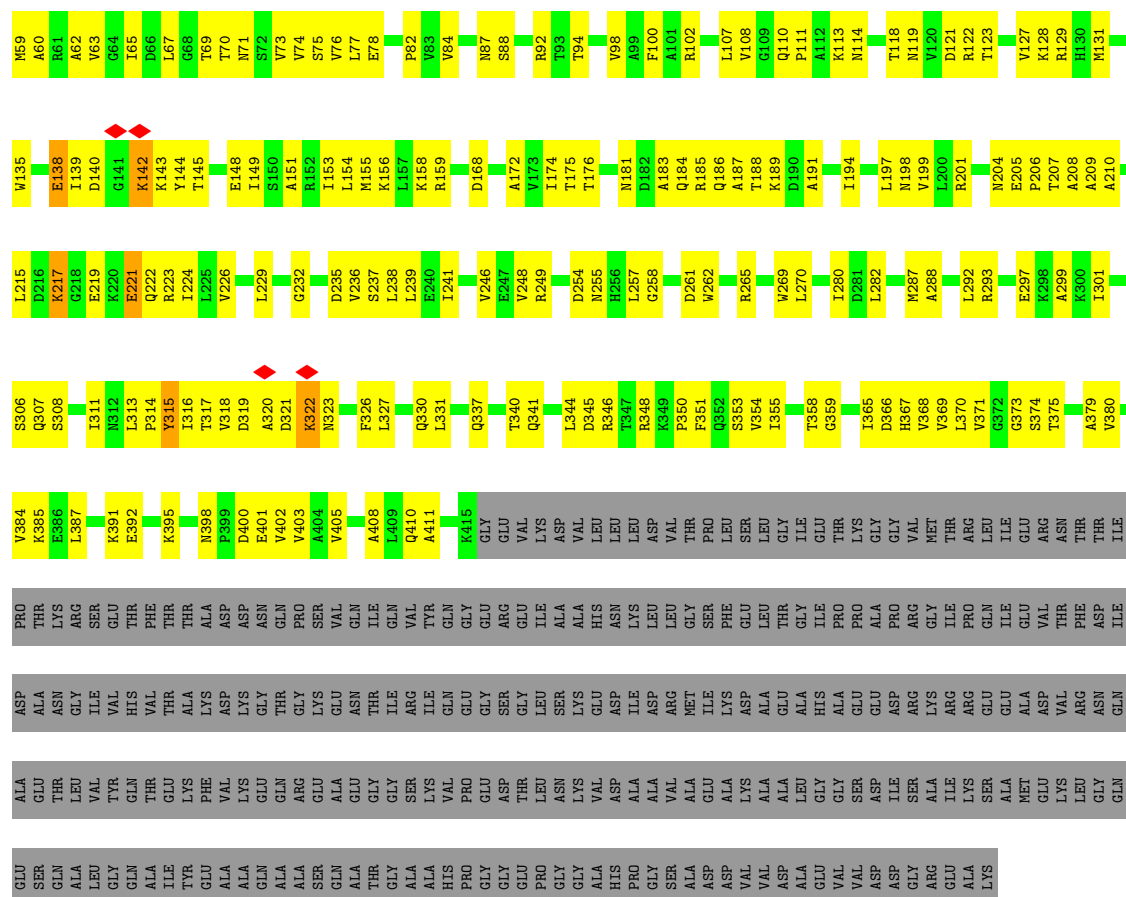




● Molecule 3: Chaperone protein DnaK



Chain K:



## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE           | Depositor |
| Imposed symmetry                     | POINT, Not provided       |           |
| Number of particles used             | 45000                     | Depositor |
| Resolution determination method      | OTHER                     | Depositor |
| CTF correction method                | NONE                      | Depositor |
| Microscope                           | FEI TITAN KRIOS           | Depositor |
| Voltage (kV)                         | 300                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 2                         | Depositor |
| Minimum defocus (nm)                 | Not provided              |           |
| Maximum defocus (nm)                 | Not provided              |           |
| Magnification                        | Not provided              |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value                    | 50.570                    | Depositor |
| Minimum map value                    | -13.833                   | Depositor |
| Average map value                    | 0.042                     | Depositor |
| Map value standard deviation         | 1.510                     | Depositor |
| Recommended contour level            | 7.1                       | Depositor |
| Map size ( $\text{\AA}$ )            | 386.64, 386.64, 386.64    | wwPDB     |
| Map dimensions                       | 360, 360, 360             | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0          | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.074, 1.074, 1.074       | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, AGS

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     | 0.32         | 0/5286  | 0.53        | 1/7126 (0.0%)  |
| 1   | B     | 0.30         | 0/5271  | 0.60        | 6/7106 (0.1%)  |
| 1   | C     | 0.29         | 0/5288  | 0.53        | 0/7130         |
| 1   | D     | 0.28         | 0/4380  | 0.53        | 0/5914         |
| 1   | E     | 0.22         | 0/4286  | 0.49        | 1/5786 (0.0%)  |
| 1   | F     | 0.19         | 0/4276  | 0.47        | 0/5774         |
| 3   | I     | 0.42         | 0/2727  | 0.68        | 1/3695 (0.0%)  |
| 3   | J     | 0.42         | 0/2727  | 0.67        | 0/3695         |
| 3   | K     | 0.42         | 0/2727  | 0.68        | 0/3695         |
| All | All   | 0.31         | 0/36968 | 0.56        | 9/49921 (0.0%) |

There are no bond length outliers.

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | B     | 388 | PRO  | CB-CA-C  | 9.93  | 127.95      | 111.56   |
| 1   | B     | 388 | PRO  | CA-N-CD  | -9.63 | 98.51       | 112.00   |
| 1   | B     | 413 | ILE  | N-CA-C   | -8.53 | 104.86      | 113.47   |
| 3   | I     | 321 | ASP  | CA-C-O   | -6.36 | 114.15      | 120.82   |
| 1   | B     | 386 | PHE  | CA-CB-CG | -6.30 | 107.50      | 113.80   |
| 1   | A     | 413 | ILE  | N-CA-C   | -6.05 | 107.00      | 111.90   |
| 1   | B     | 477 | LYS  | CB-CA-C  | -5.52 | 102.22      | 110.88   |
| 1   | E     | 805 | ARG  | CB-CG-CD | -5.06 | 99.66       | 111.30   |
| 1   | B     | 478 | GLU  | N-CA-C   | -5.01 | 105.81      | 111.28   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5222  | 0        | 5289     | 195     | 0            |
| 1   | B     | 5207  | 0        | 5264     | 181     | 0            |
| 1   | C     | 5224  | 0        | 5278     | 191     | 0            |
| 1   | D     | 4321  | 0        | 4378     | 135     | 0            |
| 1   | E     | 4230  | 0        | 4290     | 165     | 0            |
| 1   | F     | 4219  | 0        | 4283     | 144     | 0            |
| 2   | N     | 130   | 0        | 31       | 2       | 0            |
| 3   | I     | 2694  | 0        | 2716     | 182     | 0            |
| 3   | J     | 2694  | 0        | 2718     | 178     | 0            |
| 3   | K     | 2694  | 0        | 2718     | 172     | 0            |
| 4   | A     | 62    | 0        | 24       | 7       | 0            |
| 4   | B     | 62    | 0        | 24       | 7       | 0            |
| 4   | C     | 62    | 0        | 24       | 10      | 0            |
| 4   | D     | 62    | 0        | 24       | 13      | 0            |
| 4   | E     | 31    | 0        | 12       | 14      | 0            |
| 4   | F     | 31    | 0        | 12       | 3       | 0            |
| 5   | E     | 27    | 0        | 12       | 3       | 0            |
| 5   | F     | 27    | 0        | 12       | 2       | 0            |
| All | All   | 36999 | 0        | 37109    | 1464    | 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 20.

All (1464) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:E:801:VAL:HG23 | 1:E:802:TYR:CE1 | 1.38                     | 1.55              |
| 3:I:222:GLN:NE2  | 3:I:241:ILE:CG2 | 1.69                     | 1.54              |
| 3:I:222:GLN:NE2  | 3:I:241:ILE:CB  | 1.68                     | 1.49              |
| 1:D:301:LYS:HG2  | 1:D:333:ARG:NH2 | 1.27                     | 1.43              |
| 1:E:801:VAL:HG23 | 1:E:802:TYR:CD1 | 1.52                     | 1.42              |
| 1:B:342:PRO:O    | 1:B:387:LEU:CD1 | 1.67                     | 1.41              |
| 1:D:303:MET:CE   | 1:D:308:GLU:CB  | 1.99                     | 1.40              |
| 1:D:301:LYS:CG   | 1:D:333:ARG:NH2 | 1.86                     | 1.38              |
| 1:D:303:MET:CE   | 1:D:308:GLU:HG3 | 1.51                     | 1.38              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:801:VAL:CG2  | 1:E:802:TYR:CE1  | 2.07                     | 1.37              |
| 1:D:303:MET:HE2  | 1:D:308:GLU:CB   | 1.53                     | 1.37              |
| 1:D:303:MET:CE   | 1:D:308:GLU:CG   | 2.02                     | 1.36              |
| 3:I:222:GLN:NE2  | 3:I:241:ILE:HB   | 1.20                     | 1.36              |
| 1:C:476:LEU:HD23 | 1:C:510:VAL:CG1  | 1.57                     | 1.31              |
| 3:J:217:LYS:CD   | 3:J:366:ASP:HB3  | 1.67                     | 1.24              |
| 1:D:303:MET:HE2  | 1:D:308:GLU:CG   | 1.63                     | 1.23              |
| 1:C:476:LEU:CD2  | 1:C:510:VAL:HG13 | 1.67                     | 1.22              |
| 3:I:319:ASP:OD2  | 3:I:325:LEU:HG   | 1.43                     | 1.17              |
| 1:D:303:MET:HE2  | 1:D:308:GLU:HB2  | 1.25                     | 1.17              |
| 1:A:501:GLU:HA   | 3:I:315:TYR:HD2  | 1.11                     | 1.16              |
| 1:B:473:VAL:HG21 | 1:B:517:ALA:HB1  | 1.20                     | 1.16              |
| 1:C:501:GLU:HA   | 3:K:315:TYR:HD2  | 1.11                     | 1.15              |
| 1:B:501:GLU:HA   | 3:J:315:TYR:HD2  | 1.11                     | 1.15              |
| 1:B:342:PRO:O    | 1:B:387:LEU:HD13 | 1.39                     | 1.13              |
| 1:B:473:VAL:HG21 | 1:B:517:ALA:CB   | 1.79                     | 1.12              |
| 1:A:406:ILE:HD12 | 1:A:529:LEU:HD21 | 1.29                     | 1.12              |
| 1:A:500:ALA:HB2  | 3:I:316:ILE:O    | 1.48                     | 1.11              |
| 1:B:500:ALA:HB2  | 3:J:316:ILE:O    | 1.48                     | 1.11              |
| 1:D:303:MET:HE1  | 1:D:308:GLU:HB3  | 1.13                     | 1.08              |
| 1:D:303:MET:HE3  | 1:D:308:GLU:HG3  | 1.26                     | 1.08              |
| 1:C:480:LEU:HD13 | 1:C:510:VAL:CG1  | 1.83                     | 1.08              |
| 1:C:476:LEU:O    | 1:C:479:GLN:HB3  | 1.52                     | 1.07              |
| 3:J:319:ASP:HB3  | 3:J:325:LEU:HG   | 1.15                     | 1.07              |
| 3:I:222:GLN:NE2  | 3:I:241:ILE:HG21 | 1.69                     | 1.07              |
| 1:B:342:PRO:O    | 1:B:387:LEU:HD11 | 1.56                     | 1.06              |
| 1:D:573:ILE:O    | 4:D:902:AGS:N6   | 1.87                     | 1.06              |
| 1:F:311:LEU:HD11 | 1:F:334:PHE:HZ   | 1.18                     | 1.06              |
| 3:I:319:ASP:OD2  | 3:I:325:LEU:CG   | 2.04                     | 1.06              |
| 1:C:477:LYS:HA   | 1:C:480:LEU:HB3  | 1.36                     | 1.06              |
| 1:A:465:ASN:O    | 1:A:466:GLU:C    | 1.96                     | 1.05              |
| 3:J:217:LYS:HD3  | 3:J:366:ASP:HB3  | 1.34                     | 1.05              |
| 3:K:217:LYS:HE2  | 3:K:217:LYS:HA   | 1.36                     | 1.04              |
| 3:I:222:GLN:CD   | 3:I:241:ILE:HB   | 1.84                     | 1.03              |
| 1:B:476:LEU:HD11 | 1:B:513:LYS:HD3  | 1.38                     | 1.02              |
| 1:D:303:MET:HE1  | 1:D:308:GLU:CB   | 1.75                     | 1.01              |
| 3:I:222:GLN:NE2  | 3:I:241:ILE:HG22 | 1.72                     | 1.00              |
| 1:E:801:VAL:CG2  | 1:E:802:TYR:HE1  | 1.71                     | 1.00              |
| 1:C:476:LEU:O    | 1:C:480:LEU:N    | 1.95                     | 1.00              |
| 3:I:319:ASP:CG   | 3:I:325:LEU:HG   | 1.87                     | 1.00              |
| 1:C:480:LEU:HD13 | 1:C:510:VAL:HG12 | 1.43                     | 0.99              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:211:GLY:N    | 4:E:901:AGS:O1B  | 1.92                     | 0.98              |
| 1:B:389:ASP:OD2  | 1:C:332:ARG:HD2  | 1.64                     | 0.98              |
| 1:D:301:LYS:CG   | 1:D:333:ARG:HH22 | 1.59                     | 0.98              |
| 1:A:431:SER:HA   | 1:A:442:LEU:CD1  | 1.94                     | 0.97              |
| 1:D:301:LYS:CG   | 1:D:333:ARG:HH21 | 1.70                     | 0.97              |
| 1:D:301:LYS:HG3  | 1:D:333:ARG:HH21 | 1.28                     | 0.96              |
| 1:E:180:VAL:HA   | 4:E:901:AGS:C2   | 1.94                     | 0.95              |
| 1:B:378:SER:O    | 1:B:390:LYS:HE3  | 1.65                     | 0.95              |
| 1:C:477:LYS:HA   | 1:C:480:LEU:CB   | 1.96                     | 0.94              |
| 1:A:431:SER:HA   | 1:A:442:LEU:HD11 | 1.51                     | 0.92              |
| 3:J:319:ASP:CB   | 3:J:325:LEU:HG   | 1.97                     | 0.92              |
| 1:C:476:LEU:HD21 | 1:C:510:VAL:HG22 | 1.49                     | 0.92              |
| 3:I:222:GLN:HG2  | 3:I:241:ILE:O    | 1.70                     | 0.92              |
| 1:C:501:GLU:HA   | 3:K:315:TYR:CD2  | 2.04                     | 0.91              |
| 1:A:501:GLU:HA   | 3:I:315:TYR:CD2  | 2.04                     | 0.91              |
| 3:I:313:LEU:O    | 3:I:326:PHE:HB2  | 1.71                     | 0.91              |
| 1:A:406:ILE:HD12 | 1:A:529:LEU:CD2  | 2.00                     | 0.91              |
| 3:K:313:LEU:O    | 3:K:326:PHE:HB2  | 1.71                     | 0.91              |
| 1:B:387:LEU:HB3  | 1:B:388:PRO:HD2  | 1.53                     | 0.90              |
| 1:B:501:GLU:HA   | 3:J:315:TYR:CD2  | 2.04                     | 0.90              |
| 1:D:301:LYS:HG3  | 1:D:333:ARG:NH2  | 1.79                     | 0.90              |
| 3:J:313:LEU:O    | 3:J:326:PHE:HB2  | 1.71                     | 0.90              |
| 1:F:304:LEU:HD22 | 1:F:311:LEU:CD2  | 2.02                     | 0.90              |
| 1:A:427:GLU:OE2  | 1:A:446:ARG:NH2  | 2.05                     | 0.89              |
| 3:K:280:ILE:HG21 | 3:K:317:THR:HG21 | 1.54                     | 0.89              |
| 1:E:804:ALA:CB   | 1:E:807:LEU:HD12 | 2.03                     | 0.89              |
| 1:C:471:GLU:O    | 1:C:475:ASP:CB   | 2.21                     | 0.88              |
| 1:A:466:GLU:OE1  | 1:A:466:GLU:N    | 2.07                     | 0.88              |
| 1:C:476:LEU:O    | 1:C:479:GLN:CB   | 2.20                     | 0.88              |
| 1:F:311:LEU:HD11 | 1:F:334:PHE:CZ   | 2.07                     | 0.87              |
| 1:E:209:GLY:HA2  | 4:E:901:AGS:O2G  | 1.72                     | 0.87              |
| 1:D:301:LYS:HG2  | 1:D:333:ARG:HH22 | 0.77                     | 0.87              |
| 1:B:500:ALA:HB2  | 3:J:316:ILE:C    | 2.00                     | 0.86              |
| 1:A:500:ALA:HB2  | 3:I:316:ILE:C    | 2.00                     | 0.85              |
| 1:C:472:ILE:HD12 | 1:C:473:VAL:H    | 1.41                     | 0.85              |
| 1:E:801:VAL:HG21 | 1:E:802:TYR:HE1  | 1.42                     | 0.85              |
| 1:C:476:LEU:CD2  | 1:C:510:VAL:HG22 | 2.07                     | 0.84              |
| 3:J:318:VAL:CG2  | 3:J:322:LYS:HA   | 2.05                     | 0.84              |
| 1:E:801:VAL:CG2  | 1:E:802:TYR:CD1  | 2.49                     | 0.84              |
| 1:A:465:ASN:O    | 1:A:467:LYS:N    | 2.09                     | 0.84              |
| 1:E:801:VAL:HG21 | 1:E:802:TYR:CE1  | 2.12                     | 0.83              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:303:MET:CE   | 1:D:308:GLU:HB3  | 1.79                     | 0.83              |
| 1:C:473:VAL:O    | 1:C:514:LEU:HD21 | 1.79                     | 0.83              |
| 1:B:473:VAL:HG13 | 1:B:514:LEU:HD13 | 1.58                     | 0.83              |
| 1:B:280:LEU:HD23 | 1:B:313:GLY:HA3  | 1.59                     | 0.82              |
| 1:B:476:LEU:HD21 | 1:B:510:VAL:CG1  | 2.10                     | 0.82              |
| 1:D:303:MET:HE2  | 1:D:308:GLU:HG3  | 1.30                     | 0.82              |
| 1:B:476:LEU:CD1  | 1:B:513:LYS:HD3  | 2.09                     | 0.82              |
| 3:J:217:LYS:HD2  | 3:J:366:ASP:HB3  | 1.62                     | 0.82              |
| 1:C:471:GLU:O    | 1:C:475:ASP:N    | 2.12                     | 0.81              |
| 1:A:532:GLU:N    | 1:A:532:GLU:OE1  | 2.13                     | 0.81              |
| 1:F:605:PHE:HB3  | 1:F:751:LEU:HB2  | 1.62                     | 0.81              |
| 1:A:442:LEU:HD23 | 1:A:442:LEU:O    | 1.81                     | 0.80              |
| 1:C:476:LEU:O    | 1:C:479:GLN:CA   | 2.29                     | 0.80              |
| 3:I:319:ASP:OD2  | 3:I:325:LEU:CD1  | 2.29                     | 0.80              |
| 1:D:573:ILE:HD11 | 1:D:763:ARG:NH1  | 1.98                     | 0.79              |
| 1:A:406:ILE:CD1  | 1:A:529:LEU:HD21 | 2.10                     | 0.79              |
| 1:C:500:ALA:HB2  | 3:K:316:ILE:O    | 1.82                     | 0.79              |
| 1:E:757:ASN:HB3  | 1:E:760:GLU:HB2  | 1.65                     | 0.79              |
| 3:K:217:LYS:O    | 3:K:217:LYS:NZ   | 2.13                     | 0.79              |
| 1:E:180:VAL:HA   | 4:E:901:AGS:N1   | 1.98                     | 0.78              |
| 3:I:222:GLN:CG   | 3:I:241:ILE:HB   | 2.14                     | 0.78              |
| 1:A:466:GLU:O    | 1:A:469:ALA:N    | 2.16                     | 0.78              |
| 1:C:280:LEU:HD23 | 1:C:313:GLY:HA3  | 1.65                     | 0.78              |
| 1:B:342:PRO:C    | 1:B:387:LEU:HD13 | 2.08                     | 0.77              |
| 1:C:501:GLU:CA   | 3:K:315:TYR:HD2  | 1.97                     | 0.76              |
| 4:D:901:AGS:S1G  | 1:E:332:ARG:NH1  | 2.59                     | 0.76              |
| 3:J:217:LYS:HD3  | 3:J:366:ASP:CB   | 2.13                     | 0.76              |
| 1:E:805:ARG:CB   | 1:E:806:PRO:CD   | 2.64                     | 0.76              |
| 3:J:318:VAL:HG22 | 3:J:322:LYS:HA   | 1.68                     | 0.76              |
| 1:D:572:VAL:HG22 | 1:D:615:GLU:OE1  | 1.86                     | 0.76              |
| 3:I:308:SER:OG   | 3:I:331:LEU:O    | 2.03                     | 0.76              |
| 1:B:473:VAL:CG1  | 1:B:514:LEU:CD1  | 2.64                     | 0.76              |
| 1:C:513:LYS:HA   | 1:C:513:LYS:HE3  | 1.68                     | 0.76              |
| 3:J:280:ILE:HG21 | 3:J:317:THR:HG21 | 1.68                     | 0.75              |
| 1:F:304:LEU:HD22 | 1:F:311:LEU:HD21 | 1.68                     | 0.75              |
| 1:B:476:LEU:HD21 | 1:B:510:VAL:HG13 | 1.69                     | 0.75              |
| 4:B:902:AGS:S1G  | 1:C:746:ARG:NH2  | 2.60                     | 0.75              |
| 3:I:280:ILE:HG21 | 3:I:317:THR:HG21 | 1.68                     | 0.75              |
| 3:J:308:SER:OG   | 3:J:331:LEU:O    | 2.03                     | 0.74              |
| 1:B:501:GLU:CA   | 3:J:315:TYR:HD2  | 1.97                     | 0.74              |
| 1:E:804:ALA:HB2  | 1:E:807:LEU:HD12 | 1.70                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:472:ILE:O    | 1:C:473:VAL:C    | 2.30                     | 0.74              |
| 3:I:159:ARG:NH1  | 3:I:168:ASP:OD2  | 2.21                     | 0.74              |
| 1:A:501:GLU:CA   | 3:I:315:TYR:HD2  | 1.97                     | 0.74              |
| 3:I:100:PHE:CD2  | 3:I:139:ILE:HG21 | 2.23                     | 0.73              |
| 3:K:100:PHE:CD2  | 3:K:139:ILE:HG21 | 2.23                     | 0.73              |
| 1:B:476:LEU:HD12 | 1:B:513:LYS:NZ   | 2.02                     | 0.73              |
| 3:J:159:ARG:NH1  | 3:J:168:ASP:OD2  | 2.21                     | 0.73              |
| 3:J:100:PHE:CD2  | 3:J:139:ILE:HG21 | 2.23                     | 0.73              |
| 4:C:901:AGS:S1G  | 1:D:746:ARG:NH2  | 2.61                     | 0.73              |
| 1:C:547:GLY:H    | 1:C:671:ARG:HH21 | 1.35                     | 0.73              |
| 1:A:504:TYR:CE1  | 3:I:318:VAL:HB   | 2.24                     | 0.73              |
| 1:C:504:TYR:CE1  | 3:K:318:VAL:HB   | 2.24                     | 0.73              |
| 1:E:283:ILE:HG22 | 1:E:284:VAL:HG13 | 1.70                     | 0.73              |
| 3:K:159:ARG:NH1  | 3:K:168:ASP:OD2  | 2.21                     | 0.73              |
| 3:K:217:LYS:HA   | 3:K:217:LYS:CE   | 2.18                     | 0.73              |
| 1:B:476:LEU:C    | 1:B:476:LEU:HD23 | 2.14                     | 0.72              |
| 1:A:427:GLU:HG2  | 1:A:445:LEU:HD22 | 1.70                     | 0.72              |
| 3:I:235:ASP:OD1  | 3:I:237:SER:OG   | 2.07                     | 0.72              |
| 1:A:442:LEU:HD23 | 1:A:442:LEU:C    | 2.15                     | 0.72              |
| 1:B:378:SER:O    | 1:B:390:LYS:CE   | 2.36                     | 0.72              |
| 1:C:477:LYS:O    | 1:C:480:LEU:N    | 2.23                     | 0.72              |
| 1:F:236:THR:OG1  | 1:F:272:GLN:O    | 2.07                     | 0.72              |
| 1:F:681:ILE:HG12 | 1:F:718:LEU:HD23 | 1.71                     | 0.72              |
| 3:I:176:THR:OG1  | 3:I:204:ASN:OD1  | 2.07                     | 0.72              |
| 3:J:235:ASP:OD1  | 3:J:237:SER:OG   | 2.07                     | 0.72              |
| 1:C:469:ALA:O    | 1:C:473:VAL:HG22 | 1.90                     | 0.72              |
| 3:I:129:ARG:NH2  | 3:I:232:GLY:O    | 2.24                     | 0.71              |
| 1:D:545:TRP:HD1  | 1:D:546:THR:HG23 | 1.53                     | 0.71              |
| 1:F:212:LYS:HD3  | 1:F:314:ALA:HB1  | 1.72                     | 0.71              |
| 3:J:217:LYS:CE   | 3:J:366:ASP:HB3  | 2.20                     | 0.71              |
| 3:K:176:THR:OG1  | 3:K:204:ASN:OD1  | 2.07                     | 0.71              |
| 3:I:113:LYS:NZ   | 3:I:297:GLU:OE1  | 2.19                     | 0.71              |
| 3:J:209:ALA:HB1  | 3:J:369:VAL:HG11 | 1.73                     | 0.71              |
| 3:K:129:ARG:NH2  | 3:K:232:GLY:O    | 2.24                     | 0.71              |
| 3:K:209:ALA:HB1  | 3:K:369:VAL:HG11 | 1.73                     | 0.71              |
| 1:C:822:MET:HB3  | 1:C:828:VAL:HG21 | 1.72                     | 0.71              |
| 4:C:902:AGS:S1G  | 1:D:333:ARG:NH1  | 2.64                     | 0.71              |
| 1:D:301:LYS:HG2  | 1:D:301:LYS:O    | 1.89                     | 0.71              |
| 3:I:128:LYS:NZ   | 3:I:205:GLU:OE2  | 2.23                     | 0.71              |
| 3:J:129:ARG:NH2  | 3:J:232:GLY:O    | 2.23                     | 0.71              |
| 3:K:219:GLU:CD   | 3:K:219:GLU:H    | 1.96                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:235:ASP:OD1  | 3:K:237:SER:OG   | 2.07                     | 0.71              |
| 3:K:308:SER:OG   | 3:K:331:LEU:O    | 2.03                     | 0.71              |
| 1:A:427:GLU:HB2  | 1:A:445:LEU:HD21 | 1.72                     | 0.70              |
| 1:E:805:ARG:CB   | 1:E:806:PRO:HD3  | 2.21                     | 0.70              |
| 1:F:573:ILE:H    | 4:F:901:AGS:HN62 | 1.39                     | 0.70              |
| 1:C:477:LYS:C    | 1:C:479:GLN:N    | 2.47                     | 0.70              |
| 1:D:573:ILE:HG22 | 4:D:902:AGS:N1   | 2.05                     | 0.70              |
| 1:E:802:TYR:HB2  | 1:E:805:ARG:HD2  | 1.72                     | 0.70              |
| 3:J:176:THR:OG1  | 3:J:204:ASN:OD1  | 2.07                     | 0.70              |
| 1:E:180:VAL:HA   | 4:E:901:AGS:H2   | 1.72                     | 0.70              |
| 1:D:775:ARG:NH1  | 1:E:593:VAL:O    | 2.25                     | 0.69              |
| 1:E:804:ALA:HB1  | 1:E:807:LEU:HD12 | 1.72                     | 0.69              |
| 4:B:901:AGS:S1G  | 1:C:333:ARG:NH1  | 2.62                     | 0.69              |
| 3:I:209:ALA:HB1  | 3:I:369:VAL:HG11 | 1.73                     | 0.69              |
| 3:K:128:LYS:NZ   | 3:K:205:GLU:OE2  | 2.23                     | 0.69              |
| 1:A:469:ALA:HB1  | 1:A:519:PRO:HG3  | 1.73                     | 0.69              |
| 1:B:341:GLU:HG3  | 1:B:387:LEU:HD12 | 1.74                     | 0.69              |
| 1:E:613:LYS:HA   | 1:E:753:PHE:HE2  | 1.57                     | 0.69              |
| 1:C:471:GLU:O    | 1:C:475:ASP:HB2  | 1.93                     | 0.69              |
| 1:A:561:LEU:O    | 1:A:587:ARG:NH2  | 2.25                     | 0.69              |
| 1:C:476:LEU:O    | 1:C:479:GLN:C    | 2.36                     | 0.69              |
| 3:J:217:LYS:CD   | 3:J:366:ASP:CB   | 2.60                     | 0.69              |
| 1:A:445:LEU:O    | 1:A:445:LEU:HD23 | 1.91                     | 0.69              |
| 1:B:501:GLU:OE2  | 1:B:506:ARG:NH2  | 2.25                     | 0.69              |
| 1:A:501:GLU:OE2  | 1:A:506:ARG:NH2  | 2.25                     | 0.69              |
| 1:C:501:GLU:OE2  | 1:C:506:ARG:NH2  | 2.25                     | 0.69              |
| 1:E:207:GLU:HB3  | 1:E:208:PRO:HD2  | 1.75                     | 0.69              |
| 3:K:63:VAL:HG12  | 3:K:76:VAL:HG12  | 1.75                     | 0.69              |
| 1:E:784:GLN:HE22 | 1:E:786:SER:HB3  | 1.58                     | 0.69              |
| 3:I:122:ARG:NH1  | 3:I:140:ASP:OD1  | 2.26                     | 0.69              |
| 1:E:228:VAL:O    | 1:E:233:ARG:NH2  | 2.26                     | 0.68              |
| 1:A:465:ASN:O    | 1:A:468:ASN:N    | 2.26                     | 0.68              |
| 3:J:63:VAL:HG12  | 3:J:76:VAL:HG12  | 1.75                     | 0.68              |
| 3:I:142:LYS:CG   | 3:I:143:LYS:N    | 2.57                     | 0.68              |
| 3:J:122:ARG:NH1  | 3:J:140:ASP:OD1  | 2.26                     | 0.68              |
| 1:A:410:PRO:HG3  | 1:A:463:TRP:CD1  | 2.29                     | 0.68              |
| 1:C:478:GLU:OE2  | 1:C:478:GLU:HA   | 1.93                     | 0.68              |
| 3:K:122:ARG:NH1  | 3:K:140:ASP:OD1  | 2.27                     | 0.68              |
| 3:K:142:LYS:CG   | 3:K:143:LYS:N    | 2.57                     | 0.68              |
| 1:C:473:VAL:HA   | 1:C:514:LEU:CD2  | 2.24                     | 0.68              |
| 1:F:693:LEU:O    | 1:F:746:ARG:NH1  | 2.27                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:63:VAL:HG12  | 3:I:76:VAL:HG12  | 1.75                     | 0.68              |
| 1:D:301:LYS:H    | 1:D:302:PRO:HD3  | 1.59                     | 0.68              |
| 1:E:211:GLY:H    | 4:E:901:AGS:PB   | 2.17                     | 0.68              |
| 1:A:194:LEU:O    | 1:A:310:ARG:NH1  | 2.27                     | 0.68              |
| 1:C:566:ASP:O    | 1:C:570:LYS:NZ   | 2.27                     | 0.68              |
| 3:I:223:ARG:HD2  | 3:I:238:LEU:HD22 | 1.76                     | 0.68              |
| 1:C:199:LYS:HD2  | 1:C:333:ARG:HA   | 1.76                     | 0.67              |
| 1:F:267:LYS:NZ   | 1:F:308:GLU:OE2  | 2.26                     | 0.67              |
| 3:J:223:ARG:HD2  | 3:J:238:LEU:HD22 | 1.76                     | 0.67              |
| 3:K:223:ARG:HD2  | 3:K:238:LEU:HD22 | 1.76                     | 0.67              |
| 1:A:287:GLY:O    | 1:B:252:ARG:NH2  | 2.27                     | 0.67              |
| 3:I:371:VAL:HG12 | 3:I:402:VAL:HG11 | 1.76                     | 0.67              |
| 1:E:669:ARG:HB3  | 1:E:709:VAL:HG12 | 1.76                     | 0.67              |
| 1:F:201:ASN:HB2  | 1:F:310:ARG:O    | 1.93                     | 0.67              |
| 1:F:304:LEU:CD2  | 1:F:311:LEU:HD21 | 2.25                     | 0.67              |
| 1:F:575:GLN:HB3  | 1:F:578:ALA:HB3  | 1.76                     | 0.67              |
| 3:I:119:ASN:O    | 3:I:123:THR:N    | 2.28                     | 0.67              |
| 3:I:181:ASN:ND2  | 3:I:184:GLN:OE1  | 2.28                     | 0.67              |
| 1:C:518:LEU:N    | 1:C:518:LEU:HD12 | 2.10                     | 0.67              |
| 1:F:302:PRO:O    | 1:F:306:ARG:NH1  | 2.28                     | 0.67              |
| 3:K:371:VAL:HG12 | 3:K:402:VAL:HG11 | 1.76                     | 0.67              |
| 3:K:119:ASN:O    | 3:K:123:THR:N    | 2.28                     | 0.67              |
| 1:B:473:VAL:HG13 | 1:B:514:LEU:CD1  | 2.25                     | 0.67              |
| 3:J:181:ASN:ND2  | 3:J:184:GLN:OE1  | 2.27                     | 0.67              |
| 3:K:181:ASN:ND2  | 3:K:184:GLN:OE1  | 2.27                     | 0.67              |
| 3:I:254:ASP:OD2  | 3:I:346:ARG:NE   | 2.28                     | 0.67              |
| 1:A:466:GLU:O    | 1:A:467:LYS:C    | 2.38                     | 0.66              |
| 1:B:341:GLU:HG3  | 1:B:387:LEU:CD1  | 2.25                     | 0.66              |
| 1:D:301:LYS:N    | 1:D:302:PRO:HD3  | 2.10                     | 0.66              |
| 3:I:340:THR:O    | 3:I:344:LEU:N    | 2.28                     | 0.66              |
| 1:C:476:LEU:CD2  | 1:C:510:VAL:CG1  | 2.49                     | 0.66              |
| 1:C:476:LEU:HD21 | 1:C:510:VAL:CG2  | 2.24                     | 0.66              |
| 3:K:113:LYS:NZ   | 3:K:297:GLU:OE1  | 2.19                     | 0.66              |
| 3:K:340:THR:O    | 3:K:344:LEU:N    | 2.28                     | 0.66              |
| 1:A:476:LEU:HB2  | 1:A:514:LEU:HD13 | 1.77                     | 0.66              |
| 1:A:775:ARG:NH2  | 1:B:595:ASP:OD1  | 2.29                     | 0.66              |
| 3:J:119:ASN:O    | 3:J:123:THR:N    | 2.28                     | 0.66              |
| 3:K:77:LEU:HD11  | 3:K:408:ALA:O    | 1.95                     | 0.66              |
| 1:B:604:MET:HB2  | 1:B:718:LEU:HB2  | 1.77                     | 0.66              |
| 3:J:142:LYS:CG   | 3:J:143:LYS:N    | 2.57                     | 0.66              |
| 1:B:209:GLY:HA2  | 1:B:389:ASP:OD2  | 1.95                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:476:LEU:HD23 | 1:C:510:VAL:CB   | 2.26                     | 0.66              |
| 1:F:394:LEU:HD21 | 1:F:538:ILE:HG23 | 1.78                     | 0.66              |
| 1:B:566:ASP:O    | 1:B:570:LYS:NZ   | 2.28                     | 0.66              |
| 3:I:77:LEU:HD11  | 3:I:408:ALA:O    | 1.96                     | 0.66              |
| 3:J:371:VAL:HG12 | 3:J:402:VAL:HG11 | 1.76                     | 0.66              |
| 3:J:77:LEU:HD11  | 3:J:408:ALA:O    | 1.95                     | 0.66              |
| 3:J:110:GLN:O    | 3:J:114:ASN:ND2  | 2.29                     | 0.65              |
| 3:J:340:THR:O    | 3:J:344:LEU:N    | 2.28                     | 0.65              |
| 3:K:110:GLN:O    | 3:K:114:ASN:ND2  | 2.29                     | 0.65              |
| 1:A:167:ASP:OD1  | 1:A:168:LEU:N    | 2.30                     | 0.65              |
| 1:A:427:GLU:CG   | 1:A:445:LEU:HD22 | 2.25                     | 0.65              |
| 3:K:254:ASP:OD2  | 3:K:346:ARG:NE   | 2.28                     | 0.65              |
| 1:C:477:LYS:O    | 1:C:478:GLU:C    | 2.38                     | 0.65              |
| 1:D:575:GLN:NE2  | 1:D:611:VAL:HG12 | 2.12                     | 0.65              |
| 1:F:220:ALA:HB2  | 1:F:237:ILE:HD11 | 1.79                     | 0.65              |
| 1:C:836:VAL:HG12 | 1:C:845:LEU:HG   | 1.78                     | 0.65              |
| 1:F:229:PRO:HG2  | 1:F:232:LEU:HD13 | 1.77                     | 0.65              |
| 1:D:301:LYS:N    | 1:D:302:PRO:CD   | 2.60                     | 0.65              |
| 1:E:362:HIS:O    | 1:E:403:ARG:NH1  | 2.29                     | 0.65              |
| 3:K:280:ILE:HG21 | 3:K:317:THR:CG2  | 2.27                     | 0.65              |
| 1:D:301:LYS:O    | 1:D:333:ARG:NH2  | 2.29                     | 0.64              |
| 1:A:406:ILE:CD1  | 1:A:529:LEU:CD2  | 2.72                     | 0.64              |
| 1:C:473:VAL:O    | 1:C:514:LEU:CD2  | 2.45                     | 0.64              |
| 1:E:639:TYR:OH   | 1:E:663:GLN:OE1  | 2.14                     | 0.64              |
| 3:J:254:ASP:OD2  | 3:J:346:ARG:NE   | 2.28                     | 0.64              |
| 1:A:702:THR:HG22 | 1:A:708:THR:HG22 | 1.79                     | 0.64              |
| 1:E:284:VAL:HG12 | 1:E:297:GLY:HA2  | 1.78                     | 0.64              |
| 1:E:805:ARG:HB3  | 1:E:806:PRO:HD3  | 1.78                     | 0.64              |
| 3:I:110:GLN:O    | 3:I:114:ASN:ND2  | 2.29                     | 0.64              |
| 1:F:565:GLU:OE2  | 1:F:587:ARG:NH2  | 2.30                     | 0.64              |
| 3:K:129:ARG:NE   | 3:K:255:ASN:O    | 2.31                     | 0.64              |
| 1:C:727:SER:HB3  | 1:C:730:GLN:HE21 | 1.62                     | 0.64              |
| 1:D:631:MET:HE3  | 1:D:633:ARG:HB3  | 1.78                     | 0.64              |
| 1:F:280:LEU:HD22 | 1:F:313:GLY:HA3  | 1.80                     | 0.64              |
| 3:I:129:ARG:NE   | 3:I:255:ASN:O    | 2.31                     | 0.64              |
| 1:F:304:LEU:CD2  | 1:F:311:LEU:CD2  | 2.75                     | 0.64              |
| 1:A:430:LEU:HD23 | 1:A:445:LEU:HD13 | 1.80                     | 0.64              |
| 1:E:386:PHE:O    | 1:E:390:LYS:CB   | 2.45                     | 0.64              |
| 1:F:304:LEU:HD13 | 1:F:311:LEU:HD23 | 1.78                     | 0.64              |
| 3:J:129:ARG:NE   | 3:J:255:ASN:O    | 2.31                     | 0.64              |
| 1:B:605:PHE:HB3  | 1:B:751:LEU:HB2  | 1.78                     | 0.64              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:303:MET:CE   | 1:D:308:GLU:HB2  | 1.98                     | 0.64              |
| 3:K:60:ALA:HB2   | 3:K:77:LEU:HD12  | 1.80                     | 0.64              |
| 3:K:142:LYS:HG3  | 3:K:143:LYS:H    | 1.63                     | 0.64              |
| 1:E:610:GLY:HA3  | 1:E:803:GLY:HA3  | 1.80                     | 0.64              |
| 1:F:696:LEU:O    | 1:F:746:ARG:NH1  | 2.31                     | 0.64              |
| 3:I:60:ALA:HB2   | 3:I:77:LEU:HD12  | 1.80                     | 0.64              |
| 3:J:92:ARG:NE    | 3:J:401:GLU:OE2  | 2.29                     | 0.64              |
| 3:J:128:LYS:NZ   | 3:J:205:GLU:OE2  | 2.23                     | 0.64              |
| 1:A:647:ARG:NH2  | 1:B:702:THR:O    | 2.31                     | 0.63              |
| 3:K:145:THR:OG1  | 3:K:148:GLU:OE1  | 2.16                     | 0.63              |
| 1:A:638:GLU:OE1  | 1:A:647:ARG:NH2  | 2.31                     | 0.63              |
| 1:B:805:ARG:NH1  | 4:B:902:AGS:S1G  | 2.70                     | 0.63              |
| 1:C:536:ASP:OD2  | 1:C:552:ARG:NH2  | 2.32                     | 0.63              |
| 3:I:142:LYS:HG3  | 3:I:143:LYS:H    | 1.63                     | 0.63              |
| 3:J:113:LYS:NZ   | 3:J:297:GLU:OE1  | 2.19                     | 0.63              |
| 3:J:142:LYS:HG3  | 3:J:143:LYS:H    | 1.63                     | 0.63              |
| 3:I:92:ARG:NE    | 3:I:401:GLU:OE2  | 2.29                     | 0.63              |
| 3:J:60:ALA:HB2   | 3:J:77:LEU:HD12  | 1.80                     | 0.63              |
| 1:A:256:GLU:OE1  | 1:A:256:GLU:N    | 2.26                     | 0.63              |
| 1:A:500:ALA:CB   | 3:I:316:ILE:C    | 2.71                     | 0.63              |
| 1:C:476:LEU:HD23 | 1:C:510:VAL:HG13 | 0.72                     | 0.63              |
| 1:E:252:ARG:HH12 | 2:N:11:UNK:HA    | 1.62                     | 0.63              |
| 1:E:609:THR:OG1  | 5:E:902:ADP:O2B  | 2.17                     | 0.63              |
| 1:E:666:GLU:OE2  | 1:E:669:ARG:NH2  | 2.32                     | 0.63              |
| 1:F:304:LEU:HD22 | 1:F:311:LEU:HD22 | 1.80                     | 0.63              |
| 1:B:473:VAL:CG2  | 1:B:517:ALA:HB1  | 2.13                     | 0.63              |
| 1:D:568:LEU:HD23 | 1:D:579:VAL:HG13 | 1.79                     | 0.63              |
| 1:E:209:GLY:CA   | 4:E:901:AGS:O2G  | 2.41                     | 0.63              |
| 3:K:219:GLU:OE2  | 3:K:219:GLU:N    | 2.26                     | 0.63              |
| 4:C:902:AGS:O2G  | 4:C:902:AGS:O1B  | 2.17                     | 0.63              |
| 4:B:901:AGS:O2G  | 4:B:901:AGS:O1B  | 2.17                     | 0.63              |
| 1:C:476:LEU:CD2  | 1:C:510:VAL:CG2  | 2.76                     | 0.63              |
| 1:D:573:ILE:HG22 | 4:D:902:AGS:C6   | 2.28                     | 0.63              |
| 1:F:263:LEU:HB3  | 1:F:303:MET:HE1  | 1.80                     | 0.63              |
| 3:J:172:ALA:N    | 3:J:198:ASN:O    | 2.32                     | 0.63              |
| 1:A:466:GLU:O    | 1:A:468:ASN:N    | 2.32                     | 0.62              |
| 1:A:503:ARG:NH2  | 3:I:316:ILE:O    | 2.32                     | 0.62              |
| 1:C:472:ILE:HD12 | 1:C:473:VAL:N    | 2.14                     | 0.62              |
| 1:E:769:LEU:HA   | 1:E:772:LEU:HG   | 1.80                     | 0.62              |
| 3:J:355:ILE:O    | 3:J:359:GLY:N    | 2.31                     | 0.62              |
| 1:B:665:THR:HG23 | 1:B:709:VAL:HG21 | 1.81                     | 0.62              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:145:THR:OG1  | 3:I:148:GLU:OE1  | 2.16                     | 0.62              |
| 3:I:172:ALA:N    | 3:I:198:ASN:O    | 2.32                     | 0.62              |
| 3:I:319:ASP:OD2  | 3:I:325:LEU:HD11 | 1.98                     | 0.62              |
| 1:B:503:ARG:NH2  | 3:J:316:ILE:O    | 2.32                     | 0.62              |
| 4:D:901:AGS:O2A  | 4:D:901:AGS:O2B  | 2.18                     | 0.62              |
| 3:K:355:ILE:O    | 3:K:359:GLY:N    | 2.31                     | 0.62              |
| 3:J:368:VAL:HG23 | 3:J:391:LYS:HE3  | 1.81                     | 0.62              |
| 1:A:460:THR:O    | 1:A:464:GLN:HB2  | 2.00                     | 0.62              |
| 1:C:472:ILE:O    | 1:C:475:ASP:N    | 2.33                     | 0.62              |
| 1:C:605:PHE:HB3  | 1:C:751:LEU:HB2  | 1.81                     | 0.62              |
| 1:B:476:LEU:HA   | 1:B:479:GLN:HE21 | 1.63                     | 0.62              |
| 1:F:316:THR:OG1  | 1:F:318:ASP:OD1  | 2.14                     | 0.62              |
| 3:I:142:LYS:HG3  | 3:I:143:LYS:N    | 2.15                     | 0.62              |
| 3:K:280:ILE:CG2  | 3:K:317:THR:HG21 | 2.27                     | 0.62              |
| 1:A:210:VAL:HG13 | 1:A:341:GLU:HA   | 1.82                     | 0.62              |
| 1:C:197:ARG:HG2  | 1:C:198:THR:HG23 | 1.80                     | 0.62              |
| 3:I:385:LYS:NZ   | 3:I:392:GLU:OE1  | 2.33                     | 0.62              |
| 3:J:145:THR:OG1  | 3:J:148:GLU:OE1  | 2.16                     | 0.62              |
| 3:K:368:VAL:HG23 | 3:K:391:LYS:HE3  | 1.81                     | 0.62              |
| 1:B:500:ALA:CB   | 3:J:316:ILE:C    | 2.71                     | 0.61              |
| 3:I:236:VAL:HG11 | 3:I:351:PHE:HA   | 1.82                     | 0.61              |
| 3:K:172:ALA:N    | 3:K:198:ASN:O    | 2.32                     | 0.61              |
| 3:K:385:LYS:NZ   | 3:K:392:GLU:OE1  | 2.33                     | 0.61              |
| 1:E:184:ASP:OD1  | 1:E:222:ARG:NH1  | 2.33                     | 0.61              |
| 3:K:217:LYS:HE2  | 3:K:217:LYS:CA   | 2.21                     | 0.61              |
| 1:A:608:PRO:O    | 1:A:613:LYS:NZ   | 2.33                     | 0.61              |
| 3:I:355:ILE:O    | 3:I:359:GLY:N    | 2.31                     | 0.61              |
| 3:J:385:LYS:NZ   | 3:J:392:GLU:OE1  | 2.33                     | 0.61              |
| 3:K:142:LYS:HG3  | 3:K:143:LYS:N    | 2.15                     | 0.61              |
| 1:A:378:SER:OG   | 1:A:390:LYS:HG3  | 2.01                     | 0.61              |
| 3:K:221:GLU:HA   | 3:K:241:ILE:O    | 2.01                     | 0.61              |
| 1:A:409:ARG:NH2  | 1:A:414:ASP:OD1  | 2.32                     | 0.61              |
| 1:B:477:LYS:O    | 1:B:480:LEU:HB3  | 2.01                     | 0.61              |
| 3:J:139:ILE:HG22 | 3:J:139:ILE:O    | 2.00                     | 0.61              |
| 3:J:142:LYS:HG3  | 3:J:143:LYS:N    | 2.15                     | 0.61              |
| 3:K:139:ILE:HG22 | 3:K:139:ILE:O    | 2.00                     | 0.61              |
| 1:A:365:ARG:O    | 1:A:532:GLU:HB2  | 2.01                     | 0.61              |
| 1:B:473:VAL:HG11 | 1:B:514:LEU:CD1  | 2.31                     | 0.61              |
| 1:F:603:PHE:HB3  | 1:F:748:ASP:HB2  | 1.82                     | 0.61              |
| 3:I:139:ILE:HG22 | 3:I:139:ILE:O    | 2.00                     | 0.61              |
| 1:C:393:ASP:OD1  | 1:D:196:ARG:NH2  | 2.28                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:788:PRO:HB2  | 1:D:838:VAL:HG21 | 1.82                     | 0.61              |
| 1:E:374:ALA:HB2  | 1:E:538:ILE:HD13 | 1.83                     | 0.61              |
| 1:C:476:LEU:CD2  | 1:C:510:VAL:CB   | 2.79                     | 0.61              |
| 1:C:496:LEU:HD21 | 3:K:316:ILE:HG23 | 1.82                     | 0.61              |
| 3:K:236:VAL:HG11 | 3:K:351:PHE:HA   | 1.83                     | 0.61              |
| 1:E:563:ARG:HH21 | 1:E:567:GLU:HB2  | 1.66                     | 0.61              |
| 3:I:63:VAL:CG1   | 3:I:76:VAL:HG12  | 2.31                     | 0.61              |
| 3:I:368:VAL:HG23 | 3:I:391:LYS:HE3  | 1.81                     | 0.61              |
| 3:J:236:VAL:HG11 | 3:J:351:PHE:HA   | 1.83                     | 0.61              |
| 3:K:63:VAL:CG1   | 3:K:76:VAL:HG12  | 2.31                     | 0.61              |
| 1:B:341:GLU:CG   | 1:B:387:LEU:HD12 | 2.30                     | 0.60              |
| 1:C:167:ASP:OD1  | 1:C:168:LEU:N    | 2.34                     | 0.60              |
| 1:E:281:HIS:O    | 1:E:323:HIS:ND1  | 2.26                     | 0.60              |
| 4:B:902:AGS:O1B  | 4:B:902:AGS:O2G  | 2.18                     | 0.60              |
| 1:D:572:VAL:CG2  | 1:D:615:GLU:OE1  | 2.49                     | 0.60              |
| 1:E:801:VAL:C    | 1:E:802:TYR:CD1  | 2.79                     | 0.60              |
| 3:K:92:ARG:NE    | 3:K:401:GLU:OE2  | 2.28                     | 0.60              |
| 3:K:307:GLN:OE1  | 3:K:307:GLN:N    | 2.34                     | 0.60              |
| 1:A:435:ASP:OD1  | 1:A:436:GLU:N    | 2.34                     | 0.60              |
| 1:B:341:GLU:CD   | 1:B:387:LEU:HG   | 2.27                     | 0.60              |
| 1:C:480:LEU:HB2  | 1:C:510:VAL:HG11 | 1.84                     | 0.60              |
| 1:E:659:GLU:OE1  | 1:E:659:GLU:N    | 2.33                     | 0.60              |
| 3:J:307:GLN:N    | 3:J:307:GLN:OE1  | 2.34                     | 0.60              |
| 3:K:314:PRO:O    | 3:K:315:TYR:O    | 2.20                     | 0.60              |
| 1:E:818:GLN:HE21 | 1:E:845:LEU:HD12 | 1.66                     | 0.60              |
| 3:I:307:GLN:OE1  | 3:I:307:GLN:N    | 2.34                     | 0.60              |
| 1:D:303:MET:HE1  | 1:D:308:GLU:CG   | 2.12                     | 0.60              |
| 1:E:386:PHE:O    | 1:E:390:LYS:HB2  | 2.01                     | 0.60              |
| 4:A:901:AGS:O2G  | 4:A:901:AGS:O1B  | 2.18                     | 0.60              |
| 1:B:473:VAL:CG1  | 1:B:514:LEU:HD13 | 2.27                     | 0.60              |
| 1:C:608:PRO:HG2  | 1:C:611:VAL:HG21 | 1.84                     | 0.60              |
| 1:D:380:ARG:NH1  | 1:D:381:TYR:OH   | 2.35                     | 0.60              |
| 1:E:546:THR:HG23 | 1:E:548:ILE:H    | 1.67                     | 0.60              |
| 1:A:365:ARG:HH21 | 1:A:531:GLU:HB2  | 1.67                     | 0.59              |
| 1:D:300:ILE:HD13 | 1:D:300:ILE:O    | 2.01                     | 0.59              |
| 1:F:538:ILE:O    | 1:F:542:VAL:HG23 | 2.02                     | 0.59              |
| 1:F:548:ILE:HD12 | 1:F:549:PRO:HD2  | 1.84                     | 0.59              |
| 3:J:63:VAL:CG1   | 3:J:76:VAL:HG12  | 2.31                     | 0.59              |
| 3:J:314:PRO:O    | 3:J:315:TYR:O    | 2.20                     | 0.59              |
| 1:A:427:GLU:OE2  | 1:A:446:ARG:CZ   | 2.50                     | 0.59              |
| 1:F:311:LEU:HD12 | 1:F:311:LEU:O    | 2.02                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:476:LEU:O    | 1:C:479:GLN:N    | 2.36                     | 0.59              |
| 4:C:901:AGS:O1B  | 4:C:901:AGS:O2G  | 2.20                     | 0.59              |
| 3:I:314:PRO:O    | 3:I:315:TYR:O    | 2.20                     | 0.59              |
| 3:J:108:VAL:O    | 3:J:156:LYS:NZ   | 2.36                     | 0.59              |
| 1:B:411:VAL:O    | 1:B:412:GLU:HG2  | 2.01                     | 0.59              |
| 4:D:902:AGS:O1B  | 4:D:902:AGS:O2G  | 2.19                     | 0.59              |
| 1:F:621:ALA:HB2  | 1:F:631:MET:HE3  | 1.84                     | 0.59              |
| 1:F:779:ARG:HH21 | 1:F:823:LEU:HG   | 1.66                     | 0.59              |
| 1:C:414:ASP:OD1  | 1:C:418:ARG:NH1  | 2.36                     | 0.59              |
| 1:C:477:LYS:O    | 1:C:479:GLN:N    | 2.36                     | 0.59              |
| 1:A:463:TRP:HB2  | 1:A:528:MET:HE1  | 1.84                     | 0.59              |
| 1:B:242:LEU:HD11 | 1:B:283:ILE:HG13 | 1.85                     | 0.59              |
| 4:B:902:AGS:O2A  | 4:B:902:AGS:O2B  | 2.20                     | 0.59              |
| 3:K:184:GLN:O    | 3:K:188:THR:HG23 | 2.03                     | 0.59              |
| 1:B:726:GLY:HA3  | 1:B:730:GLN:HB2  | 1.85                     | 0.59              |
| 1:C:476:LEU:C    | 1:C:479:GLN:HB3  | 2.25                     | 0.59              |
| 1:C:480:LEU:HD13 | 1:C:510:VAL:HG11 | 1.78                     | 0.59              |
| 1:E:698:GLU:OE2  | 1:E:700:ARG:NH1  | 2.35                     | 0.59              |
| 1:F:344:VAL:HG13 | 1:F:375:ALA:HB1  | 1.85                     | 0.59              |
| 1:F:345:GLU:HA   | 1:F:348:ILE:HD12 | 1.85                     | 0.59              |
| 1:A:654:GLY:HA2  | 1:F:656:VAL:HB   | 1.84                     | 0.58              |
| 3:K:258:GLY:N    | 3:K:261:ASP:OD1  | 2.36                     | 0.58              |
| 1:A:545:TRP:CD1  | 1:A:546:THR:HG23 | 2.38                     | 0.58              |
| 1:A:702:THR:O    | 1:F:647:ARG:NH2  | 2.36                     | 0.58              |
| 1:E:765:VAL:O    | 1:E:769:LEU:HG   | 2.03                     | 0.58              |
| 3:I:184:GLN:O    | 3:I:188:THR:HG23 | 2.03                     | 0.58              |
| 3:J:258:GLY:N    | 3:J:261:ASP:OD1  | 2.36                     | 0.58              |
| 1:A:196:ARG:NH2  | 1:F:397:GLU:OE2  | 2.36                     | 0.58              |
| 1:A:427:GLU:CG   | 1:A:445:LEU:CD2  | 2.80                     | 0.58              |
| 1:B:645:VAL:HG11 | 1:B:691:VAL:HG21 | 1.84                     | 0.58              |
| 1:C:471:GLU:O    | 1:C:475:ASP:CA   | 2.51                     | 0.58              |
| 1:E:221:GLN:HA   | 1:E:224:VAL:HG12 | 1.85                     | 0.58              |
| 3:I:151:ALA:C    | 3:I:155:MET:HE3  | 2.29                     | 0.58              |
| 3:K:100:PHE:HB2  | 3:K:139:ILE:HD12 | 1.84                     | 0.58              |
| 1:A:785:VAL:HA   | 1:A:836:VAL:HG22 | 1.84                     | 0.58              |
| 1:B:808:ARG:HH22 | 1:C:598:ARG:HD2  | 1.68                     | 0.58              |
| 1:E:263:LEU:HD23 | 1:E:303:MET:HG3  | 1.85                     | 0.58              |
| 1:E:611:VAL:C    | 5:E:902:ADP:N7   | 2.61                     | 0.58              |
| 1:F:189:ARG:NH1  | 1:F:192:GLN:OE1  | 2.36                     | 0.58              |
| 3:K:151:ALA:C    | 3:K:155:MET:HE3  | 2.29                     | 0.58              |
| 1:A:670:ARG:HD3  | 1:B:317:LEU:HD21 | 1.84                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:518:LEU:HD12 | 1:C:518:LEU:H    | 1.69                     | 0.58              |
| 4:C:901:AGS:O2A  | 4:C:901:AGS:O2B  | 2.19                     | 0.58              |
| 1:F:613:LYS:NZ   | 4:F:901:AGS:O3G  | 2.37                     | 0.58              |
| 3:I:258:GLY:N    | 3:I:261:ASP:OD1  | 2.36                     | 0.58              |
| 3:K:108:VAL:O    | 3:K:156:LYS:NZ   | 2.36                     | 0.58              |
| 1:A:779:ARG:HH22 | 1:A:823:LEU:HD21 | 1.69                     | 0.58              |
| 3:J:184:GLN:O    | 3:J:188:THR:HG23 | 2.03                     | 0.58              |
| 3:J:341:GLN:O    | 3:J:341:GLN:NE2  | 2.37                     | 0.58              |
| 1:A:666:GLU:O    | 1:A:670:ARG:NH1  | 2.36                     | 0.58              |
| 1:E:805:ARG:HB3  | 1:E:806:PRO:CD   | 2.32                     | 0.58              |
| 3:I:100:PHE:HB2  | 3:I:139:ILE:HD12 | 1.85                     | 0.58              |
| 1:A:415:GLU:OE2  | 1:B:188:ARG:NH2  | 2.36                     | 0.57              |
| 3:K:341:GLN:O    | 3:K:341:GLN:NE2  | 2.37                     | 0.57              |
| 1:A:250:LYS:NZ   | 1:B:254:GLU:OE1  | 2.32                     | 0.57              |
| 1:A:321:ARG:HB3  | 1:F:670:ARG:HH22 | 1.70                     | 0.57              |
| 3:I:108:VAL:O    | 3:I:156:LYS:NZ   | 2.36                     | 0.57              |
| 3:I:206:PRO:HA   | 3:I:226:VAL:HG11 | 1.87                     | 0.57              |
| 3:J:350:PRO:O    | 3:J:353:SER:OG   | 2.19                     | 0.57              |
| 1:A:427:GLU:OE2  | 1:A:446:ARG:NE   | 2.38                     | 0.57              |
| 3:I:341:GLN:O    | 3:I:341:GLN:NE2  | 2.37                     | 0.57              |
| 3:J:151:ALA:C    | 3:J:155:MET:HE3  | 2.29                     | 0.57              |
| 1:A:445:LEU:HD23 | 1:A:445:LEU:C    | 2.29                     | 0.57              |
| 1:A:653:PRO:HA   | 1:A:658:TYR:CZ   | 2.40                     | 0.57              |
| 1:C:274:ILE:HG12 | 1:C:310:ARG:HD3  | 1.85                     | 0.57              |
| 3:K:350:PRO:O    | 3:K:353:SER:OG   | 2.19                     | 0.57              |
| 1:B:469:ALA:O    | 1:B:472:ILE:HG22 | 2.04                     | 0.57              |
| 1:D:769:LEU:HD13 | 1:D:785:VAL:HG21 | 1.87                     | 0.57              |
| 1:E:571:ARG:NH2  | 1:E:628:GLU:OE1  | 2.32                     | 0.57              |
| 1:F:279:GLU:HB3  | 1:F:281:HIS:NE2  | 2.20                     | 0.57              |
| 3:J:100:PHE:HB2  | 3:J:139:ILE:HD12 | 1.85                     | 0.57              |
| 3:K:209:ALA:HB2  | 3:K:371:VAL:HG11 | 1.87                     | 0.57              |
| 1:A:411:VAL:O    | 1:A:412:GLU:HG2  | 2.05                     | 0.57              |
| 1:C:472:ILE:CD1  | 1:C:473:VAL:H    | 2.13                     | 0.57              |
| 1:C:518:LEU:H    | 1:C:518:LEU:CD1  | 2.18                     | 0.57              |
| 1:E:801:VAL:C    | 1:E:802:TYR:HD1  | 2.13                     | 0.57              |
| 3:I:209:ALA:HB2  | 3:I:371:VAL:HG11 | 1.87                     | 0.57              |
| 1:A:465:ASN:O    | 1:A:466:GLU:O    | 2.21                     | 0.57              |
| 1:B:161:LEU:O    | 1:B:165:SER:OG   | 2.19                     | 0.57              |
| 1:D:299:MET:O    | 1:D:302:PRO:CD   | 2.53                     | 0.57              |
| 3:K:313:LEU:HB2  | 3:K:316:ILE:HD11 | 1.86                     | 0.57              |
| 1:A:378:SER:HB2  | 1:A:394:LEU:HD11 | 1.87                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:757:ASN:HB2  | 1:C:760:GLU:HG3  | 1.87                     | 0.57              |
| 3:K:185:ARG:NH2  | 3:K:204:ASN:OD1  | 2.38                     | 0.57              |
| 3:K:341:GLN:NE2  | 3:K:345:ASP:OD1  | 2.38                     | 0.57              |
| 1:A:465:ASN:C    | 1:A:467:LYS:N    | 2.58                     | 0.56              |
| 1:C:505:GLY:O    | 1:C:509:GLU:HB2  | 2.05                     | 0.56              |
| 3:I:341:GLN:NE2  | 3:I:345:ASP:OD1  | 2.38                     | 0.56              |
| 3:K:207:THR:HG23 | 3:K:246:VAL:HG11 | 1.87                     | 0.56              |
| 1:C:476:LEU:HG   | 1:C:479:GLN:OE1  | 2.04                     | 0.56              |
| 3:J:102:ARG:NH2  | 3:J:121:ASP:OD1  | 2.39                     | 0.56              |
| 1:A:496:LEU:HD22 | 3:I:288:ALA:HA   | 1.86                     | 0.56              |
| 1:A:549:PRO:HB2  | 1:A:590:ARG:HH12 | 1.70                     | 0.56              |
| 1:A:669:ARG:NH2  | 1:B:325:GLU:OE1  | 2.30                     | 0.56              |
| 1:E:691:VAL:O    | 1:E:695:VAL:HG23 | 2.04                     | 0.56              |
| 1:E:802:TYR:CD1  | 1:E:802:TYR:N    | 2.73                     | 0.56              |
| 1:F:604:MET:HB2  | 1:F:718:LEU:HB2  | 1.87                     | 0.56              |
| 3:I:392:GLU:OE2  | 3:I:395:LYS:NZ   | 2.37                     | 0.56              |
| 3:J:113:LYS:O    | 3:J:293:ARG:NH2  | 2.38                     | 0.56              |
| 3:J:206:PRO:HA   | 3:J:226:VAL:HG11 | 1.87                     | 0.56              |
| 1:A:202:PRO:HG2  | 1:A:312:VAL:HG23 | 1.88                     | 0.56              |
| 3:I:113:LYS:O    | 3:I:293:ARG:NH2  | 2.38                     | 0.56              |
| 3:I:185:ARG:NH2  | 3:I:204:ASN:OD1  | 2.38                     | 0.56              |
| 3:K:102:ARG:NH2  | 3:K:121:ASP:OD1  | 2.39                     | 0.56              |
| 3:K:206:PRO:HA   | 3:K:226:VAL:HG11 | 1.87                     | 0.56              |
| 1:B:473:VAL:HG11 | 1:B:514:LEU:HD12 | 1.87                     | 0.56              |
| 1:C:496:LEU:HD22 | 3:K:288:ALA:HA   | 1.86                     | 0.56              |
| 1:E:772:LEU:HA   | 1:E:775:ARG:HG2  | 1.88                     | 0.56              |
| 3:K:257:LEU:HD12 | 3:K:258:GLY:H    | 1.71                     | 0.56              |
| 3:I:257:LEU:HD12 | 3:I:258:GLY:H    | 1.70                     | 0.56              |
| 3:J:185:ARG:NH2  | 3:J:204:ASN:OD1  | 2.38                     | 0.56              |
| 3:J:341:GLN:NE2  | 3:J:345:ASP:OD1  | 2.38                     | 0.56              |
| 1:A:769:LEU:HD13 | 1:A:785:VAL:HG21 | 1.88                     | 0.56              |
| 1:E:180:VAL:CA   | 4:E:901:AGS:N1   | 2.68                     | 0.56              |
| 1:F:603:PHE:HA   | 1:F:747:LEU:HD22 | 1.87                     | 0.56              |
| 3:I:191:ALA:HA   | 3:I:194:ILE:HD12 | 1.87                     | 0.56              |
| 3:I:207:THR:HG23 | 3:I:246:VAL:HG11 | 1.87                     | 0.56              |
| 3:J:207:THR:HG23 | 3:J:246:VAL:HG11 | 1.87                     | 0.56              |
| 3:J:380:VAL:O    | 3:J:384:VAL:HG23 | 2.06                     | 0.56              |
| 3:K:191:ALA:HA   | 3:K:194:ILE:HD12 | 1.88                     | 0.56              |
| 1:B:341:GLU:OE1  | 1:B:387:LEU:HG   | 2.06                     | 0.56              |
| 1:B:476:LEU:HD21 | 1:B:510:VAL:HG12 | 1.88                     | 0.56              |
| 3:K:113:LYS:O    | 3:K:293:ARG:NH2  | 2.38                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:326:LYS:NZ   | 1:C:327:ASP:OD1  | 2.35                     | 0.56              |
| 1:C:476:LEU:HD21 | 1:C:510:VAL:HA   | 1.87                     | 0.56              |
| 1:E:213:THR:OG1  | 4:E:901:AGS:O2A  | 2.23                     | 0.56              |
| 3:I:102:ARG:NH2  | 3:I:121:ASP:OD1  | 2.39                     | 0.56              |
| 3:I:380:VAL:O    | 3:I:384:VAL:HG23 | 2.06                     | 0.56              |
| 1:B:347:THR:HG23 | 1:B:388:PRO:HD3  | 1.88                     | 0.56              |
| 1:B:608:PRO:O    | 1:B:613:LYS:NZ   | 2.39                     | 0.56              |
| 1:A:595:ASP:OD2  | 1:F:775:ARG:NH2  | 2.39                     | 0.55              |
| 1:B:471:GLU:OE1  | 1:B:471:GLU:HA   | 2.04                     | 0.55              |
| 1:C:471:GLU:O    | 1:C:475:ASP:HB3  | 2.05                     | 0.55              |
| 1:E:167:ASP:OD1  | 1:E:170:ALA:N    | 2.31                     | 0.55              |
| 1:E:726:GLY:HA3  | 1:E:730:GLN:HG3  | 1.87                     | 0.55              |
| 1:F:786:SER:HB2  | 1:F:788:PRO:HD2  | 1.88                     | 0.55              |
| 3:J:326:PHE:CD1  | 3:J:327:LEU:N    | 2.74                     | 0.55              |
| 3:K:261:ASP:O    | 3:K:265:ARG:NH1  | 2.39                     | 0.55              |
| 1:A:235:LYS:NZ   | 1:A:271:GLY:O    | 2.30                     | 0.55              |
| 1:B:267:LYS:HB2  | 1:B:303:MET:HE1  | 1.88                     | 0.55              |
| 1:E:720:SER:OG   | 1:E:721:ASN:N    | 2.39                     | 0.55              |
| 3:I:319:ASP:HB3  | 3:I:325:LEU:HD12 | 1.86                     | 0.55              |
| 1:A:431:SER:CA   | 1:A:442:LEU:HD11 | 2.30                     | 0.55              |
| 1:B:480:LEU:HG   | 1:B:484:ARG:CZ   | 2.36                     | 0.55              |
| 1:C:635:ASP:OD2  | 1:D:700:ARG:NH1  | 2.35                     | 0.55              |
| 3:J:261:ASP:O    | 3:J:265:ARG:NH1  | 2.39                     | 0.55              |
| 1:A:386:PHE:C    | 1:A:390:LYS:HD2  | 2.32                     | 0.55              |
| 1:B:496:LEU:HD22 | 3:J:288:ALA:HA   | 1.86                     | 0.55              |
| 1:D:767:ILE:O    | 1:D:771:GLN:HG3  | 2.07                     | 0.55              |
| 3:J:209:ALA:HB2  | 3:J:371:VAL:HG11 | 1.87                     | 0.55              |
| 3:J:392:GLU:OE2  | 3:J:395:LYS:NZ   | 2.37                     | 0.55              |
| 1:B:342:PRO:C    | 1:B:387:LEU:CD1  | 2.68                     | 0.55              |
| 1:E:275:THR:OG1  | 1:E:276:PHE:N    | 2.37                     | 0.55              |
| 1:F:310:ARG:HA   | 1:F:310:ARG:HE   | 1.71                     | 0.55              |
| 3:I:208:ALA:HB3  | 3:I:403:VAL:HG13 | 1.89                     | 0.55              |
| 3:I:261:ASP:O    | 3:I:265:ARG:NH1  | 2.39                     | 0.55              |
| 3:J:208:ALA:HB3  | 3:J:403:VAL:HG13 | 1.89                     | 0.55              |
| 1:A:410:PRO:CD   | 1:A:463:TRP:NE1  | 2.69                     | 0.55              |
| 1:A:561:LEU:HD21 | 1:A:590:ARG:HG3  | 1.89                     | 0.55              |
| 1:D:575:GLN:HE21 | 1:D:611:VAL:HG12 | 1.71                     | 0.55              |
| 3:I:326:PHE:CD1  | 3:I:327:LEU:N    | 2.74                     | 0.55              |
| 1:B:703:ASP:OD1  | 1:B:703:ASP:N    | 2.39                     | 0.55              |
| 1:E:656:VAL:HG22 | 2:N:25:UNK:HA    | 1.89                     | 0.55              |
| 3:J:257:LEU:HD12 | 3:J:258:GLY:H    | 1.70                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:208:ALA:HB3  | 3:K:403:VAL:HG13 | 1.89                     | 0.55              |
| 1:A:442:LEU:HD21 | 1:A:446:ARG:CZ   | 2.37                     | 0.55              |
| 1:E:814:ALA:O    | 1:E:818:GLN:HB3  | 2.06                     | 0.55              |
| 3:J:191:ALA:HA   | 3:J:194:ILE:HD12 | 1.87                     | 0.55              |
| 3:K:282:LEU:HD12 | 3:K:292:LEU:HD11 | 1.89                     | 0.55              |
| 3:K:326:PHE:CD1  | 3:K:327:LEU:N    | 2.74                     | 0.55              |
| 1:A:276:PHE:HD1  | 1:A:312:VAL:HG13 | 1.71                     | 0.55              |
| 1:B:347:THR:CG2  | 1:B:388:PRO:HD3  | 2.37                     | 0.55              |
| 1:B:476:LEU:HA   | 1:B:479:GLN:HB3  | 1.88                     | 0.55              |
| 1:E:566:ASP:O    | 1:E:570:LYS:N    | 2.39                     | 0.55              |
| 1:E:726:GLY:H    | 1:E:730:GLN:HE21 | 1.55                     | 0.55              |
| 1:A:287:GLY:HA2  | 1:A:296:ALA:HB3  | 1.88                     | 0.54              |
| 1:D:299:MET:O    | 1:D:302:PRO:HD3  | 2.08                     | 0.54              |
| 3:K:392:GLU:OE2  | 3:K:395:LYS:NZ   | 2.37                     | 0.54              |
| 1:A:181:ILE:HD12 | 1:A:181:ILE:H    | 1.72                     | 0.54              |
| 3:J:67:LEU:O     | 3:J:128:LYS:NZ   | 2.26                     | 0.54              |
| 1:A:504:TYR:CD1  | 3:I:318:VAL:HB   | 2.41                     | 0.54              |
| 3:K:380:VAL:O    | 3:K:384:VAL:HG23 | 2.06                     | 0.54              |
| 1:B:545:TRP:HB2  | 1:C:189:ARG:NH2  | 2.22                     | 0.54              |
| 1:C:509:GLU:OE1  | 1:C:509:GLU:HA   | 2.06                     | 0.54              |
| 1:E:191:VAL:HG23 | 1:E:232:LEU:HD13 | 1.89                     | 0.54              |
| 1:F:310:ARG:HA   | 1:F:310:ARG:NE   | 2.22                     | 0.54              |
| 3:I:350:PRO:O    | 3:I:353:SER:OG   | 2.19                     | 0.54              |
| 1:A:808:ARG:NH1  | 4:A:902:AGS:O3'  | 2.40                     | 0.54              |
| 1:B:557:GLU:OE1  | 1:B:590:ARG:NH2  | 2.41                     | 0.54              |
| 1:D:163:LYS:NZ   | 1:D:164:TYR:OH   | 2.41                     | 0.54              |
| 1:B:504:TYR:CE2  | 3:J:317:THR:HA   | 2.42                     | 0.54              |
| 1:C:263:LEU:HD11 | 1:C:300:ILE:HG22 | 1.88                     | 0.54              |
| 1:E:805:ARG:HB2  | 1:E:806:PRO:CD   | 2.38                     | 0.54              |
| 4:D:901:AGS:O2G  | 4:D:901:AGS:O1B  | 2.26                     | 0.54              |
| 1:E:809:ARG:HA   | 1:E:812:GLN:HG2  | 1.89                     | 0.54              |
| 3:I:131:MET:HE3  | 3:I:187:ALA:HB1  | 1.90                     | 0.54              |
| 1:A:614:THR:OG1  | 4:A:902:AGS:O1B  | 2.24                     | 0.54              |
| 1:B:476:LEU:CD1  | 1:B:513:LYS:CD   | 2.83                     | 0.54              |
| 1:D:565:GLU:OE2  | 1:D:587:ARG:NH2  | 2.31                     | 0.54              |
| 1:D:685:HIS:O    | 1:D:687:ASP:N    | 2.34                     | 0.54              |
| 4:A:902:AGS:O1B  | 4:A:902:AGS:O2G  | 2.24                     | 0.54              |
| 1:B:476:LEU:CD2  | 1:B:510:VAL:HG13 | 2.38                     | 0.54              |
| 1:B:799:ASP:O    | 1:B:801:VAL:N    | 2.33                     | 0.54              |
| 1:C:298:ASN:HB2  | 1:C:301:LYS:HE3  | 1.90                     | 0.54              |
| 1:D:799:ASP:N    | 1:D:799:ASP:OD1  | 2.42                     | 0.54              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:342:PRO:HG2  | 1:E:388:PRO:HG3  | 1.89                     | 0.53              |
| 3:I:282:LEU:HD12 | 3:I:292:LEU:HD11 | 1.89                     | 0.53              |
| 1:A:634:ILE:HD11 | 1:A:678:PHE:HE1  | 1.73                     | 0.53              |
| 1:D:575:GLN:NE2  | 1:D:611:VAL:CG1  | 2.71                     | 0.53              |
| 3:K:131:MET:HE3  | 3:K:187:ALA:HB1  | 1.90                     | 0.53              |
| 1:B:476:LEU:O    | 1:B:480:LEU:N    | 2.40                     | 0.53              |
| 3:K:186:GLN:OE1  | 3:K:189:LYS:NZ   | 2.39                     | 0.53              |
| 1:B:501:GLU:HG3  | 3:J:315:TYR:CD2  | 2.44                     | 0.53              |
| 1:C:194:LEU:HD21 | 1:C:274:ILE:HG21 | 1.91                     | 0.53              |
| 1:C:477:LYS:C    | 1:C:480:LEU:H    | 2.16                     | 0.53              |
| 1:C:477:LYS:HG3  | 1:C:480:LEU:CD2  | 2.39                     | 0.53              |
| 1:F:318:ASP:O    | 1:F:322:LYS:HG2  | 2.08                     | 0.53              |
| 1:A:501:GLU:HG3  | 3:I:315:TYR:CD2  | 2.44                     | 0.53              |
| 1:A:741:PRO:O    | 1:A:745:ASN:HB2  | 2.09                     | 0.53              |
| 1:C:501:GLU:HG3  | 3:K:315:TYR:CD2  | 2.44                     | 0.53              |
| 1:F:222:ARG:HH22 | 1:F:228:VAL:HG12 | 1.72                     | 0.53              |
| 1:A:786:SER:OG   | 1:A:788:PRO:HD2  | 2.09                     | 0.53              |
| 1:D:386:PHE:O    | 1:D:390:LYS:HB3  | 2.09                     | 0.53              |
| 3:K:84:VAL:HG12  | 3:K:92:ARG:HB3   | 1.91                     | 0.53              |
| 3:K:148:GLU:HG3  | 3:K:194:ILE:HD13 | 1.91                     | 0.53              |
| 3:K:321:ASP:O    | 3:K:322:LYS:HB2  | 2.08                     | 0.53              |
| 1:B:300:ILE:HD11 | 1:B:309:LEU:HD11 | 1.90                     | 0.53              |
| 1:A:504:TYR:CE2  | 3:I:317:THR:HA   | 2.43                     | 0.53              |
| 1:C:826:GLY:O    | 1:C:827:GLN:HG2  | 2.08                     | 0.53              |
| 1:D:573:ILE:O    | 1:D:573:ILE:HG23 | 2.08                     | 0.53              |
| 1:E:819:LEU:O    | 1:E:823:LEU:HG   | 2.08                     | 0.53              |
| 3:I:297:GLU:O    | 3:I:301:ILE:HD12 | 2.09                     | 0.53              |
| 1:A:726:GLY:HA3  | 1:A:730:GLN:HB2  | 1.91                     | 0.53              |
| 1:C:507:ILE:O    | 1:C:511:GLU:HG3  | 2.09                     | 0.53              |
| 1:D:539:ALA:HA   | 1:D:542:VAL:HG12 | 1.91                     | 0.53              |
| 1:E:740:LYS:HG3  | 1:E:742:GLU:HG3  | 1.90                     | 0.53              |
| 1:F:234:ASP:O    | 1:F:236:THR:N    | 2.42                     | 0.53              |
| 1:F:843:ASP:N    | 1:F:843:ASP:OD1  | 2.41                     | 0.53              |
| 3:K:100:PHE:CG   | 3:K:139:ILE:HG13 | 2.44                     | 0.53              |
| 1:A:196:ARG:HG2  | 1:A:197:ARG:H    | 1.74                     | 0.53              |
| 1:C:381:TYR:HE2  | 1:C:550:ALA:HB2  | 1.72                     | 0.53              |
| 1:C:500:ALA:HB2  | 3:K:316:ILE:C    | 2.33                     | 0.53              |
| 3:J:186:GLN:OE1  | 3:J:189:LYS:NZ   | 2.38                     | 0.53              |
| 3:K:373:GLY:N    | 3:K:400:ASP:OD1  | 2.42                     | 0.53              |
| 1:C:430:LEU:HD22 | 1:C:442:LEU:HD13 | 1.91                     | 0.52              |
| 1:C:477:LYS:CA   | 1:C:480:LEU:H    | 2.21                     | 0.52              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:513:LYS:HE3  | 1:C:513:LYS:CA   | 2.37                     | 0.52              |
| 1:D:681:ILE:HG21 | 1:D:718:LEU:HD12 | 1.90                     | 0.52              |
| 1:E:242:LEU:HD11 | 1:E:283:ILE:HD11 | 1.92                     | 0.52              |
| 1:E:181:ILE:H    | 1:E:181:ILE:HD12 | 1.74                     | 0.52              |
| 1:E:301:LYS:HE2  | 1:E:330:LEU:HD13 | 1.91                     | 0.52              |
| 1:E:805:ARG:HB2  | 1:E:806:PRO:HD3  | 1.90                     | 0.52              |
| 1:F:210:VAL:HG11 | 1:F:339:VAL:HG21 | 1.91                     | 0.52              |
| 3:J:282:LEU:HD12 | 3:J:292:LEU:HD11 | 1.89                     | 0.52              |
| 3:I:67:LEU:O     | 3:I:128:LYS:NZ   | 2.26                     | 0.52              |
| 3:I:84:VAL:HG12  | 3:I:92:ARG:HB3   | 1.91                     | 0.52              |
| 3:K:67:LEU:O     | 3:K:128:LYS:NZ   | 2.26                     | 0.52              |
| 1:B:476:LEU:HD12 | 1:B:513:LYS:HZ3  | 1.73                     | 0.52              |
| 1:B:646:ALA:HA   | 1:B:649:ILE:HG22 | 1.91                     | 0.52              |
| 3:J:84:VAL:HG12  | 3:J:92:ARG:HB3   | 1.91                     | 0.52              |
| 1:C:477:LYS:HG3  | 1:C:480:LEU:HD23 | 1.91                     | 0.52              |
| 1:D:573:ILE:C    | 4:D:902:AGS:HN62 | 2.15                     | 0.52              |
| 1:D:826:GLY:O    | 1:D:827:GLN:HG2  | 2.10                     | 0.52              |
| 3:I:100:PHE:CG   | 3:I:139:ILE:HG13 | 2.44                     | 0.52              |
| 3:J:217:LYS:HD2  | 3:J:366:ASP:CB   | 2.37                     | 0.52              |
| 3:K:241:ILE:HG12 | 3:K:246:VAL:HG13 | 1.91                     | 0.52              |
| 1:B:476:LEU:O    | 1:B:479:GLN:HB3  | 2.10                     | 0.52              |
| 3:J:131:MET:HE3  | 3:J:187:ALA:HB1  | 1.90                     | 0.52              |
| 3:J:297:GLU:O    | 3:J:301:ILE:HD12 | 2.09                     | 0.52              |
| 3:I:241:ILE:HG12 | 3:I:246:VAL:HG13 | 1.91                     | 0.52              |
| 3:J:100:PHE:CG   | 3:J:139:ILE:HG13 | 2.44                     | 0.52              |
| 3:J:241:ILE:HG12 | 3:J:246:VAL:HG13 | 1.91                     | 0.52              |
| 1:B:341:GLU:CG   | 1:B:387:LEU:CD1  | 2.87                     | 0.52              |
| 1:C:720:SER:OG   | 1:C:721:ASN:N    | 2.40                     | 0.52              |
| 1:F:319:GLU:O    | 1:F:323:HIS:HB2  | 2.10                     | 0.52              |
| 1:D:692:LEU:HA   | 1:D:695:VAL:HB   | 1.92                     | 0.52              |
| 1:F:352:ARG:O    | 1:F:355:LYS:NZ   | 2.33                     | 0.52              |
| 3:K:297:GLU:O    | 3:K:301:ILE:HD12 | 2.09                     | 0.52              |
| 1:A:710:ASP:OD1  | 1:A:710:ASP:N    | 2.40                     | 0.52              |
| 4:A:902:AGS:S1G  | 1:B:746:ARG:NH2  | 2.75                     | 0.52              |
| 1:F:308:GLU:N    | 1:F:308:GLU:OE1  | 2.43                     | 0.52              |
| 1:F:350:ILE:HG12 | 5:F:902:ADP:N1   | 2.24                     | 0.52              |
| 1:F:403:ARG:HA   | 1:F:406:ILE:HD12 | 1.91                     | 0.52              |
| 1:B:480:LEU:HG   | 1:B:484:ARG:NH1  | 2.25                     | 0.51              |
| 1:C:477:LYS:HA   | 1:C:480:LEU:HB2  | 1.90                     | 0.51              |
| 3:I:280:ILE:HG21 | 3:I:317:THR:CG2  | 2.39                     | 0.51              |
| 3:J:148:GLU:HG3  | 3:J:194:ILE:HD13 | 1.91                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:472:ILE:HA   | 1:C:475:ASP:HB3  | 1.92                     | 0.51              |
| 1:E:167:ASP:OD1  | 1:E:169:THR:N    | 2.43                     | 0.51              |
| 1:F:785:VAL:HA   | 1:F:836:VAL:HG12 | 1.92                     | 0.51              |
| 3:K:326:PHE:HD1  | 3:K:327:LEU:N    | 2.08                     | 0.51              |
| 1:A:213:THR:O    | 1:A:217:GLU:HG2  | 2.10                     | 0.51              |
| 1:B:455:LYS:HG3  | 1:B:459:LEU:HD13 | 1.91                     | 0.51              |
| 1:E:710:ASP:OD1  | 1:E:710:ASP:N    | 2.42                     | 0.51              |
| 1:A:476:LEU:CB   | 1:A:514:LEU:HD13 | 2.39                     | 0.51              |
| 1:B:480:LEU:HD11 | 1:B:507:ILE:HG23 | 1.92                     | 0.51              |
| 1:B:504:TYR:CB   | 3:J:324:PRO:HG3  | 2.41                     | 0.51              |
| 1:E:179:PRO:O    | 4:E:901:AGS:H2   | 2.11                     | 0.51              |
| 1:A:361:HIS:CD2  | 1:B:197:ARG:HB2  | 2.46                     | 0.51              |
| 1:C:546:THR:O    | 1:C:548:ILE:N    | 2.43                     | 0.51              |
| 1:C:732:LEU:O    | 1:C:736:ARG:NH2  | 2.43                     | 0.51              |
| 1:D:763:ARG:O    | 1:D:767:ILE:HG12 | 2.10                     | 0.51              |
| 1:E:614:THR:O    | 1:E:618:LYS:HG3  | 2.11                     | 0.51              |
| 1:F:579:VAL:HA   | 1:F:582:VAL:HG12 | 1.93                     | 0.51              |
| 3:J:308:SER:OG   | 3:J:330:GLN:NE2  | 2.44                     | 0.51              |
| 1:A:504:TYR:CB   | 3:I:324:PRO:HG3  | 2.41                     | 0.51              |
| 1:A:745:ASN:ND2  | 1:F:805:ARG:HD2  | 2.25                     | 0.51              |
| 1:E:318:ASP:OD1  | 1:E:319:GLU:N    | 2.42                     | 0.51              |
| 1:E:805:ARG:N    | 1:E:806:PRO:HD2  | 2.25                     | 0.51              |
| 3:I:326:PHE:HD1  | 3:I:327:LEU:N    | 2.08                     | 0.51              |
| 3:J:326:PHE:HD1  | 3:J:327:LEU:N    | 2.09                     | 0.51              |
| 1:D:205:ILE:HD12 | 1:D:336:GLN:HB3  | 1.93                     | 0.51              |
| 1:D:633:ARG:NH2  | 1:D:679:ASP:OD2  | 2.44                     | 0.51              |
| 3:I:223:ARG:N    | 3:I:366:ASP:OD2  | 2.43                     | 0.51              |
| 1:B:434:GLU:OE1  | 1:B:434:GLU:N    | 2.43                     | 0.51              |
| 1:D:277:ILE:HD12 | 1:D:311:LEU:HD11 | 1.92                     | 0.51              |
| 3:I:148:GLU:HG3  | 3:I:194:ILE:HD13 | 1.91                     | 0.51              |
| 1:A:194:LEU:HD11 | 1:A:310:ARG:HB3  | 1.93                     | 0.51              |
| 1:A:666:GLU:HB3  | 1:A:670:ARG:HH12 | 1.75                     | 0.51              |
| 1:E:386:PHE:O    | 1:E:390:LYS:HB3  | 2.11                     | 0.51              |
| 3:I:71:ASN:ND2   | 3:I:400:ASP:OD1  | 2.44                     | 0.51              |
| 3:K:71:ASN:ND2   | 3:K:400:ASP:OD1  | 2.44                     | 0.51              |
| 1:B:441:ARG:NH2  | 1:C:368:ASP:OD1  | 2.44                     | 0.50              |
| 1:B:487:SER:HA   | 1:B:502:LEU:HD13 | 1.94                     | 0.50              |
| 1:B:504:TYR:HB2  | 3:J:324:PRO:HG3  | 1.93                     | 0.50              |
| 1:F:232:LEU:O    | 1:F:234:ASP:N    | 2.42                     | 0.50              |
| 3:I:158:LYS:NZ   | 3:I:168:ASP:OD2  | 2.45                     | 0.50              |
| 3:J:71:ASN:ND2   | 3:J:400:ASP:OD1  | 2.44                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:280:ILE:HG21 | 3:J:317:THR:CG2  | 2.39                     | 0.50              |
| 3:J:299:ALA:HB2  | 3:J:311:ILE:HD11 | 1.93                     | 0.50              |
| 1:C:643:HIS:HD2  | 1:D:652:PRO:HG3  | 1.76                     | 0.50              |
| 1:C:799:ASP:O    | 1:C:801:VAL:N    | 2.38                     | 0.50              |
| 1:E:355:LYS:HG3  | 1:E:366:ILE:HG13 | 1.92                     | 0.50              |
| 3:J:158:LYS:NZ   | 3:J:168:ASP:OD2  | 2.45                     | 0.50              |
| 3:K:299:ALA:HB2  | 3:K:311:ILE:HD11 | 1.93                     | 0.50              |
| 1:A:421:ARG:O    | 1:A:425:ILE:HG13 | 2.11                     | 0.50              |
| 1:C:427:GLU:O    | 1:C:431:SER:OG   | 2.29                     | 0.50              |
| 3:I:299:ALA:HB2  | 3:I:311:ILE:HD11 | 1.93                     | 0.50              |
| 3:J:62:ALA:HB3   | 3:J:411:ALA:HB1  | 1.94                     | 0.50              |
| 3:K:308:SER:OG   | 3:K:330:GLN:NE2  | 2.44                     | 0.50              |
| 1:C:487:SER:HA   | 1:C:502:LEU:HD13 | 1.94                     | 0.50              |
| 1:D:322:LYS:HE3  | 1:D:323:HIS:CD2  | 2.46                     | 0.50              |
| 1:D:785:VAL:HA   | 1:D:836:VAL:HG22 | 1.94                     | 0.50              |
| 1:E:563:ARG:NH2  | 1:E:567:GLU:HB2  | 2.25                     | 0.50              |
| 1:F:222:ARG:HH11 | 1:F:227:ASP:HB2  | 1.76                     | 0.50              |
| 1:F:234:ASP:C    | 1:F:236:THR:H    | 2.19                     | 0.50              |
| 3:J:257:LEU:HD12 | 3:J:258:GLY:N    | 2.26                     | 0.50              |
| 1:A:643:HIS:HB2  | 1:B:655:TYR:CZ   | 2.47                     | 0.50              |
| 1:B:470:ILE:CB   | 1:B:519:PRO:HG2  | 2.41                     | 0.50              |
| 3:K:217:LYS:CE   | 3:K:217:LYS:CA   | 2.86                     | 0.50              |
| 3:K:257:LEU:HD12 | 3:K:258:GLY:N    | 2.26                     | 0.50              |
| 1:A:410:PRO:HD3  | 1:A:463:TRP:NE1  | 2.26                     | 0.50              |
| 1:A:455:LYS:O    | 1:A:459:LEU:HB2  | 2.11                     | 0.50              |
| 1:A:692:LEU:HA   | 1:A:695:VAL:HB   | 1.94                     | 0.50              |
| 1:B:476:LEU:CD2  | 1:B:510:VAL:CG1  | 2.85                     | 0.50              |
| 1:B:659:GLU:CD   | 1:B:659:GLU:H    | 2.19                     | 0.50              |
| 1:D:259:LEU:HD23 | 1:D:299:MET:SD   | 2.52                     | 0.50              |
| 1:A:321:ARG:HB3  | 1:F:670:ARG:NH2  | 2.25                     | 0.50              |
| 3:I:257:LEU:HD12 | 3:I:258:GLY:N    | 2.26                     | 0.50              |
| 3:K:127:VAL:HG23 | 3:K:135:TRP:CD1  | 2.47                     | 0.50              |
| 1:A:410:PRO:HG3  | 1:A:463:TRP:NE1  | 2.27                     | 0.50              |
| 1:C:242:LEU:HD11 | 1:C:283:ILE:HG13 | 1.93                     | 0.50              |
| 1:C:518:LEU:N    | 1:C:518:LEU:CD1  | 2.73                     | 0.50              |
| 1:E:650:GLY:O    | 1:E:704:GLY:HA3  | 2.12                     | 0.50              |
| 3:K:158:LYS:NZ   | 3:K:168:ASP:OD2  | 2.45                     | 0.50              |
| 1:A:487:SER:HA   | 1:A:502:LEU:HD13 | 1.94                     | 0.50              |
| 1:C:822:MET:HG2  | 1:C:827:GLN:HE21 | 1.77                     | 0.50              |
| 1:F:779:ARG:HE   | 1:F:823:LEU:HD21 | 1.77                     | 0.50              |
| 1:B:812:GLN:HE22 | 1:C:594:SER:HA   | 1.77                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:460:THR:O    | 1:C:464:GLN:HG2  | 2.12                     | 0.49              |
| 1:C:554:LEU:HD23 | 1:C:554:LEU:H    | 1.77                     | 0.49              |
| 1:C:812:GLN:HB3  | 1:D:588:ARG:NH1  | 2.27                     | 0.49              |
| 1:E:534:GLY:H    | 1:E:537:ASP:HB3  | 1.77                     | 0.49              |
| 3:K:100:PHE:CB   | 3:K:139:ILE:HD12 | 2.42                     | 0.49              |
| 1:D:172:ALA:HB2  | 1:D:177:LEU:HD12 | 1.93                     | 0.49              |
| 1:D:194:LEU:HD11 | 1:D:310:ARG:HB3  | 1.94                     | 0.49              |
| 1:D:605:PHE:HB3  | 1:D:751:LEU:HB2  | 1.94                     | 0.49              |
| 1:E:804:ALA:HB1  | 1:E:807:LEU:HB2  | 1.93                     | 0.49              |
| 1:E:820:ALA:HA   | 1:E:823:LEU:HD12 | 1.94                     | 0.49              |
| 1:F:537:ASP:O    | 1:F:541:VAL:HG23 | 2.12                     | 0.49              |
| 3:I:62:ALA:HB3   | 3:I:411:ALA:HB1  | 1.94                     | 0.49              |
| 3:I:84:VAL:HG11  | 3:I:401:GLU:HG2  | 1.94                     | 0.49              |
| 3:I:100:PHE:CB   | 3:I:139:ILE:HD12 | 2.42                     | 0.49              |
| 1:B:423:LEU:HD22 | 1:B:445:LEU:HD11 | 1.94                     | 0.49              |
| 1:F:183:ARG:NH1  | 1:F:340:GLY:O    | 2.41                     | 0.49              |
| 1:C:436:GLU:OE2  | 1:C:780:ARG:NH1  | 2.44                     | 0.49              |
| 1:C:573:ILE:H    | 4:C:901:AGS:HN62 | 1.60                     | 0.49              |
| 1:D:720:SER:OG   | 1:D:721:ASN:N    | 2.46                     | 0.49              |
| 1:E:784:GLN:NE2  | 1:E:785:VAL:O    | 2.45                     | 0.49              |
| 3:I:151:ALA:O    | 3:I:155:MET:HE3  | 2.13                     | 0.49              |
| 3:I:308:SER:OG   | 3:I:330:GLN:NE2  | 2.44                     | 0.49              |
| 1:A:504:TYR:HB2  | 3:I:324:PRO:HG3  | 1.93                     | 0.49              |
| 1:C:407:ASP:CG   | 1:C:408:SER:H    | 2.20                     | 0.49              |
| 1:E:365:ARG:HH11 | 1:E:532:GLU:HB3  | 1.77                     | 0.49              |
| 1:E:761:LEU:HD12 | 1:E:794:ALA:HB1  | 1.94                     | 0.49              |
| 3:K:62:ALA:HB3   | 3:K:411:ALA:HB1  | 1.94                     | 0.49              |
| 3:I:87:ASN:OD1   | 3:I:88:SER:N     | 2.46                     | 0.49              |
| 3:I:127:VAL:HG23 | 3:I:135:TRP:CD1  | 2.47                     | 0.49              |
| 3:J:59:MET:HE2   | 3:J:78:GLU:CA    | 2.43                     | 0.49              |
| 1:A:646:ALA:HA   | 1:A:649:ILE:HG22 | 1.95                     | 0.49              |
| 1:E:681:ILE:HG12 | 1:E:718:LEU:HD23 | 1.93                     | 0.49              |
| 1:F:387:LEU:HA   | 1:F:390:LYS:HE2  | 1.95                     | 0.49              |
| 3:I:148:GLU:OE1  | 3:I:148:GLU:N    | 2.46                     | 0.49              |
| 3:J:69:THR:HG21  | 3:J:232:GLY:O    | 2.12                     | 0.49              |
| 3:J:151:ALA:O    | 3:J:155:MET:HE3  | 2.13                     | 0.49              |
| 3:K:69:THR:HG21  | 3:K:232:GLY:O    | 2.12                     | 0.49              |
| 1:A:608:PRO:HG2  | 1:A:611:VAL:HG21 | 1.94                     | 0.49              |
| 1:B:539:ALA:HA   | 1:B:542:VAL:HG12 | 1.94                     | 0.49              |
| 1:C:645:VAL:HG21 | 1:C:691:VAL:HG21 | 1.95                     | 0.49              |
| 1:D:303:MET:HE3  | 1:D:308:GLU:CG   | 2.04                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:69:THR:HG21  | 3:I:232:GLY:O    | 2.12                     | 0.49              |
| 1:C:355:LYS:HD3  | 1:C:371:LEU:HD11 | 1.95                     | 0.49              |
| 1:D:299:MET:HG2  | 1:D:300:ILE:N    | 2.28                     | 0.49              |
| 1:F:571:ARG:HG2  | 1:F:619:ALA:HB2  | 1.95                     | 0.49              |
| 3:J:84:VAL:HG11  | 3:J:401:GLU:HG2  | 1.94                     | 0.49              |
| 3:J:127:VAL:HG23 | 3:J:135:TRP:CD1  | 2.47                     | 0.49              |
| 3:J:373:GLY:N    | 3:J:400:ASP:OD1  | 2.42                     | 0.49              |
| 3:K:87:ASN:OD1   | 3:K:88:SER:N     | 2.46                     | 0.49              |
| 1:A:365:ARG:C    | 1:A:532:GLU:HB2  | 2.38                     | 0.49              |
| 1:D:304:LEU:HD21 | 1:D:311:LEU:HD22 | 1.95                     | 0.49              |
| 1:E:837:ASN:N    | 1:E:845:LEU:O    | 2.44                     | 0.49              |
| 3:J:87:ASN:OD1   | 3:J:88:SER:N     | 2.46                     | 0.49              |
| 3:J:174:ILE:HG13 | 3:J:199:VAL:HG22 | 1.94                     | 0.49              |
| 3:K:84:VAL:HG11  | 3:K:401:GLU:HG2  | 1.94                     | 0.49              |
| 3:K:257:LEU:HD11 | 3:K:262:TRP:NE1  | 2.28                     | 0.49              |
| 1:B:475:ASP:O    | 1:B:479:GLN:N    | 2.45                     | 0.48              |
| 1:E:365:ARG:NH1  | 1:E:531:GLU:O    | 2.46                     | 0.48              |
| 1:B:539:ALA:HB1  | 1:B:550:ALA:O    | 2.13                     | 0.48              |
| 1:B:685:HIS:O    | 1:B:687:ASP:N    | 2.44                     | 0.48              |
| 1:F:201:ASN:CB   | 1:F:310:ARG:O    | 2.59                     | 0.48              |
| 1:F:304:LEU:CD1  | 1:F:311:LEU:HD23 | 2.43                     | 0.48              |
| 3:K:174:ILE:HG13 | 3:K:199:VAL:HG22 | 1.94                     | 0.48              |
| 1:C:414:ASP:O    | 1:C:417:GLU:HG3  | 2.14                     | 0.48              |
| 3:K:151:ALA:O    | 3:K:155:MET:HE3  | 2.13                     | 0.48              |
| 1:A:180:VAL:HG11 | 1:A:218:GLY:HA3  | 1.94                     | 0.48              |
| 1:D:248:GLY:O    | 1:D:258:ARG:NH2  | 2.39                     | 0.48              |
| 1:D:278:ASP:OD1  | 1:D:279:GLU:N    | 2.46                     | 0.48              |
| 3:I:59:MET:HE2   | 3:I:78:GLU:CA    | 2.43                     | 0.48              |
| 3:I:186:GLN:OE1  | 3:I:189:LYS:NZ   | 2.39                     | 0.48              |
| 3:J:100:PHE:CB   | 3:J:139:ILE:HD12 | 2.42                     | 0.48              |
| 3:J:148:GLU:OE1  | 3:J:148:GLU:N    | 2.46                     | 0.48              |
| 3:K:59:MET:HE2   | 3:K:78:GLU:CA    | 2.43                     | 0.48              |
| 1:B:355:LYS:HD3  | 1:B:371:LEU:HD11 | 1.95                     | 0.48              |
| 1:B:362:HIS:O    | 1:B:364:VAL:N    | 2.46                     | 0.48              |
| 1:D:778:GLN:HG2  | 1:D:779:ARG:HD2  | 1.94                     | 0.48              |
| 3:I:239:LEU:HG   | 3:I:248:VAL:HG22 | 1.95                     | 0.48              |
| 3:I:373:GLY:N    | 3:I:400:ASP:OD1  | 2.42                     | 0.48              |
| 1:A:477:LYS:HE3  | 1:A:514:LEU:HD11 | 1.96                     | 0.48              |
| 1:A:564:MET:HE1  | 1:A:586:VAL:HG21 | 1.95                     | 0.48              |
| 1:B:678:PHE:HB2  | 1:B:718:LEU:HD23 | 1.94                     | 0.48              |
| 1:C:203:VAL:HG22 | 1:C:280:LEU:HD21 | 1.96                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:148:GLU:OE1  | 3:K:148:GLU:N    | 2.46                     | 0.48              |
| 1:C:260:LYS:HA   | 1:C:260:LYS:HD3  | 1.71                     | 0.48              |
| 1:D:613:LYS:HG2  | 1:D:753:PHE:CD2  | 2.48                     | 0.48              |
| 1:D:817:ASP:O    | 1:D:821:LYS:HG2  | 2.14                     | 0.48              |
| 1:F:350:ILE:HG23 | 5:F:902:ADP:C2   | 2.48                     | 0.48              |
| 1:F:792:TRP:HE1  | 1:F:796:ARG:HH11 | 1.62                     | 0.48              |
| 3:K:368:VAL:HG23 | 3:K:391:LYS:CE   | 2.44                     | 0.48              |
| 1:C:259:LEU:HD23 | 1:C:299:MET:HE3  | 1.96                     | 0.48              |
| 1:E:575:GLN:NE2  | 1:E:754:GLU:O    | 2.46                     | 0.48              |
| 3:I:100:PHE:O    | 3:I:122:ARG:NE   | 2.47                     | 0.48              |
| 3:I:176:THR:HG21 | 3:I:185:ARG:HG2  | 1.96                     | 0.48              |
| 1:C:476:LEU:HA   | 1:C:479:GLN:HB3  | 1.95                     | 0.48              |
| 1:E:193:VAL:HG11 | 1:E:202:PRO:HB3  | 1.95                     | 0.48              |
| 1:E:582:VAL:O    | 1:E:586:VAL:HG23 | 2.13                     | 0.48              |
| 3:J:257:LEU:HD11 | 3:J:262:TRP:NE1  | 2.28                     | 0.48              |
| 3:J:287:MET:HE2  | 3:J:287:MET:N    | 2.29                     | 0.48              |
| 3:K:287:MET:N    | 3:K:287:MET:HE2  | 2.29                     | 0.48              |
| 1:A:466:GLU:N    | 1:A:466:GLU:CD   | 2.70                     | 0.48              |
| 4:A:901:AGS:O2A  | 4:A:901:AGS:O2B  | 2.32                     | 0.48              |
| 1:C:181:ILE:CD1  | 1:C:353:GLY:HA3  | 2.44                     | 0.48              |
| 1:D:386:PHE:O    | 1:D:390:LYS:CB   | 2.62                     | 0.48              |
| 1:D:768:GLN:HG3  | 1:D:807:LEU:HD22 | 1.96                     | 0.48              |
| 1:F:222:ARG:HD2  | 1:F:227:ASP:HB2  | 1.96                     | 0.48              |
| 3:K:215:LEU:O    | 3:K:222:GLN:NE2  | 2.45                     | 0.48              |
| 5:E:902:ADP:H2'  | 5:E:902:ADP:N3   | 2.29                     | 0.47              |
| 3:I:174:ILE:HG13 | 3:I:199:VAL:HG22 | 1.95                     | 0.47              |
| 3:I:257:LEU:HD11 | 3:I:262:TRP:NE1  | 2.28                     | 0.47              |
| 3:J:151:ALA:HA   | 3:J:154:LEU:HD12 | 1.96                     | 0.47              |
| 1:B:500:ALA:HB3  | 3:J:316:ILE:N    | 2.29                     | 0.47              |
| 1:B:799:ASP:C    | 1:B:801:VAL:H    | 2.22                     | 0.47              |
| 1:D:235:LYS:HE2  | 1:D:272:GLN:HA   | 1.95                     | 0.47              |
| 1:D:573:ILE:N    | 4:D:902:AGS:HN62 | 2.12                     | 0.47              |
| 1:F:303:MET:HE2  | 1:F:303:MET:HB3  | 1.70                     | 0.47              |
| 3:K:239:LEU:HG   | 3:K:248:VAL:HG22 | 1.96                     | 0.47              |
| 1:B:727:SER:OG   | 1:B:728:ALA:N    | 2.47                     | 0.47              |
| 1:C:477:LYS:CG   | 1:C:480:LEU:HD23 | 2.44                     | 0.47              |
| 1:F:648:LEU:HD12 | 1:F:649:ILE:HG12 | 1.96                     | 0.47              |
| 3:J:215:LEU:HD13 | 3:J:367:HIS:CB   | 2.44                     | 0.47              |
| 1:A:442:LEU:C    | 1:A:442:LEU:CD2  | 2.85                     | 0.47              |
| 1:A:678:PHE:HB2  | 1:A:718:LEU:HG   | 1.96                     | 0.47              |
| 1:C:490:ALA:O    | 1:C:495:ASP:N    | 2.46                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:684:ALA:HB1  | 1:E:688:VAL:HG11 | 1.97                     | 0.47              |
| 1:F:389:ASP:OD1  | 1:F:390:LYS:N    | 2.47                     | 0.47              |
| 3:I:287:MET:N    | 3:I:287:MET:HE2  | 2.29                     | 0.47              |
| 3:J:176:THR:HG21 | 3:J:185:ARG:HG2  | 1.96                     | 0.47              |
| 3:J:239:LEU:HG   | 3:J:248:VAL:HG22 | 1.95                     | 0.47              |
| 3:J:368:VAL:HG23 | 3:J:391:LYS:CE   | 2.44                     | 0.47              |
| 3:K:282:LEU:HD13 | 3:K:288:ALA:HB1  | 1.96                     | 0.47              |
| 1:A:381:TYR:HD2  | 1:A:542:VAL:HG11 | 1.80                     | 0.47              |
| 1:A:669:ARG:HH22 | 1:B:325:GLU:CD   | 2.19                     | 0.47              |
| 1:B:695:VAL:HG13 | 1:B:711:PHE:HD2  | 1.79                     | 0.47              |
| 1:F:207:GLU:O    | 1:F:210:VAL:HG23 | 2.14                     | 0.47              |
| 1:F:822:MET:HE3  | 1:F:828:VAL:HG21 | 1.96                     | 0.47              |
| 3:I:223:ARG:HG3  | 3:I:365:ILE:HG23 | 1.97                     | 0.47              |
| 3:I:282:LEU:HD13 | 3:I:288:ALA:HB1  | 1.96                     | 0.47              |
| 1:A:612:GLY:O    | 1:A:615:GLU:N    | 2.48                     | 0.47              |
| 1:D:575:GLN:OE1  | 1:D:575:GLN:HA   | 2.15                     | 0.47              |
| 1:E:648:LEU:HA   | 1:E:663:GLN:H    | 1.79                     | 0.47              |
| 1:E:749:ASP:OD1  | 1:E:749:ASP:N    | 2.47                     | 0.47              |
| 3:J:100:PHE:O    | 3:J:122:ARG:NE   | 2.47                     | 0.47              |
| 3:K:151:ALA:HA   | 3:K:154:LEU:HD12 | 1.96                     | 0.47              |
| 1:A:184:ASP:OD1  | 1:A:185:ASN:N    | 2.47                     | 0.47              |
| 1:A:393:ASP:OD2  | 1:B:335:GLN:NE2  | 2.47                     | 0.47              |
| 1:A:634:ILE:HD11 | 1:A:678:PHE:CE1  | 2.49                     | 0.47              |
| 1:B:761:LEU:HD12 | 1:B:764:ILE:HB   | 1.97                     | 0.47              |
| 1:C:646:ALA:HA   | 1:C:649:ILE:HG22 | 1.97                     | 0.47              |
| 1:D:177:LEU:HD22 | 1:D:217:GLU:HG2  | 1.95                     | 0.47              |
| 1:D:634:ILE:HD11 | 1:D:678:PHE:CE2  | 2.50                     | 0.47              |
| 1:E:538:ILE:O    | 1:E:542:VAL:HG23 | 2.15                     | 0.47              |
| 1:E:727:SER:OG   | 1:E:728:ALA:N    | 2.48                     | 0.47              |
| 1:E:769:LEU:HD11 | 1:E:790:LYS:HG2  | 1.97                     | 0.47              |
| 1:F:349:GLY:HA2  | 1:F:352:ARG:HD2  | 1.95                     | 0.47              |
| 3:I:368:VAL:HG23 | 3:I:391:LYS:CE   | 2.44                     | 0.47              |
| 3:J:217:LYS:HE3  | 3:J:366:ASP:HB3  | 1.93                     | 0.47              |
| 3:J:282:LEU:HD13 | 3:J:288:ALA:HB1  | 1.96                     | 0.47              |
| 3:K:370:LEU:HD13 | 3:K:375:THR:O    | 2.15                     | 0.47              |
| 1:A:490:ALA:O    | 1:A:495:ASP:N    | 2.46                     | 0.47              |
| 1:D:666:GLU:OE2  | 1:D:669:ARG:NH2  | 2.48                     | 0.47              |
| 1:E:542:VAL:O    | 1:E:546:THR:HG22 | 2.15                     | 0.47              |
| 3:K:87:ASN:HD22  | 3:K:94:THR:HG1   | 1.63                     | 0.47              |
| 1:B:594:SER:OG   | 1:B:595:ASP:N    | 2.47                     | 0.47              |
| 1:B:821:LYS:HB2  | 1:B:821:LYS:HE3  | 1.64                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:197:ARG:HG2  | 1:D:198:THR:HG23 | 1.96                     | 0.47              |
| 1:F:368:ASP:O    | 1:F:372:VAL:HG22 | 2.15                     | 0.47              |
| 1:F:403:ARG:HD2  | 1:F:406:ILE:HD12 | 1.97                     | 0.47              |
| 3:K:100:PHE:O    | 3:K:122:ARG:NE   | 2.47                     | 0.47              |
| 1:D:682:GLU:HG2  | 1:D:683:LYS:HD2  | 1.97                     | 0.47              |
| 3:I:59:MET:HE2   | 3:I:78:GLU:HA    | 1.97                     | 0.47              |
| 3:K:215:LEU:HD13 | 3:K:367:HIS:CB   | 2.44                     | 0.47              |
| 3:K:371:VAL:HG12 | 3:K:402:VAL:CG1  | 2.44                     | 0.47              |
| 1:C:477:LYS:O    | 1:C:481:GLU:N    | 2.37                     | 0.46              |
| 1:D:301:LYS:CD   | 1:D:333:ARG:NH2  | 2.71                     | 0.46              |
| 3:I:215:LEU:HD13 | 3:I:367:HIS:CB   | 2.44                     | 0.46              |
| 3:I:370:LEU:HD13 | 3:I:375:THR:O    | 2.15                     | 0.46              |
| 3:I:371:VAL:HG12 | 3:I:402:VAL:CG1  | 2.44                     | 0.46              |
| 3:J:59:MET:HE2   | 3:J:78:GLU:HA    | 1.97                     | 0.46              |
| 3:K:176:THR:HG21 | 3:K:185:ARG:HG2  | 1.96                     | 0.46              |
| 3:K:223:ARG:HG3  | 3:K:365:ILE:HG23 | 1.97                     | 0.46              |
| 1:A:276:PHE:CD1  | 1:A:312:VAL:HG13 | 2.51                     | 0.46              |
| 1:A:356:ASP:O    | 1:A:360:VAL:HG23 | 2.15                     | 0.46              |
| 1:B:229:PRO:O    | 1:B:233:ARG:HG3  | 2.15                     | 0.46              |
| 1:C:437:ALA:O    | 1:C:441:ARG:NH1  | 2.48                     | 0.46              |
| 1:C:480:LEU:HD13 | 1:C:510:VAL:CB   | 2.43                     | 0.46              |
| 3:J:139:ILE:HB   | 3:J:144:TYR:CE2  | 2.51                     | 0.46              |
| 1:A:459:LEU:HD22 | 1:A:459:LEU:HA   | 1.76                     | 0.46              |
| 1:E:613:LYS:HA   | 1:E:753:PHE:CE2  | 2.45                     | 0.46              |
| 3:I:151:ALA:HA   | 3:I:154:LEU:HD12 | 1.96                     | 0.46              |
| 3:J:384:VAL:O    | 3:J:388:THR:OG1  | 2.31                     | 0.46              |
| 3:K:139:ILE:HB   | 3:K:144:TYR:CE2  | 2.51                     | 0.46              |
| 1:A:500:ALA:HB3  | 3:I:316:ILE:N    | 2.30                     | 0.46              |
| 1:A:685:HIS:O    | 1:A:687:ASP:N    | 2.43                     | 0.46              |
| 1:A:695:VAL:HG13 | 1:A:711:PHE:HD2  | 1.80                     | 0.46              |
| 1:B:342:PRO:O    | 1:B:387:LEU:HD12 | 1.95                     | 0.46              |
| 1:B:606:LEU:HB3  | 1:B:720:SER:HB3  | 1.98                     | 0.46              |
| 3:I:158:LYS:HB2  | 3:I:197:LEU:HD21 | 1.98                     | 0.46              |
| 3:K:257:LEU:HD11 | 3:K:262:TRP:CD1  | 2.50                     | 0.46              |
| 1:B:676:VAL:HB   | 1:B:716:LEU:HD23 | 1.98                     | 0.46              |
| 4:C:902:AGS:O2A  | 4:C:902:AGS:O2B  | 2.34                     | 0.46              |
| 1:E:786:SER:C    | 1:E:790:LYS:HE2  | 2.40                     | 0.46              |
| 3:K:59:MET:HE2   | 3:K:78:GLU:HA    | 1.97                     | 0.46              |
| 3:K:87:ASN:ND2   | 3:K:94:THR:OG1   | 2.47                     | 0.46              |
| 1:A:373:ALA:HA   | 1:A:376:THR:HG22 | 1.97                     | 0.46              |
| 1:E:263:LEU:HD21 | 1:E:300:ILE:HG22 | 1.96                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:798:PHE:CE2  | 1:E:800:PRO:HB3  | 2.49                     | 0.46              |
| 3:J:370:LEU:HD13 | 3:J:375:THR:O    | 2.15                     | 0.46              |
| 3:K:82:PRO:CB    | 3:K:405:VAL:HG13 | 2.46                     | 0.46              |
| 1:B:785:VAL:HA   | 1:B:836:VAL:HG22 | 1.97                     | 0.46              |
| 1:C:609:THR:OG1  | 4:C:901:AGS:S1G  | 2.71                     | 0.46              |
| 1:C:792:TRP:HE1  | 1:C:796:ARG:NH2  | 2.14                     | 0.46              |
| 1:D:809:ARG:NH1  | 1:D:813:GLN:HB3  | 2.31                     | 0.46              |
| 1:E:792:TRP:HE3  | 1:E:793:LEU:HD12 | 1.81                     | 0.46              |
| 3:I:82:PRO:CB    | 3:I:405:VAL:HG13 | 2.46                     | 0.46              |
| 3:I:257:LEU:HD11 | 3:I:262:TRP:CD1  | 2.51                     | 0.46              |
| 3:J:223:ARG:HG3  | 3:J:365:ILE:HG23 | 1.97                     | 0.46              |
| 1:B:476:LEU:HD12 | 1:B:513:LYS:HZ2  | 1.80                     | 0.46              |
| 1:C:378:SER:OG   | 1:C:390:LYS:HG3  | 2.16                     | 0.46              |
| 1:D:305:ALA:HB2  | 1:D:333:ARG:CG   | 2.46                     | 0.46              |
| 1:F:276:PHE:HA   | 1:F:312:VAL:HG13 | 1.97                     | 0.46              |
| 1:A:365:ARG:NH2  | 1:A:531:GLU:HB2  | 2.29                     | 0.46              |
| 1:D:789:ALA:HB2  | 1:D:838:VAL:HG22 | 1.98                     | 0.46              |
| 3:I:139:ILE:HB   | 3:I:144:TYR:CE2  | 2.51                     | 0.46              |
| 1:A:805:ARG:HD2  | 1:B:745:ASN:ND2  | 2.31                     | 0.46              |
| 1:B:490:ALA:O    | 1:B:495:ASP:N    | 2.46                     | 0.46              |
| 1:C:277:ILE:HD12 | 1:C:311:LEU:HD11 | 1.97                     | 0.46              |
| 3:K:221:GLU:HG2  | 3:K:222:GLN:N    | 2.31                     | 0.46              |
| 3:K:318:VAL:HG22 | 3:K:320:ALA:H    | 1.81                     | 0.46              |
| 3:K:341:GLN:HA   | 3:K:344:LEU:HD12 | 1.98                     | 0.46              |
| 1:B:358:TYR:HE1  | 1:C:197:ARG:HH21 | 1.63                     | 0.45              |
| 1:B:380:ARG:NH2  | 1:B:596:PRO:O    | 2.49                     | 0.45              |
| 1:C:594:SER:OG   | 1:C:595:ASP:N    | 2.48                     | 0.45              |
| 1:F:786:SER:O    | 1:F:790:LYS:HG3  | 2.16                     | 0.45              |
| 3:J:82:PRO:CB    | 3:J:405:VAL:HG13 | 2.46                     | 0.45              |
| 3:J:215:LEU:O    | 3:J:222:GLN:NE2  | 2.45                     | 0.45              |
| 3:K:181:ASN:N    | 3:K:184:GLN:OE1  | 2.46                     | 0.45              |
| 1:D:220:ALA:HB2  | 1:D:237:ILE:HD11 | 1.97                     | 0.45              |
| 1:E:161:LEU:HD22 | 1:E:261:ALA:HB1  | 1.97                     | 0.45              |
| 1:F:255:PHE:O    | 1:F:258:ARG:HG2  | 2.17                     | 0.45              |
| 1:A:278:ASP:OD1  | 1:A:278:ASP:N    | 2.49                     | 0.45              |
| 1:A:434:GLU:H    | 1:A:434:GLU:CD   | 2.25                     | 0.45              |
| 1:A:633:ARG:NH2  | 1:B:698:GLU:OE2  | 2.49                     | 0.45              |
| 1:B:497:ALA:HA   | 3:J:315:TYR:O    | 2.16                     | 0.45              |
| 3:J:238:LEU:CB   | 3:J:358:THR:HG21 | 2.47                     | 0.45              |
| 3:J:325:LEU:HD23 | 3:J:325:LEU:HA   | 1.85                     | 0.45              |
| 3:K:319:ASP:N    | 3:K:323:ASN:O    | 2.32                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:474:ARG:NH1  | 1:A:475:ASP:OD1  | 2.45                     | 0.45              |
| 1:A:681:ILE:HG12 | 1:A:718:LEU:HD23 | 1.98                     | 0.45              |
| 1:B:666:GLU:OE2  | 1:B:669:ARG:NE   | 2.45                     | 0.45              |
| 1:D:699:GLY:HA2  | 1:D:711:PHE:HB2  | 1.97                     | 0.45              |
| 1:D:822:MET:HG3  | 1:D:827:GLN:HE21 | 1.81                     | 0.45              |
| 1:F:263:LEU:HD23 | 1:F:266:ILE:HD12 | 1.99                     | 0.45              |
| 1:F:373:ALA:HB3  | 1:F:538:ILE:HD12 | 1.98                     | 0.45              |
| 1:F:382:ILE:HD11 | 1:F:542:VAL:HA   | 1.99                     | 0.45              |
| 3:I:102:ARG:NH2  | 3:I:118:THR:O    | 2.45                     | 0.45              |
| 3:I:238:LEU:CB   | 3:I:358:THR:HG21 | 2.46                     | 0.45              |
| 3:J:257:LEU:HD11 | 3:J:262:TRP:CD1  | 2.50                     | 0.45              |
| 1:D:778:GLN:NE2  | 1:E:592:GLY:O    | 2.49                     | 0.45              |
| 3:K:238:LEU:CB   | 3:K:358:THR:HG21 | 2.46                     | 0.45              |
| 1:B:249:SER:HB2  | 1:C:252:ARG:HH21 | 1.82                     | 0.45              |
| 1:D:299:MET:C    | 1:D:301:LYS:H    | 2.25                     | 0.45              |
| 3:K:201:ARG:NH1  | 3:K:410:GLN:OE1  | 2.50                     | 0.45              |
| 1:A:389:ASP:OD1  | 1:A:390:LYS:N    | 2.49                     | 0.45              |
| 1:E:726:GLY:N    | 1:E:730:GLN:HE21 | 2.15                     | 0.45              |
| 1:E:744:ILE:HA   | 1:E:747:LEU:HD13 | 1.98                     | 0.45              |
| 3:J:181:ASN:N    | 3:J:184:GLN:OE1  | 2.46                     | 0.45              |
| 1:A:497:ALA:HA   | 3:I:315:TYR:O    | 2.16                     | 0.45              |
| 1:B:473:VAL:CG2  | 1:B:517:ALA:CB   | 2.72                     | 0.45              |
| 1:E:304:LEU:HA   | 1:E:309:LEU:HD21 | 1.97                     | 0.45              |
| 1:E:322:LYS:O    | 1:E:326:LYS:HG2  | 2.16                     | 0.45              |
| 1:F:379:ASP:OD1  | 1:F:380:ARG:N    | 2.45                     | 0.45              |
| 1:F:573:ILE:HG23 | 1:F:763:ARG:HH21 | 1.80                     | 0.45              |
| 3:J:201:ARG:NH1  | 3:J:410:GLN:OE1  | 2.50                     | 0.45              |
| 3:J:371:VAL:HG12 | 3:J:402:VAL:CG1  | 2.44                     | 0.45              |
| 3:K:158:LYS:HB2  | 3:K:197:LEU:HD21 | 1.97                     | 0.45              |
| 1:A:364:VAL:HG21 | 1:A:402:LEU:HD23 | 1.99                     | 0.45              |
| 1:D:180:VAL:HA   | 4:D:901:AGS:N1   | 2.32                     | 0.45              |
| 1:E:200:ASN:OD1  | 1:E:201:ASN:ND2  | 2.49                     | 0.45              |
| 1:F:298:ASN:N    | 1:F:301:LYS:HD3  | 2.32                     | 0.45              |
| 1:F:694:GLN:NE2  | 1:F:701:LEU:HA   | 2.32                     | 0.45              |
| 3:I:398:ASN:O    | 3:I:402:VAL:N    | 2.50                     | 0.45              |
| 3:J:158:LYS:HB2  | 3:J:197:LEU:HD21 | 1.97                     | 0.45              |
| 1:A:427:GLU:CB   | 1:A:445:LEU:HD21 | 2.43                     | 0.45              |
| 1:B:196:ARG:HG3  | 1:B:200:ASN:HB3  | 1.98                     | 0.45              |
| 1:B:387:LEU:HB3  | 1:B:388:PRO:CD   | 2.35                     | 0.45              |
| 1:C:177:LEU:HD13 | 1:C:217:GLU:HG2  | 1.99                     | 0.45              |
| 1:C:231:SER:O    | 1:C:231:SER:OG   | 2.35                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:545:TRP:CD1  | 1:D:546:THR:HG23 | 2.43                     | 0.45              |
| 1:F:561:LEU:O    | 1:F:587:ARG:HD3  | 2.16                     | 0.45              |
| 3:I:224:ILE:HD12 | 3:I:367:HIS:HB2  | 1.99                     | 0.45              |
| 3:J:215:LEU:HD13 | 3:J:367:HIS:HB3  | 1.99                     | 0.45              |
| 1:A:406:ILE:HD12 | 1:A:529:LEU:HD11 | 1.97                     | 0.44              |
| 1:A:769:LEU:HD23 | 1:A:769:LEU:HA   | 1.80                     | 0.44              |
| 1:C:193:VAL:O    | 1:C:196:ARG:HG2  | 2.16                     | 0.44              |
| 1:C:497:ALA:HA   | 3:K:315:TYR:O    | 2.16                     | 0.44              |
| 1:F:726:GLY:HA3  | 1:F:730:GLN:HB2  | 1.99                     | 0.44              |
| 3:K:398:ASN:O    | 3:K:402:VAL:N    | 2.50                     | 0.44              |
| 1:C:267:LYS:HB3  | 1:C:267:LYS:HE2  | 1.80                     | 0.44              |
| 1:C:776:LEU:HD11 | 1:C:819:LEU:HD21 | 1.98                     | 0.44              |
| 1:C:805:ARG:NH2  | 4:C:901:AGS:S1G  | 2.89                     | 0.44              |
| 1:C:805:ARG:NH2  | 1:D:746:ARG:HH21 | 2.16                     | 0.44              |
| 1:D:299:MET:HE2  | 1:D:299:MET:HB3  | 1.70                     | 0.44              |
| 1:F:162:GLN:OE1  | 1:F:162:GLN:N    | 2.48                     | 0.44              |
| 3:K:207:THR:CG2  | 3:K:246:VAL:HG11 | 2.47                     | 0.44              |
| 1:A:463:TRP:CD2  | 1:A:463:TRP:O    | 2.70                     | 0.44              |
| 1:A:799:ASP:OD1  | 1:A:799:ASP:N    | 2.48                     | 0.44              |
| 1:C:473:VAL:CA   | 1:C:514:LEU:CD2  | 2.94                     | 0.44              |
| 1:C:476:LEU:HD21 | 1:C:510:VAL:CA   | 2.48                     | 0.44              |
| 1:C:477:LYS:C    | 1:C:479:GLN:H    | 2.23                     | 0.44              |
| 1:E:762:VAL:HA   | 1:E:765:VAL:HG12 | 1.99                     | 0.44              |
| 1:F:167:ASP:OD1  | 1:F:168:LEU:N    | 2.51                     | 0.44              |
| 3:I:98:VAL:CG2   | 3:I:153:ILE:HD11 | 2.48                     | 0.44              |
| 3:I:201:ARG:NH1  | 3:I:410:GLN:OE1  | 2.50                     | 0.44              |
| 3:I:207:THR:CG2  | 3:I:246:VAL:HG11 | 2.47                     | 0.44              |
| 3:I:341:GLN:HA   | 3:I:344:LEU:HD12 | 1.98                     | 0.44              |
| 3:J:65:ILE:HG12  | 3:J:74:VAL:HG13  | 1.99                     | 0.44              |
| 3:J:102:ARG:NH2  | 3:J:118:THR:O    | 2.45                     | 0.44              |
| 3:J:207:THR:CG2  | 3:J:246:VAL:HG11 | 2.47                     | 0.44              |
| 3:J:98:VAL:CG2   | 3:J:153:ILE:HD11 | 2.48                     | 0.44              |
| 3:J:238:LEU:C    | 3:J:239:LEU:HD12 | 2.43                     | 0.44              |
| 1:B:328:ALA:HA   | 1:B:331:GLU:HG3  | 1.99                     | 0.44              |
| 1:C:545:TRP:O    | 1:C:546:THR:OG1  | 2.36                     | 0.44              |
| 1:E:277:ILE:HG22 | 1:E:280:LEU:HB3  | 1.99                     | 0.44              |
| 1:E:372:VAL:O    | 1:E:376:THR:HG23 | 2.17                     | 0.44              |
| 3:J:341:GLN:HA   | 3:J:344:LEU:HD12 | 1.98                     | 0.44              |
| 3:J:398:ASN:O    | 3:J:402:VAL:N    | 2.50                     | 0.44              |
| 3:K:181:ASN:OD1  | 3:K:183:ALA:HB3  | 2.18                     | 0.44              |
| 1:A:303:MET:HB3  | 1:A:309:LEU:HD13 | 2.00                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:808:ARG:HH22 | 1:C:598:ARG:HH11 | 1.65                     | 0.44              |
| 1:D:693:LEU:O    | 1:D:746:ARG:NH1  | 2.50                     | 0.44              |
| 1:E:729:GLU:OE1  | 1:E:729:GLU:N    | 2.51                     | 0.44              |
| 3:J:224:ILE:HD12 | 3:J:367:HIS:HB2  | 1.99                     | 0.44              |
| 3:K:65:ILE:HG12  | 3:K:74:VAL:HG13  | 1.99                     | 0.44              |
| 3:K:224:ILE:HD12 | 3:K:367:HIS:HB2  | 1.99                     | 0.44              |
| 3:K:236:VAL:HB   | 3:K:354:VAL:HG21 | 2.00                     | 0.44              |
| 1:A:598:ARG:HG2  | 1:A:599:PRO:O    | 2.18                     | 0.44              |
| 1:A:685:HIS:C    | 1:A:687:ASP:H    | 2.26                     | 0.44              |
| 1:B:722:LEU:HA   | 1:B:722:LEU:HD23 | 1.81                     | 0.44              |
| 1:C:473:VAL:HA   | 1:C:514:LEU:HD23 | 2.00                     | 0.44              |
| 1:D:573:ILE:CG2  | 4:D:902:AGS:N6   | 2.81                     | 0.44              |
| 1:D:760:GLU:HG2  | 1:D:763:ARG:NH2  | 2.33                     | 0.44              |
| 1:E:575:GLN:O    | 1:E:579:VAL:HG23 | 2.18                     | 0.44              |
| 1:F:168:LEU:HD12 | 1:F:168:LEU:HA   | 1.86                     | 0.44              |
| 1:F:307:GLY:N    | 1:F:308:GLU:OE1  | 2.51                     | 0.44              |
| 1:F:649:ILE:HG23 | 1:F:703:ASP:HA   | 2.00                     | 0.44              |
| 3:I:60:ALA:CB    | 3:I:77:LEU:HD12  | 2.47                     | 0.44              |
| 3:J:181:ASN:OD1  | 3:J:183:ALA:HB3  | 2.18                     | 0.44              |
| 1:B:826:GLY:O    | 1:B:827:GLN:HG2  | 2.18                     | 0.44              |
| 1:C:199:LYS:HE3  | 1:C:335:GLN:HE21 | 1.82                     | 0.44              |
| 1:C:832:ASP:OD1  | 1:C:832:ASP:N    | 2.51                     | 0.44              |
| 1:E:563:ARG:C    | 1:E:565:GLU:H    | 2.26                     | 0.44              |
| 1:E:699:GLY:O    | 1:E:712:ARG:NH2  | 2.51                     | 0.44              |
| 1:E:784:GLN:HB2  | 1:E:833:THR:O    | 2.18                     | 0.44              |
| 1:F:573:ILE:O    | 4:F:901:AGS:N6   | 2.50                     | 0.44              |
| 3:I:87:ASN:ND2   | 3:I:94:THR:OG1   | 2.47                     | 0.44              |
| 3:I:181:ASN:OD1  | 3:I:183:ALA:HB3  | 2.18                     | 0.44              |
| 3:I:238:LEU:C    | 3:I:239:LEU:HD12 | 2.43                     | 0.44              |
| 1:A:364:VAL:HG22 | 1:A:532:GLU:HA   | 2.00                     | 0.44              |
| 1:B:211:GLY:HA2  | 4:B:901:AGS:O2A  | 2.17                     | 0.44              |
| 1:E:349:GLY:HA2  | 1:E:352:ARG:HG2  | 2.00                     | 0.44              |
| 3:I:249:ARG:HG3  | 3:I:358:THR:HG22 | 2.00                     | 0.44              |
| 1:A:237:ILE:HG12 | 1:A:274:ILE:HB   | 2.00                     | 0.43              |
| 1:D:613:LYS:HZ3  | 4:D:902:AGS:PB   | 2.41                     | 0.43              |
| 1:F:347:THR:HA   | 1:F:350:ILE:HD12 | 1.99                     | 0.43              |
| 1:F:367:THR:OG1  | 1:F:369:SER:OG   | 2.27                     | 0.43              |
| 1:A:819:LEU:O    | 1:A:823:LEU:HB2  | 2.18                     | 0.43              |
| 1:F:258:ARG:HG3  | 1:F:259:LEU:HD22 | 1.99                     | 0.43              |
| 3:I:65:ILE:HG12  | 3:I:74:VAL:HG13  | 1.99                     | 0.43              |
| 3:J:87:ASN:ND2   | 3:J:94:THR:OG1   | 2.47                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:215:LEU:HD13 | 3:K:367:HIS:HB3  | 1.99                     | 0.43              |
| 1:A:539:ALA:HB1  | 1:A:550:ALA:O    | 2.18                     | 0.43              |
| 1:A:792:TRP:HE1  | 1:A:796:ARG:CZ   | 2.31                     | 0.43              |
| 1:A:817:ASP:OD1  | 1:A:818:GLN:N    | 2.51                     | 0.43              |
| 1:B:341:GLU:HG3  | 1:B:387:LEU:HD11 | 2.00                     | 0.43              |
| 1:B:428:MET:HE3  | 1:B:428:MET:HB3  | 1.81                     | 0.43              |
| 1:C:757:ASN:ND2  | 1:C:760:GLU:OE2  | 2.51                     | 0.43              |
| 1:E:207:GLU:O    | 1:E:212:LYS:NZ   | 2.48                     | 0.43              |
| 1:E:302:PRO:O    | 1:E:306:ARG:NH2  | 2.51                     | 0.43              |
| 1:F:310:ARG:NE   | 1:F:310:ARG:CA   | 2.81                     | 0.43              |
| 3:I:215:LEU:HD13 | 3:I:367:HIS:HB3  | 1.99                     | 0.43              |
| 1:B:318:ASP:OD1  | 1:B:321:ARG:NE   | 2.49                     | 0.43              |
| 1:B:422:ARG:HD2  | 1:C:181:ILE:HG23 | 2.01                     | 0.43              |
| 1:B:808:ARG:NH2  | 1:C:598:ARG:HD2  | 2.32                     | 0.43              |
| 1:C:513:LYS:HE3  | 1:C:513:LYS:O    | 2.19                     | 0.43              |
| 1:D:647:ARG:NH2  | 1:E:703:ASP:O    | 2.52                     | 0.43              |
| 1:E:173:ARG:HE   | 1:E:224:VAL:HG23 | 1.82                     | 0.43              |
| 3:I:236:VAL:HB   | 3:I:354:VAL:HG21 | 2.00                     | 0.43              |
| 3:J:60:ALA:CB    | 3:J:77:LEU:HD12  | 2.47                     | 0.43              |
| 1:A:487:SER:CA   | 1:A:502:LEU:HD13 | 2.49                     | 0.43              |
| 1:B:634:ILE:HD11 | 1:B:678:PHE:CE2  | 2.54                     | 0.43              |
| 1:C:508:PRO:O    | 1:C:512:LYS:HG3  | 2.19                     | 0.43              |
| 1:D:792:TRP:CZ3  | 1:D:843:ASP:HB2  | 2.53                     | 0.43              |
| 1:E:201:ASN:HB2  | 1:E:311:LEU:O    | 2.18                     | 0.43              |
| 1:E:636:MET:HB3  | 1:E:684:ALA:HB2  | 2.00                     | 0.43              |
| 1:F:278:ASP:OD1  | 1:F:279:GLU:HG2  | 2.19                     | 0.43              |
| 3:J:236:VAL:HB   | 3:J:354:VAL:HG21 | 2.00                     | 0.43              |
| 3:K:98:VAL:CG2   | 3:K:153:ILE:HD11 | 2.48                     | 0.43              |
| 3:K:249:ARG:HG3  | 3:K:358:THR:HG22 | 2.00                     | 0.43              |
| 1:B:553:LEU:HD21 | 1:B:590:ARG:HB3  | 2.01                     | 0.43              |
| 1:D:659:GLU:H    | 1:D:659:GLU:CD   | 2.23                     | 0.43              |
| 1:F:365:ARG:HB2  | 1:F:532:GLU:HB2  | 2.00                     | 0.43              |
| 1:F:761:LEU:HD23 | 1:F:761:LEU:HA   | 1.82                     | 0.43              |
| 1:F:827:GLN:H    | 1:F:829:HIS:CE1  | 2.37                     | 0.43              |
| 3:I:181:ASN:N    | 3:I:184:GLN:OE1  | 2.45                     | 0.43              |
| 3:J:249:ARG:HG3  | 3:J:358:THR:HG22 | 2.00                     | 0.43              |
| 3:K:238:LEU:C    | 3:K:239:LEU:HD12 | 2.43                     | 0.43              |
| 1:C:281:HIS:NE2  | 1:C:319:GLU:OE1  | 2.51                     | 0.43              |
| 1:C:411:VAL:O    | 1:C:412:GLU:HG2  | 2.19                     | 0.43              |
| 1:C:476:LEU:CA   | 1:C:479:GLN:HB3  | 2.47                     | 0.43              |
| 1:C:487:SER:CA   | 1:C:502:LEU:HD13 | 2.49                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:389:ASP:OD1  | 1:D:390:LYS:N    | 2.51                     | 0.43              |
| 1:F:235:LYS:HA   | 1:F:235:LYS:HD3  | 1.70                     | 0.43              |
| 1:F:344:VAL:HG22 | 1:F:387:LEU:HD21 | 2.00                     | 0.43              |
| 1:F:632:VAL:HG12 | 1:F:676:VAL:HG23 | 2.01                     | 0.43              |
| 1:B:199:LYS:HE3  | 1:B:332:ARG:O    | 2.18                     | 0.43              |
| 1:B:562:LEU:HD23 | 1:B:562:LEU:HA   | 1.84                     | 0.43              |
| 1:B:631:MET:HE2  | 1:B:633:ARG:NH1  | 2.32                     | 0.43              |
| 1:C:423:LEU:HD22 | 1:C:445:LEU:HD11 | 2.00                     | 0.43              |
| 1:D:240:LEU:HD23 | 1:D:277:ILE:HD11 | 2.01                     | 0.43              |
| 1:E:180:VAL:HG13 | 4:E:901:AGS:C6   | 2.49                     | 0.43              |
| 1:E:802:TYR:CB   | 1:E:805:ARG:HD2  | 2.46                     | 0.43              |
| 1:F:211:GLY:O    | 1:F:215:ILE:HG13 | 2.18                     | 0.43              |
| 3:J:365:ILE:HG22 | 3:J:391:LYS:HE2  | 2.01                     | 0.43              |
| 1:E:783:LEU:HA   | 1:E:834:VAL:HG22 | 2.00                     | 0.43              |
| 1:F:554:LEU:HB3  | 1:F:557:GLU:HG2  | 2.01                     | 0.43              |
| 3:I:98:VAL:HG21  | 3:I:149:ILE:HG22 | 2.01                     | 0.43              |
| 3:K:60:ALA:CB    | 3:K:77:LEU:HD12  | 2.47                     | 0.43              |
| 1:A:196:ARG:HD2  | 1:A:198:THR:O    | 2.18                     | 0.43              |
| 1:A:321:ARG:NH1  | 1:F:659:GLU:O    | 2.42                     | 0.43              |
| 1:C:276:PHE:HA   | 1:C:312:VAL:O    | 2.19                     | 0.43              |
| 1:C:546:THR:O    | 1:C:546:THR:OG1  | 2.36                     | 0.43              |
| 1:D:213:THR:HG22 | 1:D:217:GLU:OE1  | 2.19                     | 0.43              |
| 1:F:703:ASP:OD1  | 1:F:703:ASP:N    | 2.51                     | 0.43              |
| 3:J:98:VAL:HG21  | 3:J:149:ILE:HG22 | 2.01                     | 0.43              |
| 3:J:257:LEU:HD11 | 3:J:262:TRP:HE1  | 1.84                     | 0.43              |
| 3:K:98:VAL:HG21  | 3:K:149:ILE:HG22 | 2.01                     | 0.43              |
| 3:K:102:ARG:NH2  | 3:K:118:THR:O    | 2.45                     | 0.43              |
| 1:A:180:VAL:HG21 | 1:A:218:GLY:HA2  | 2.00                     | 0.42              |
| 1:A:211:GLY:HA2  | 4:A:901:AGS:O2A  | 2.18                     | 0.42              |
| 1:A:242:LEU:HA   | 1:A:245:MET:HB3  | 2.01                     | 0.42              |
| 1:A:573:ILE:HD11 | 1:A:767:ILE:HD12 | 2.00                     | 0.42              |
| 1:B:321:ARG:HA   | 1:B:325:GLU:HB2  | 2.00                     | 0.42              |
| 1:B:332:ARG:HH21 | 1:B:333:ARG:NH2  | 2.17                     | 0.42              |
| 1:B:435:ASP:OD1  | 1:B:436:GLU:N    | 2.52                     | 0.42              |
| 1:B:476:LEU:CG   | 1:B:510:VAL:HG13 | 2.49                     | 0.42              |
| 1:B:480:LEU:CD1  | 1:B:507:ILE:HG23 | 2.49                     | 0.42              |
| 1:C:363:GLY:O    | 1:C:403:ARG:NH1  | 2.51                     | 0.42              |
| 1:C:790:LYS:HE3  | 1:C:790:LYS:HB2  | 1.83                     | 0.42              |
| 1:D:204:LEU:HD23 | 1:D:337:VAL:HB   | 2.01                     | 0.42              |
| 1:D:636:MET:HE1  | 1:D:688:VAL:HG11 | 2.01                     | 0.42              |
| 3:I:306:SER:OG   | 3:I:308:SER:O    | 2.37                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:238:LEU:O    | 3:J:249:ARG:N    | 2.52                     | 0.42              |
| 1:B:358:TYR:CD1  | 1:C:197:ARG:HD3  | 2.53                     | 0.42              |
| 1:B:487:SER:CA   | 1:B:502:LEU:HD13 | 2.49                     | 0.42              |
| 1:C:642:LYS:HB3  | 1:C:642:LYS:HE3  | 1.90                     | 0.42              |
| 3:J:306:SER:OG   | 3:J:308:SER:O    | 2.37                     | 0.42              |
| 1:B:226:GLY:O    | 1:B:233:ARG:NH1  | 2.52                     | 0.42              |
| 1:C:211:GLY:HA2  | 4:C:902:AGS:O2A  | 2.19                     | 0.42              |
| 1:C:321:ARG:HA   | 1:C:325:GLU:HB3  | 2.01                     | 0.42              |
| 1:C:472:ILE:H    | 1:C:472:ILE:HG13 | 1.61                     | 0.42              |
| 1:C:677:LEU:HD22 | 1:C:679:ASP:OD1  | 2.19                     | 0.42              |
| 1:F:343:SER:O    | 1:F:347:THR:HG23 | 2.19                     | 0.42              |
| 3:I:222:GLN:HG3  | 3:I:241:ILE:HB   | 1.94                     | 0.42              |
| 3:J:221:GLU:CD   | 3:J:222:GLN:N    | 2.78                     | 0.42              |
| 1:A:645:VAL:HG22 | 1:A:688:VAL:HG22 | 2.00                     | 0.42              |
| 1:B:778:GLN:N    | 1:B:778:GLN:OE1  | 2.53                     | 0.42              |
| 1:C:476:LEU:HD21 | 1:C:510:VAL:CB   | 2.47                     | 0.42              |
| 1:D:280:LEU:HD23 | 1:D:313:GLY:HA3  | 2.00                     | 0.42              |
| 1:E:799:ASP:O    | 1:E:801:VAL:N    | 2.49                     | 0.42              |
| 1:F:300:ILE:HD11 | 1:F:309:LEU:HD11 | 2.02                     | 0.42              |
| 3:I:229:LEU:HD23 | 3:I:374:SER:CB   | 2.50                     | 0.42              |
| 1:A:532:GLU:OE1  | 1:A:532:GLU:CA   | 2.68                     | 0.42              |
| 1:A:545:TRP:O    | 1:A:547:GLY:N    | 2.53                     | 0.42              |
| 1:A:578:ALA:HA   | 1:A:751:LEU:HD13 | 2.01                     | 0.42              |
| 1:A:682:GLU:OE2  | 1:A:683:LYS:NZ   | 2.51                     | 0.42              |
| 1:F:351:LEU:O    | 1:F:355:LYS:N    | 2.47                     | 0.42              |
| 1:F:387:LEU:HB3  | 1:F:388:PRO:HD3  | 2.00                     | 0.42              |
| 1:F:678:PHE:HB2  | 1:F:718:LEU:HG   | 2.01                     | 0.42              |
| 3:I:319:ASP:OD2  | 3:I:325:LEU:CD2  | 2.67                     | 0.42              |
| 3:K:223:ARG:N    | 3:K:366:ASP:OD2  | 2.44                     | 0.42              |
| 1:A:732:LEU:HD23 | 1:A:732:LEU:HA   | 1.77                     | 0.42              |
| 1:A:826:GLY:O    | 1:A:827:GLN:HG2  | 2.19                     | 0.42              |
| 1:B:411:VAL:C    | 1:B:413:ILE:H    | 2.28                     | 0.42              |
| 3:K:158:LYS:CB   | 3:K:197:LEU:HD21 | 2.50                     | 0.42              |
| 1:B:470:ILE:CB   | 1:B:519:PRO:CG   | 2.97                     | 0.42              |
| 1:D:575:GLN:HE22 | 1:D:611:VAL:CG1  | 2.32                     | 0.42              |
| 1:D:585:ALA:HB2  | 1:D:603:PHE:HZ   | 1.84                     | 0.42              |
| 1:E:554:LEU:HD23 | 1:E:554:LEU:HA   | 1.80                     | 0.42              |
| 1:F:651:ALA:HB3  | 1:F:657:GLY:O    | 2.19                     | 0.42              |
| 1:F:690:ASP:O    | 1:F:693:LEU:HB3  | 2.20                     | 0.42              |
| 3:K:70:THR:HG23  | 3:K:232:GLY:HA3  | 2.02                     | 0.42              |
| 3:K:238:LEU:O    | 3:K:249:ARG:N    | 2.52                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:257:LEU:HD11 | 3:K:262:TRP:HE1  | 1.84                     | 0.42              |
| 3:K:348:ARG:O    | 3:K:351:PHE:N    | 2.53                     | 0.42              |
| 1:A:660:ALA:HA   | 1:B:321:ARG:HH22 | 1.84                     | 0.42              |
| 1:B:496:LEU:HD11 | 3:J:316:ILE:HG23 | 2.01                     | 0.42              |
| 1:B:602:ALA:HA   | 1:B:716:LEU:O    | 2.20                     | 0.42              |
| 1:D:322:LYS:HE3  | 1:D:323:HIS:NE2  | 2.35                     | 0.42              |
| 1:E:207:GLU:HB3  | 1:E:208:PRO:CD   | 2.48                     | 0.42              |
| 1:F:772:LEU:O    | 1:F:776:LEU:HG   | 2.19                     | 0.42              |
| 1:F:774:LYS:HE2  | 1:F:774:LYS:HB3  | 1.90                     | 0.42              |
| 3:I:158:LYS:CB   | 3:I:197:LEU:HD21 | 2.50                     | 0.42              |
| 3:K:175:THR:HG21 | 3:K:403:VAL:CG1  | 2.50                     | 0.42              |
| 3:K:229:LEU:HD23 | 3:K:374:SER:CB   | 2.50                     | 0.42              |
| 1:A:311:LEU:O    | 1:A:311:LEU:HD23 | 2.20                     | 0.42              |
| 1:A:406:ILE:HD12 | 1:A:529:LEU:CD1  | 2.50                     | 0.42              |
| 1:A:641:GLU:O    | 1:A:644:THR:OG1  | 2.36                     | 0.42              |
| 1:B:201:ASN:ND2  | 1:B:304:LEU:HD22 | 2.35                     | 0.42              |
| 1:B:784:GLN:HB2  | 1:B:835:PRO:HB3  | 2.01                     | 0.42              |
| 1:C:386:PHE:O    | 1:C:390:LYS:HG2  | 2.20                     | 0.42              |
| 1:D:378:SER:HB2  | 1:D:390:LYS:HG2  | 2.01                     | 0.42              |
| 1:E:264:ASP:OD1  | 1:E:268:ASN:ND2  | 2.53                     | 0.42              |
| 1:E:365:ARG:O    | 1:E:533:VAL:HG12 | 2.19                     | 0.42              |
| 1:E:834:VAL:HG23 | 1:E:834:VAL:O    | 2.19                     | 0.42              |
| 1:F:694:GLN:O    | 1:F:698:GLU:HB3  | 2.20                     | 0.42              |
| 3:I:122:ARG:NH2  | 3:I:140:ASP:OD2  | 2.53                     | 0.42              |
| 3:J:175:THR:HG21 | 3:J:403:VAL:CG1  | 2.50                     | 0.42              |
| 3:J:348:ARG:HG3  | 3:J:387:LEU:HD21 | 2.02                     | 0.42              |
| 1:A:194:LEU:HD21 | 1:A:274:ILE:HG21 | 2.01                     | 0.42              |
| 1:A:355:LYS:HB2  | 1:A:371:LEU:HD11 | 2.01                     | 0.42              |
| 1:B:260:LYS:HE2  | 1:B:260:LYS:HB2  | 1.75                     | 0.42              |
| 1:C:366:ILE:HA   | 1:C:533:VAL:HG22 | 2.02                     | 0.42              |
| 1:C:480:LEU:CD1  | 1:C:510:VAL:CG1  | 2.76                     | 0.42              |
| 1:E:264:ASP:O    | 1:E:268:ASN:ND2  | 2.53                     | 0.42              |
| 1:F:244:SER:HB2  | 1:F:258:ARG:NH2  | 2.34                     | 0.42              |
| 3:K:238:LEU:HB3  | 3:K:358:THR:HG21 | 2.02                     | 0.42              |
| 3:K:348:ARG:HG3  | 3:K:387:LEU:HD21 | 2.02                     | 0.42              |
| 3:K:365:ILE:HG22 | 3:K:391:LYS:HE2  | 2.01                     | 0.42              |
| 1:A:702:THR:OG1  | 1:F:647:ARG:NH2  | 2.53                     | 0.41              |
| 1:C:194:LEU:HD11 | 1:C:310:ARG:HB3  | 2.01                     | 0.41              |
| 1:E:400:SER:OG   | 1:F:192:GLN:HG2  | 2.19                     | 0.41              |
| 1:E:775:ARG:HA   | 1:E:775:ARG:HD3  | 1.82                     | 0.41              |
| 3:J:158:LYS:CB   | 3:J:197:LEU:HD21 | 2.50                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:282:LEU:HB2  | 3:J:292:LEU:HD11 | 2.02                     | 0.41              |
| 3:J:348:ARG:O    | 3:J:351:PHE:N    | 2.53                     | 0.41              |
| 1:B:553:LEU:O    | 1:B:555:GLU:N    | 2.48                     | 0.41              |
| 1:B:583:SER:O    | 1:B:583:SER:OG   | 2.36                     | 0.41              |
| 1:C:475:ASP:O    | 1:C:479:GLN:N    | 2.53                     | 0.41              |
| 1:D:575:GLN:OE1  | 1:D:575:GLN:CA   | 2.68                     | 0.41              |
| 1:D:837:ASN:ND2  | 1:D:845:LEU:O    | 2.53                     | 0.41              |
| 4:E:901:AGS:O1A  | 1:F:332:ARG:NH1  | 2.54                     | 0.41              |
| 1:F:636:MET:HB2  | 1:F:680:GLU:O    | 2.20                     | 0.41              |
| 1:F:780:ARG:O    | 1:F:781:LEU:HD23 | 2.20                     | 0.41              |
| 3:I:238:LEU:HB3  | 3:I:358:THR:HG21 | 2.02                     | 0.41              |
| 3:J:73:VAL:HG21  | 3:J:400:ASP:HB3  | 2.01                     | 0.41              |
| 3:K:375:THR:HA   | 3:K:380:VAL:HG21 | 2.03                     | 0.41              |
| 1:B:245:MET:HE1  | 1:B:259:LEU:HD13 | 2.03                     | 0.41              |
| 1:B:418:ARG:HG2  | 1:B:421:ARG:NH2  | 2.35                     | 0.41              |
| 1:C:681:ILE:HG22 | 1:C:720:SER:HB2  | 2.02                     | 0.41              |
| 4:D:902:AGS:O2B  | 4:D:902:AGS:O2A  | 2.38                     | 0.41              |
| 1:E:278:ASP:OD1  | 1:E:278:ASP:N    | 2.50                     | 0.41              |
| 1:F:355:LYS:HB2  | 1:F:366:ILE:HD11 | 2.02                     | 0.41              |
| 3:I:70:THR:HG23  | 3:I:232:GLY:HA3  | 2.02                     | 0.41              |
| 3:I:269:TRP:CE3  | 3:I:270:LEU:HD23 | 2.56                     | 0.41              |
| 3:I:348:ARG:O    | 3:I:351:PHE:N    | 2.53                     | 0.41              |
| 3:J:398:ASN:O    | 3:J:401:GLU:N    | 2.53                     | 0.41              |
| 1:A:463:TRP:O    | 1:A:463:TRP:CG   | 2.74                     | 0.41              |
| 1:D:254:GLU:O    | 1:D:257:GLU:HG2  | 2.20                     | 0.41              |
| 1:D:358:TYR:CE1  | 1:E:197:ARG:HD3  | 2.55                     | 0.41              |
| 1:E:400:SER:OG   | 1:F:192:GLN:O    | 2.36                     | 0.41              |
| 1:F:784:GLN:O    | 1:F:835:PRO:HA   | 2.21                     | 0.41              |
| 3:I:175:THR:HG21 | 3:I:403:VAL:CG1  | 2.50                     | 0.41              |
| 3:I:238:LEU:O    | 3:I:249:ARG:N    | 2.52                     | 0.41              |
| 3:I:257:LEU:HD11 | 3:I:262:TRP:HE1  | 1.84                     | 0.41              |
| 1:A:496:LEU:HD11 | 3:I:316:ILE:HG23 | 2.01                     | 0.41              |
| 1:B:316:THR:HG21 | 1:C:329:ALA:HB2  | 2.03                     | 0.41              |
| 1:D:243:GLY:O    | 1:D:247:ALA:HB2  | 2.21                     | 0.41              |
| 1:D:300:ILE:O    | 1:D:300:ILE:CG1  | 2.68                     | 0.41              |
| 1:D:620:LEU:O    | 1:D:624:LEU:HD23 | 2.19                     | 0.41              |
| 1:D:631:MET:HE1  | 1:D:677:LEU:HD13 | 2.02                     | 0.41              |
| 1:E:260:LYS:HA   | 1:E:260:LYS:HD2  | 1.81                     | 0.41              |
| 1:F:836:VAL:HG23 | 1:F:845:LEU:HD23 | 2.02                     | 0.41              |
| 3:I:319:ASP:CG   | 3:I:325:LEU:CG   | 2.71                     | 0.41              |
| 3:J:229:LEU:HD23 | 3:J:374:SER:CB   | 2.50                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:238:LEU:HB3  | 3:J:358:THR:HG21 | 2.02                     | 0.41              |
| 3:K:73:VAL:HG21  | 3:K:400:ASP:HB3  | 2.01                     | 0.41              |
| 3:K:282:LEU:HB2  | 3:K:292:LEU:HD11 | 2.02                     | 0.41              |
| 1:B:342:PRO:N    | 1:B:387:LEU:HD12 | 2.35                     | 0.41              |
| 1:B:826:GLY:C    | 1:B:828:VAL:H    | 2.28                     | 0.41              |
| 3:I:73:VAL:HG21  | 3:I:400:ASP:HB3  | 2.01                     | 0.41              |
| 3:I:365:ILE:HG22 | 3:I:391:LYS:HE2  | 2.01                     | 0.41              |
| 3:K:122:ARG:NH2  | 3:K:140:ASP:OD2  | 2.53                     | 0.41              |
| 3:K:398:ASN:O    | 3:K:401:GLU:N    | 2.54                     | 0.41              |
| 1:A:636:MET:HG3  | 1:A:681:ILE:HD12 | 2.03                     | 0.41              |
| 1:B:393:ASP:OD2  | 1:C:335:GLN:NE2  | 2.52                     | 0.41              |
| 1:B:412:GLU:O    | 1:B:413:ILE:HD13 | 2.21                     | 0.41              |
| 1:C:496:LEU:HD21 | 3:K:316:ILE:CG2  | 2.48                     | 0.41              |
| 1:E:604:MET:HB2  | 1:E:718:LEU:O    | 2.21                     | 0.41              |
| 1:E:779:ARG:O    | 1:E:830:ASP:HB3  | 2.20                     | 0.41              |
| 3:I:65:ILE:HB    | 3:I:174:ILE:HG12 | 2.03                     | 0.41              |
| 3:I:124:VAL:HG11 | 3:I:149:ILE:HG21 | 2.03                     | 0.41              |
| 3:I:375:THR:HA   | 3:I:380:VAL:HG21 | 2.03                     | 0.41              |
| 3:J:65:ILE:HB    | 3:J:174:ILE:HG12 | 2.03                     | 0.41              |
| 3:J:70:THR:HG23  | 3:J:232:GLY:HA3  | 2.02                     | 0.41              |
| 3:J:124:VAL:HG11 | 3:J:149:ILE:HG21 | 2.03                     | 0.41              |
| 3:J:375:THR:HA   | 3:J:380:VAL:HG21 | 2.03                     | 0.41              |
| 1:A:600:THR:O    | 1:A:600:THR:OG1  | 2.37                     | 0.41              |
| 1:A:691:VAL:O    | 1:A:695:VAL:HG23 | 2.21                     | 0.41              |
| 1:C:355:LYS:HE2  | 1:C:355:LYS:HB3  | 1.93                     | 0.41              |
| 1:D:237:ILE:HA   | 1:D:274:ILE:O    | 2.21                     | 0.41              |
| 1:D:365:ARG:HB2  | 1:D:532:GLU:HB2  | 2.02                     | 0.41              |
| 1:D:822:MET:HG3  | 1:D:827:GLN:NE2  | 2.35                     | 0.41              |
| 1:E:235:LYS:HD2  | 1:E:272:GLN:HB2  | 2.03                     | 0.41              |
| 1:F:575:GLN:O    | 1:F:579:VAL:HG22 | 2.21                     | 0.41              |
| 1:F:823:LEU:HD12 | 1:F:823:LEU:HA   | 1.87                     | 0.41              |
| 3:I:75:SER:O     | 3:I:408:ALA:HB2  | 2.21                     | 0.41              |
| 3:J:75:SER:O     | 3:J:408:ALA:HB2  | 2.21                     | 0.41              |
| 3:J:337:GLN:HG2  | 3:J:379:ALA:HB2  | 2.03                     | 0.41              |
| 1:A:496:LEU:HD21 | 3:I:316:ILE:HD13 | 2.03                     | 0.41              |
| 1:A:533:VAL:O    | 1:A:533:VAL:CG2  | 2.68                     | 0.41              |
| 1:A:643:HIS:HB2  | 1:B:655:TYR:OH   | 2.21                     | 0.41              |
| 1:B:277:ILE:O    | 1:B:313:GLY:HA2  | 2.21                     | 0.41              |
| 1:B:597:ASN:OD1  | 1:B:597:ASN:N    | 2.53                     | 0.41              |
| 1:B:675:VAL:HG23 | 1:B:715:ILE:HB   | 2.01                     | 0.41              |
| 1:C:543:SER:O    | 1:C:547:GLY:HA2  | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:787:LEU:HD23 | 1:C:787:LEU:HA   | 1.88                     | 0.41              |
| 1:E:352:ARG:HE   | 1:E:352:ARG:HB3  | 1.68                     | 0.41              |
| 1:E:613:LYS:HB2  | 1:E:613:LYS:HE3  | 1.84                     | 0.41              |
| 1:F:641:GLU:HG3  | 1:F:643:HIS:CE1  | 2.56                     | 0.41              |
| 3:I:210:ALA:HB2  | 3:I:224:ILE:HG21 | 2.03                     | 0.41              |
| 3:J:139:ILE:CG2  | 3:J:144:TYR:CE2  | 3.04                     | 0.41              |
| 3:J:238:LEU:HD12 | 3:J:354:VAL:HG12 | 2.03                     | 0.41              |
| 3:J:269:TRP:CE3  | 3:J:270:LEU:HD23 | 2.56                     | 0.41              |
| 3:K:210:ALA:HB2  | 3:K:224:ILE:HG21 | 2.03                     | 0.41              |
| 3:K:306:SER:OG   | 3:K:308:SER:O    | 2.37                     | 0.41              |
| 1:B:752:ILE:HD13 | 1:B:752:ILE:HA   | 1.93                     | 0.41              |
| 1:C:545:TRP:CD1  | 1:C:546:THR:HG23 | 2.56                     | 0.41              |
| 1:C:820:ALA:O    | 1:C:824:LEU:HG   | 2.21                     | 0.41              |
| 1:E:824:LEU:HD12 | 1:F:591:ALA:HB2  | 2.02                     | 0.41              |
| 3:I:65:ILE:HG23  | 3:I:74:VAL:HG22  | 2.03                     | 0.41              |
| 3:J:174:ILE:H    | 3:J:199:VAL:HG13 | 1.86                     | 0.41              |
| 3:K:107:LEU:HD13 | 3:K:111:PRO:O    | 2.21                     | 0.41              |
| 3:K:174:ILE:H    | 3:K:199:VAL:HG13 | 1.86                     | 0.41              |
| 3:K:269:TRP:CE3  | 3:K:270:LEU:HD23 | 2.55                     | 0.41              |
| 1:A:500:ALA:HB1  | 1:A:504:TYR:HD2  | 1.86                     | 0.40              |
| 1:B:374:ALA:HA   | 1:B:538:ILE:HG21 | 2.02                     | 0.40              |
| 1:C:472:ILE:O    | 1:C:474:ARG:N    | 2.54                     | 0.40              |
| 1:C:759:GLU:OE1  | 1:C:759:GLU:N    | 2.46                     | 0.40              |
| 1:E:368:ASP:O    | 1:E:372:VAL:HG12 | 2.21                     | 0.40              |
| 1:F:311:LEU:O    | 1:F:311:LEU:CG   | 2.70                     | 0.40              |
| 3:I:282:LEU:HB2  | 3:I:292:LEU:HD11 | 2.03                     | 0.40              |
| 3:J:65:ILE:HG23  | 3:J:74:VAL:HG22  | 2.03                     | 0.40              |
| 3:J:209:ALA:CB   | 3:J:371:VAL:HG11 | 2.51                     | 0.40              |
| 3:K:269:TRP:CZ3  | 3:K:270:LEU:HD23 | 2.57                     | 0.40              |
| 1:A:322:LYS:HB3  | 1:A:323:HIS:HD2  | 1.86                     | 0.40              |
| 1:A:327:ASP:O    | 1:A:329:ALA:N    | 2.54                     | 0.40              |
| 1:A:697:ASP:OD2  | 1:F:805:ARG:NH1  | 2.54                     | 0.40              |
| 1:D:593:VAL:HG23 | 1:D:593:VAL:O    | 2.21                     | 0.40              |
| 1:E:213:THR:HG23 | 4:E:901:AGS:O2B  | 2.20                     | 0.40              |
| 1:E:253:GLY:C    | 1:E:255:PHE:H    | 2.29                     | 0.40              |
| 1:F:739:PHE:HB2  | 1:F:744:ILE:HD11 | 2.04                     | 0.40              |
| 3:I:174:ILE:H    | 3:I:199:VAL:HG13 | 1.86                     | 0.40              |
| 3:I:348:ARG:HG3  | 3:I:387:LEU:HD21 | 2.02                     | 0.40              |
| 3:K:337:GLN:HG2  | 3:K:379:ALA:HB2  | 2.03                     | 0.40              |
| 1:C:246:VAL:HG12 | 1:C:246:VAL:O    | 2.20                     | 0.40              |
| 1:C:500:ALA:HB1  | 1:C:504:TYR:HD2  | 1.86                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:334:PHE:HD1  | 1:E:334:PHE:HA   | 1.80                     | 0.40              |
| 1:E:609:THR:OG1  | 1:E:610:GLY:N    | 2.54                     | 0.40              |
| 3:J:122:ARG:NH2  | 3:J:140:ASP:OD2  | 2.53                     | 0.40              |
| 3:J:210:ALA:HB2  | 3:J:224:ILE:HG21 | 2.03                     | 0.40              |
| 3:K:139:ILE:CG2  | 3:K:144:TYR:CE2  | 3.04                     | 0.40              |
| 1:B:478:GLU:O    | 1:B:481:GLU:HB2  | 2.20                     | 0.40              |
| 1:B:766:ASP:OD1  | 1:B:790:LYS:HD3  | 2.20                     | 0.40              |
| 1:D:666:GLU:OE1  | 1:D:669:ARG:NH1  | 2.54                     | 0.40              |
| 1:E:534:GLY:H    | 1:E:537:ASP:CB   | 2.34                     | 0.40              |
| 1:F:183:ARG:O    | 1:F:187:ILE:HG12 | 2.21                     | 0.40              |
| 1:F:761:LEU:HD12 | 1:F:798:PHE:HD1  | 1.86                     | 0.40              |
| 3:I:139:ILE:CG2  | 3:I:144:TYR:CE2  | 3.04                     | 0.40              |
| 3:I:238:LEU:HD12 | 3:I:354:VAL:HG12 | 2.03                     | 0.40              |
| 3:I:325:LEU:HD23 | 3:I:325:LEU:HA   | 1.85                     | 0.40              |
| 3:I:398:ASN:O    | 3:I:401:GLU:N    | 2.54                     | 0.40              |
| 1:A:575:GLN:O    | 1:A:579:VAL:HG23 | 2.22                     | 0.40              |
| 1:D:184:ASP:OD1  | 1:D:185:ASN:N    | 2.54                     | 0.40              |
| 1:E:212:LYS:HG3  | 4:E:901:AGS:PB   | 2.62                     | 0.40              |
| 1:E:729:GLU:H    | 1:E:729:GLU:CD   | 2.29                     | 0.40              |
| 3:K:75:SER:O     | 3:K:408:ALA:HB2  | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | A     | 668/848 (79%) | 590 (88%) | 76 (11%) | 2 (0%)   | 36          | 72 |
| 1   | B     | 666/848 (78%) | 605 (91%) | 60 (9%)  | 1 (0%)   | 43          | 78 |
| 1   | C     | 669/848 (79%) | 592 (88%) | 72 (11%) | 5 (1%)   | 18          | 56 |
| 1   | D     | 556/848 (66%) | 480 (86%) | 75 (14%) | 1 (0%)   | 43          | 78 |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | E     | 540/848 (64%)   | 477 (88%)  | 62 (12%)  | 1 (0%)   | 43          | 78 |
| 1   | F     | 538/848 (63%)   | 472 (88%)  | 65 (12%)  | 1 (0%)   | 43          | 78 |
| 3   | I     | 355/625 (57%)   | 318 (90%)  | 34 (10%)  | 3 (1%)   | 16          | 54 |
| 3   | J     | 355/625 (57%)   | 318 (90%)  | 33 (9%)   | 4 (1%)   | 11          | 46 |
| 3   | K     | 355/625 (57%)   | 317 (89%)  | 34 (10%)  | 4 (1%)   | 11          | 46 |
| All | All   | 4702/6963 (68%) | 4169 (89%) | 511 (11%) | 22 (0%)  | 26          | 63 |

All (22) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 466 | GLU  |
| 1   | B     | 388 | PRO  |
| 1   | C     | 516 | ALA  |
| 3   | I     | 315 | TYR  |
| 3   | I     | 322 | LYS  |
| 3   | J     | 217 | LYS  |
| 3   | J     | 315 | TYR  |
| 3   | K     | 221 | GLU  |
| 3   | K     | 315 | TYR  |
| 3   | K     | 322 | LYS  |
| 1   | C     | 547 | GLY  |
| 1   | C     | 473 | VAL  |
| 1   | C     | 478 | GLU  |
| 1   | F     | 235 | LYS  |
| 1   | A     | 465 | ASN  |
| 1   | E     | 566 | ASP  |
| 3   | J     | 324 | PRO  |
| 3   | J     | 138 | GLU  |
| 3   | K     | 138 | GLU  |
| 1   | C     | 472 | ILE  |
| 1   | D     | 302 | PRO  |
| 3   | I     | 324 | PRO  |

### 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     | 549/682 (80%)   | 540 (98%)  | 9 (2%)   | 55          | 70 |
| 1   | B     | 547/682 (80%)   | 541 (99%)  | 6 (1%)   | 65          | 76 |
| 1   | C     | 548/682 (80%)   | 537 (98%)  | 11 (2%)  | 48          | 66 |
| 1   | D     | 455/682 (67%)   | 449 (99%)  | 6 (1%)   | 61          | 74 |
| 1   | E     | 448/682 (66%)   | 445 (99%)  | 3 (1%)   | 76          | 81 |
| 1   | F     | 448/682 (66%)   | 446 (100%) | 2 (0%)   | 84          | 84 |
| 3   | I     | 291/500 (58%)   | 286 (98%)  | 5 (2%)   | 53          | 69 |
| 3   | J     | 291/500 (58%)   | 288 (99%)  | 3 (1%)   | 68          | 78 |
| 3   | K     | 291/500 (58%)   | 288 (99%)  | 3 (1%)   | 68          | 78 |
| All | All   | 3868/5592 (69%) | 3820 (99%) | 48 (1%)  | 61          | 75 |

All (48) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 444 | LYS  |
| 1   | A     | 459 | LEU  |
| 1   | A     | 464 | GLN  |
| 1   | A     | 466 | GLU  |
| 1   | A     | 527 | VAL  |
| 1   | A     | 529 | LEU  |
| 1   | A     | 530 | LYS  |
| 1   | A     | 533 | VAL  |
| 1   | A     | 738 | THR  |
| 1   | B     | 388 | PRO  |
| 1   | B     | 461 | THR  |
| 1   | B     | 467 | LYS  |
| 1   | B     | 473 | VAL  |
| 1   | B     | 600 | THR  |
| 1   | B     | 674 | THR  |
| 1   | C     | 166 | THR  |
| 1   | C     | 461 | THR  |
| 1   | C     | 472 | ILE  |
| 1   | C     | 473 | VAL  |
| 1   | C     | 474 | ARG  |
| 1   | C     | 476 | LEU  |
| 1   | C     | 477 | LYS  |
| 1   | C     | 478 | GLU  |
| 1   | C     | 509 | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 510 | VAL  |
| 1   | C     | 513 | LYS  |
| 1   | D     | 275 | THR  |
| 1   | D     | 300 | ILE  |
| 1   | D     | 303 | MET  |
| 1   | D     | 333 | ARG  |
| 1   | D     | 576 | LYS  |
| 1   | D     | 644 | THR  |
| 1   | E     | 210 | VAL  |
| 1   | E     | 275 | THR  |
| 1   | E     | 802 | TYR  |
| 1   | F     | 311 | LEU  |
| 1   | F     | 738 | THR  |
| 3   | I     | 138 | GLU  |
| 3   | I     | 142 | LYS  |
| 3   | I     | 217 | LYS  |
| 3   | I     | 317 | THR  |
| 3   | I     | 318 | VAL  |
| 3   | J     | 138 | GLU  |
| 3   | J     | 142 | LYS  |
| 3   | J     | 317 | THR  |
| 3   | K     | 138 | GLU  |
| 3   | K     | 142 | LYS  |
| 3   | K     | 217 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 268 | ASN  |
| 1   | A     | 281 | HIS  |
| 1   | A     | 323 | HIS  |
| 1   | A     | 361 | HIS  |
| 1   | A     | 705 | HIS  |
| 1   | A     | 784 | GLN  |
| 1   | A     | 818 | GLN  |
| 1   | B     | 221 | GLN  |
| 1   | B     | 361 | HIS  |
| 1   | B     | 362 | HIS  |
| 1   | B     | 479 | GLN  |
| 1   | B     | 575 | GLN  |
| 1   | B     | 685 | HIS  |
| 1   | B     | 705 | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 812 | GLN  |
| 1   | C     | 221 | GLN  |
| 1   | C     | 323 | HIS  |
| 1   | C     | 520 | GLN  |
| 1   | C     | 643 | HIS  |
| 1   | C     | 685 | HIS  |
| 1   | C     | 705 | HIS  |
| 1   | C     | 721 | ASN  |
| 1   | C     | 730 | GLN  |
| 1   | C     | 757 | ASN  |
| 1   | C     | 818 | GLN  |
| 1   | C     | 827 | GLN  |
| 1   | D     | 298 | ASN  |
| 1   | D     | 685 | HIS  |
| 1   | D     | 782 | GLN  |
| 1   | D     | 827 | GLN  |
| 1   | E     | 201 | ASN  |
| 1   | E     | 272 | GLN  |
| 1   | E     | 281 | HIS  |
| 1   | E     | 362 | HIS  |
| 1   | E     | 685 | HIS  |
| 1   | E     | 730 | GLN  |
| 1   | E     | 778 | GLN  |
| 1   | E     | 784 | GLN  |
| 1   | E     | 818 | GLN  |
| 1   | E     | 829 | HIS  |
| 1   | F     | 268 | ASN  |
| 1   | F     | 771 | GLN  |
| 3   | I     | 114 | ASN  |
| 3   | I     | 290 | GLN  |
| 3   | I     | 330 | GLN  |
| 3   | I     | 394 | ASN  |
| 3   | J     | 114 | ASN  |
| 3   | J     | 290 | GLN  |
| 3   | J     | 330 | GLN  |
| 3   | J     | 394 | ASN  |
| 3   | K     | 114 | ASN  |
| 3   | K     | 181 | ASN  |
| 3   | K     | 290 | GLN  |
| 3   | K     | 330 | GLN  |
| 3   | K     | 394 | ASN  |



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | ADP  | F     | 902 | -    | 28,29,29     | 1.40 | 5 (17%)  | 43,45,45    | 1.81 | 8 (18%)  |
| 4   | AGS  | C     | 901 | -    | 32,33,33     | 0.75 | 2 (6%)   | 45,52,52    | 0.73 | 1 (2%)   |
| 4   | AGS  | F     | 901 | -    | 32,33,33     | 0.62 | 1 (3%)   | 45,52,52    | 0.71 | 1 (2%)   |
| 4   | AGS  | B     | 901 | -    | 32,33,33     | 0.84 | 3 (9%)   | 45,52,52    | 0.79 | 1 (2%)   |
| 4   | AGS  | A     | 902 | -    | 32,33,33     | 0.81 | 3 (9%)   | 45,52,52    | 0.81 | 1 (2%)   |
| 4   | AGS  | A     | 901 | -    | 32,33,33     | 0.76 | 2 (6%)   | 45,52,52    | 0.76 | 1 (2%)   |
| 4   | AGS  | D     | 902 | -    | 32,33,33     | 0.57 | 1 (3%)   | 45,52,52    | 0.72 | 1 (2%)   |
| 4   | AGS  | E     | 901 | -    | 32,33,33     | 2.04 | 6 (18%)  | 45,52,52    | 1.89 | 10 (22%) |
| 4   | AGS  | D     | 901 | -    | 32,33,33     | 0.76 | 1 (3%)   | 45,52,52    | 0.75 | 1 (2%)   |
| 5   | ADP  | E     | 902 | -    | 28,29,29     | 0.54 | 0        | 43,45,45    | 0.60 | 0        |
| 4   | AGS  | B     | 902 | -    | 32,33,33     | 0.81 | 4 (12%)  | 45,52,52    | 0.81 | 1 (2%)   |
| 4   | AGS  | C     | 902 | -    | 32,33,33     | 0.83 | 3 (9%)   | 45,52,52    | 0.78 | 1 (2%)   |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | ADP  | F     | 902 | -    | -       | 0/16/32/32 | 0/3/3/3 |
| 4   | AGS  | C     | 901 | -    | -       | 4/21/38/38 | 0/3/3/3 |
| 4   | AGS  | F     | 901 | -    | -       | 7/21/38/38 | 0/3/3/3 |
| 4   | AGS  | B     | 901 | -    | -       | 4/21/38/38 | 0/3/3/3 |
| 4   | AGS  | A     | 902 | -    | -       | 5/21/38/38 | 0/3/3/3 |
| 4   | AGS  | A     | 901 | -    | -       | 5/21/38/38 | 0/3/3/3 |
| 4   | AGS  | D     | 902 | -    | -       | 3/21/38/38 | 0/3/3/3 |
| 4   | AGS  | E     | 901 | -    | -       | 2/21/38/38 | 0/3/3/3 |
| 4   | AGS  | D     | 901 | -    | -       | 6/21/38/38 | 0/3/3/3 |
| 5   | ADP  | E     | 902 | -    | -       | 7/16/32/32 | 0/3/3/3 |
| 4   | AGS  | B     | 902 | -    | -       | 5/21/38/38 | 0/3/3/3 |
| 4   | AGS  | C     | 902 | -    | -       | 2/21/38/38 | 0/3/3/3 |

All (31) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | E     | 901 | AGS  | PG-S1G | 7.96  | 2.07        | 1.90     |
| 4   | E     | 901 | AGS  | C5-C4  | 4.74  | 1.47        | 1.39     |
| 5   | F     | 902 | ADP  | C5-C4  | 4.66  | 1.47        | 1.39     |
| 4   | E     | 901 | AGS  | C5-C6  | 2.78  | 1.48        | 1.41     |
| 4   | B     | 901 | AGS  | PB-O3A | -2.75 | 1.56        | 1.59     |
| 5   | F     | 902 | ADP  | C5-C6  | 2.54  | 1.48        | 1.41     |
| 4   | C     | 902 | AGS  | PB-O3A | -2.50 | 1.56        | 1.59     |
| 5   | F     | 902 | ADP  | C5-N7  | -2.42 | 1.34        | 1.39     |
| 4   | A     | 902 | AGS  | PB-O3A | -2.41 | 1.56        | 1.59     |
| 4   | C     | 902 | AGS  | PA-O3A | -2.38 | 1.56        | 1.59     |
| 4   | E     | 901 | AGS  | C8-N7  | 2.34  | 1.36        | 1.31     |
| 4   | B     | 901 | AGS  | PA-O3A | -2.33 | 1.57        | 1.59     |
| 5   | F     | 902 | ADP  | C8-N7  | 2.31  | 1.36        | 1.31     |
| 4   | A     | 901 | AGS  | PB-O3A | -2.29 | 1.57        | 1.59     |
| 4   | E     | 901 | AGS  | C5-N7  | -2.21 | 1.35        | 1.39     |
| 4   | B     | 902 | AGS  | PB-O3B | -2.17 | 1.57        | 1.59     |
| 4   | A     | 901 | AGS  | PA-O3A | -2.14 | 1.57        | 1.59     |
| 4   | A     | 902 | AGS  | PB-O3B | -2.13 | 1.57        | 1.59     |
| 4   | C     | 901 | AGS  | PB-O3A | -2.13 | 1.57        | 1.59     |
| 4   | B     | 902 | AGS  | PA-O3A | -2.12 | 1.57        | 1.59     |
| 4   | D     | 901 | AGS  | PB-O3A | -2.11 | 1.57        | 1.59     |
| 4   | A     | 902 | AGS  | PG-S1G | 2.11  | 1.95        | 1.90     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | B     | 902 | AGS  | PB-O3A | -2.10 | 1.57        | 1.59     |
| 4   | C     | 902 | AGS  | PG-S1G | 2.10  | 1.95        | 1.90     |
| 4   | F     | 901 | AGS  | PG-S1G | 2.09  | 1.95        | 1.90     |
| 4   | E     | 901 | AGS  | PG-O2G | 2.08  | 1.61        | 1.54     |
| 4   | C     | 901 | AGS  | PA-O3A | -2.08 | 1.57        | 1.59     |
| 4   | D     | 902 | AGS  | PG-S1G | 2.06  | 1.95        | 1.90     |
| 4   | B     | 901 | AGS  | PG-S1G | 2.03  | 1.95        | 1.90     |
| 4   | B     | 902 | AGS  | PG-S1G | 2.02  | 1.95        | 1.90     |
| 5   | F     | 902 | ADP  | C4-N9  | -2.01 | 1.33        | 1.37     |

All (27) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | E     | 901 | AGS  | C5-C4-N3    | -5.86 | 118.64      | 126.72   |
| 5   | F     | 902 | ADP  | C5-C4-N3    | -5.65 | 118.94      | 126.72   |
| 4   | E     | 901 | AGS  | N3-C4-N9    | 4.62  | 135.02      | 127.17   |
| 5   | F     | 902 | ADP  | N3-C4-N9    | 4.52  | 134.86      | 127.17   |
| 4   | C     | 902 | AGS  | PB-O3B-PG   | -4.40 | 117.07      | 133.17   |
| 4   | B     | 902 | AGS  | PB-O3B-PG   | -4.39 | 117.10      | 133.17   |
| 4   | B     | 901 | AGS  | PB-O3B-PG   | -4.39 | 117.12      | 133.17   |
| 4   | A     | 902 | AGS  | PB-O3B-PG   | -4.38 | 117.16      | 133.17   |
| 4   | D     | 901 | AGS  | PB-O3B-PG   | -4.34 | 117.30      | 133.17   |
| 4   | A     | 901 | AGS  | PB-O3B-PG   | -4.17 | 117.90      | 133.17   |
| 4   | F     | 901 | AGS  | PB-O3B-PG   | -4.05 | 118.36      | 133.17   |
| 4   | C     | 901 | AGS  | PB-O3B-PG   | -3.91 | 118.87      | 133.17   |
| 4   | D     | 902 | AGS  | PB-O3B-PG   | -3.88 | 118.97      | 133.17   |
| 4   | E     | 901 | AGS  | C2-N3-C4    | 3.71  | 120.90      | 111.83   |
| 5   | F     | 902 | ADP  | C2-N3-C4    | 3.55  | 120.51      | 111.83   |
| 4   | E     | 901 | AGS  | C4-C5-N7    | -3.50 | 106.58      | 110.58   |
| 4   | E     | 901 | AGS  | PB-O3B-PG   | -3.47 | 120.46      | 133.17   |
| 5   | F     | 902 | ADP  | C4-C5-N7    | -3.30 | 106.81      | 110.58   |
| 4   | E     | 901 | AGS  | N3-C2-N1    | -3.22 | 123.70      | 128.58   |
| 5   | F     | 902 | ADP  | N3-C2-N1    | -3.18 | 123.77      | 128.58   |
| 5   | F     | 902 | ADP  | C4-N9-C8    | 2.68  | 108.56      | 105.74   |
| 4   | E     | 901 | AGS  | C4-N9-C8    | 2.59  | 108.45      | 105.74   |
| 4   | E     | 901 | AGS  | C5-N7-C8    | 2.53  | 107.43      | 103.45   |
| 4   | E     | 901 | AGS  | C3'-C2'-C1' | 2.48  | 106.14      | 101.46   |
| 5   | F     | 902 | ADP  | C5-N7-C8    | 2.41  | 107.24      | 103.45   |
| 5   | F     | 902 | ADP  | C3'-C2'-C1' | 2.35  | 105.90      | 101.46   |
| 4   | E     | 901 | AGS  | C6-C5-N7    | 2.09  | 136.12      | 132.09   |

There are no chirality outliers.

All (50) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | A     | 901 | AGS  | PB-O3B-PG-O2G   |
| 4   | A     | 901 | AGS  | PB-O3B-PG-O3G   |
| 4   | A     | 901 | AGS  | C5'-O5'-PA-O1A  |
| 4   | A     | 901 | AGS  | C5'-O5'-PA-O2A  |
| 4   | A     | 901 | AGS  | C5'-O5'-PA-O3A  |
| 4   | A     | 902 | AGS  | C5'-O5'-PA-O1A  |
| 4   | A     | 902 | AGS  | C5'-O5'-PA-O2A  |
| 4   | A     | 902 | AGS  | C5'-O5'-PA-O3A  |
| 4   | B     | 901 | AGS  | PB-O3B-PG-O2G   |
| 4   | B     | 901 | AGS  | PB-O3B-PG-O3G   |
| 4   | B     | 902 | AGS  | PB-O3B-PG-O2G   |
| 4   | B     | 902 | AGS  | PB-O3B-PG-O3G   |
| 4   | B     | 902 | AGS  | C5'-O5'-PA-O1A  |
| 4   | C     | 901 | AGS  | PB-O3B-PG-O2G   |
| 4   | C     | 901 | AGS  | PB-O3B-PG-O3G   |
| 4   | D     | 901 | AGS  | PB-O3B-PG-O2G   |
| 4   | D     | 901 | AGS  | PB-O3B-PG-O3G   |
| 4   | D     | 901 | AGS  | C5'-O5'-PA-O2A  |
| 4   | D     | 902 | AGS  | PB-O3B-PG-O2G   |
| 4   | D     | 902 | AGS  | PB-O3B-PG-O3G   |
| 4   | D     | 902 | AGS  | C5'-O5'-PA-O1A  |
| 4   | F     | 901 | AGS  | PB-O3B-PG-O2G   |
| 4   | F     | 901 | AGS  | PB-O3B-PG-O3G   |
| 4   | F     | 901 | AGS  | O4'-C4'-C5'-O5' |
| 5   | E     | 902 | ADP  | C5'-O5'-PA-O2A  |
| 5   | E     | 902 | ADP  | C5'-O5'-PA-O3A  |
| 4   | B     | 901 | AGS  | O4'-C4'-C5'-O5' |
| 4   | B     | 902 | AGS  | C3'-C4'-C5'-O5' |
| 4   | F     | 901 | AGS  | C3'-C4'-C5'-O5' |
| 4   | C     | 902 | AGS  | O4'-C4'-C5'-O5' |
| 4   | B     | 902 | AGS  | O4'-C4'-C5'-O5' |
| 5   | E     | 902 | ADP  | O4'-C4'-C5'-O5' |
| 4   | B     | 901 | AGS  | C3'-C4'-C5'-O5' |
| 4   | C     | 902 | AGS  | C3'-C4'-C5'-O5' |
| 4   | D     | 901 | AGS  | O4'-C4'-C5'-O5' |
| 4   | D     | 901 | AGS  | C5'-O5'-PA-O1A  |
| 4   | D     | 901 | AGS  | C5'-O5'-PA-O3A  |
| 4   | F     | 901 | AGS  | C5'-O5'-PA-O1A  |
| 4   | F     | 901 | AGS  | C5'-O5'-PA-O2A  |
| 4   | F     | 901 | AGS  | C5'-O5'-PA-O3A  |
| 5   | E     | 902 | ADP  | C5'-O5'-PA-O1A  |
| 4   | A     | 902 | AGS  | PA-O3A-PB-O2B   |

*Continued on next page...*

*Continued from previous page...*

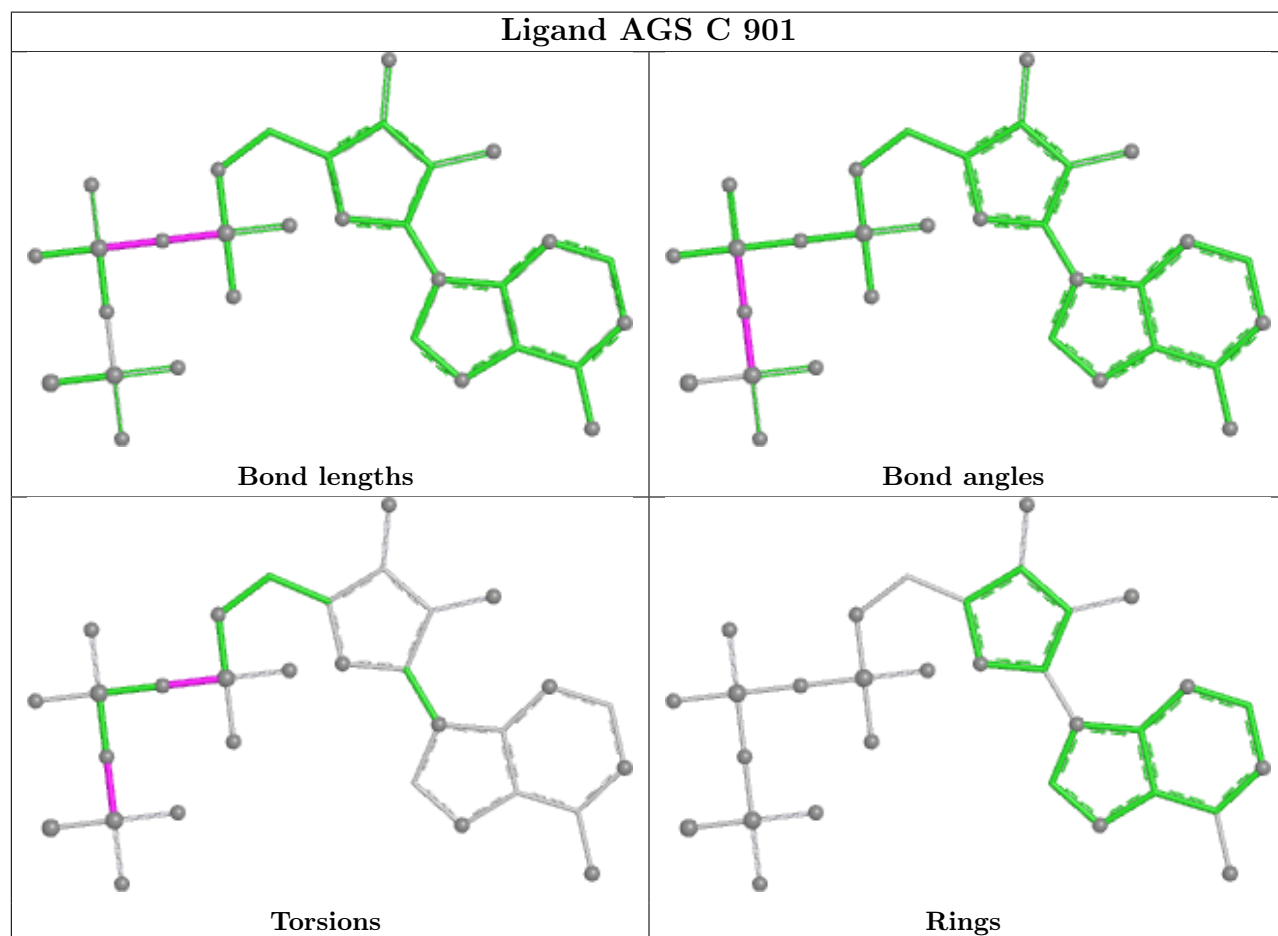
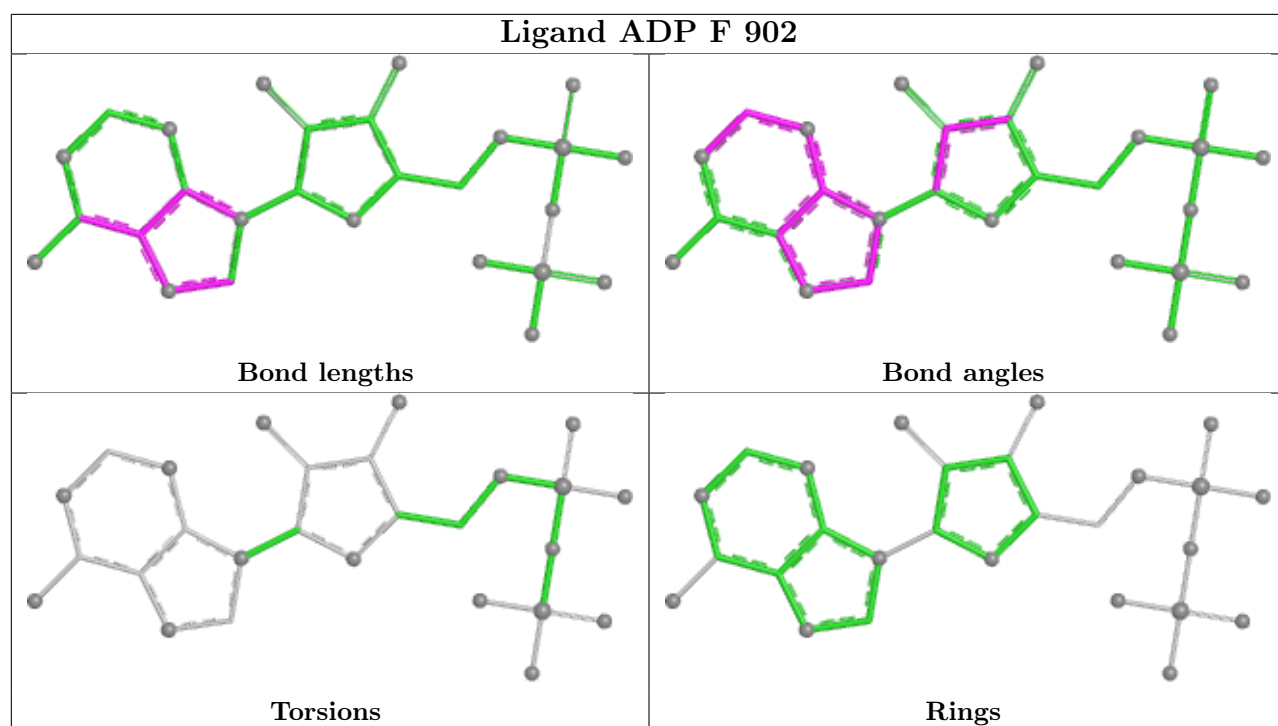
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | E     | 902 | ADP  | C2'-C1'-N9-C8   |
| 4   | C     | 901 | AGS  | PB-O3A-PA-O2A   |
| 5   | E     | 902 | ADP  | C2'-C1'-N9-C4   |
| 4   | A     | 902 | AGS  | PA-O3A-PB-O1B   |
| 4   | C     | 901 | AGS  | PB-O3A-PA-O1A   |
| 4   | E     | 901 | AGS  | PA-O3A-PB-O1B   |
| 4   | E     | 901 | AGS  | PA-O3A-PB-O2B   |
| 5   | E     | 902 | ADP  | C3'-C4'-C5'-O5' |

There are no ring outliers.

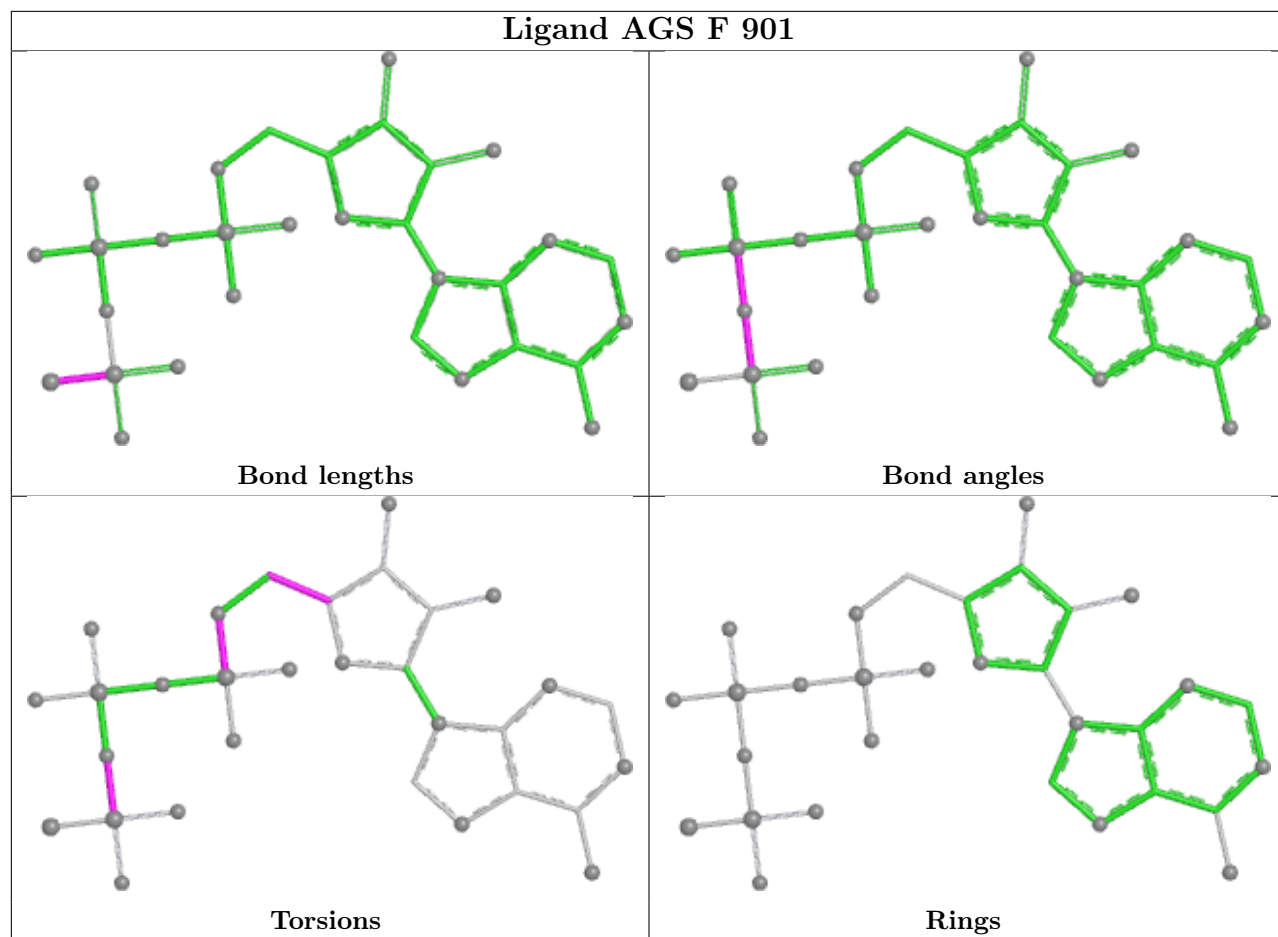
12 monomers are involved in 59 short contacts:

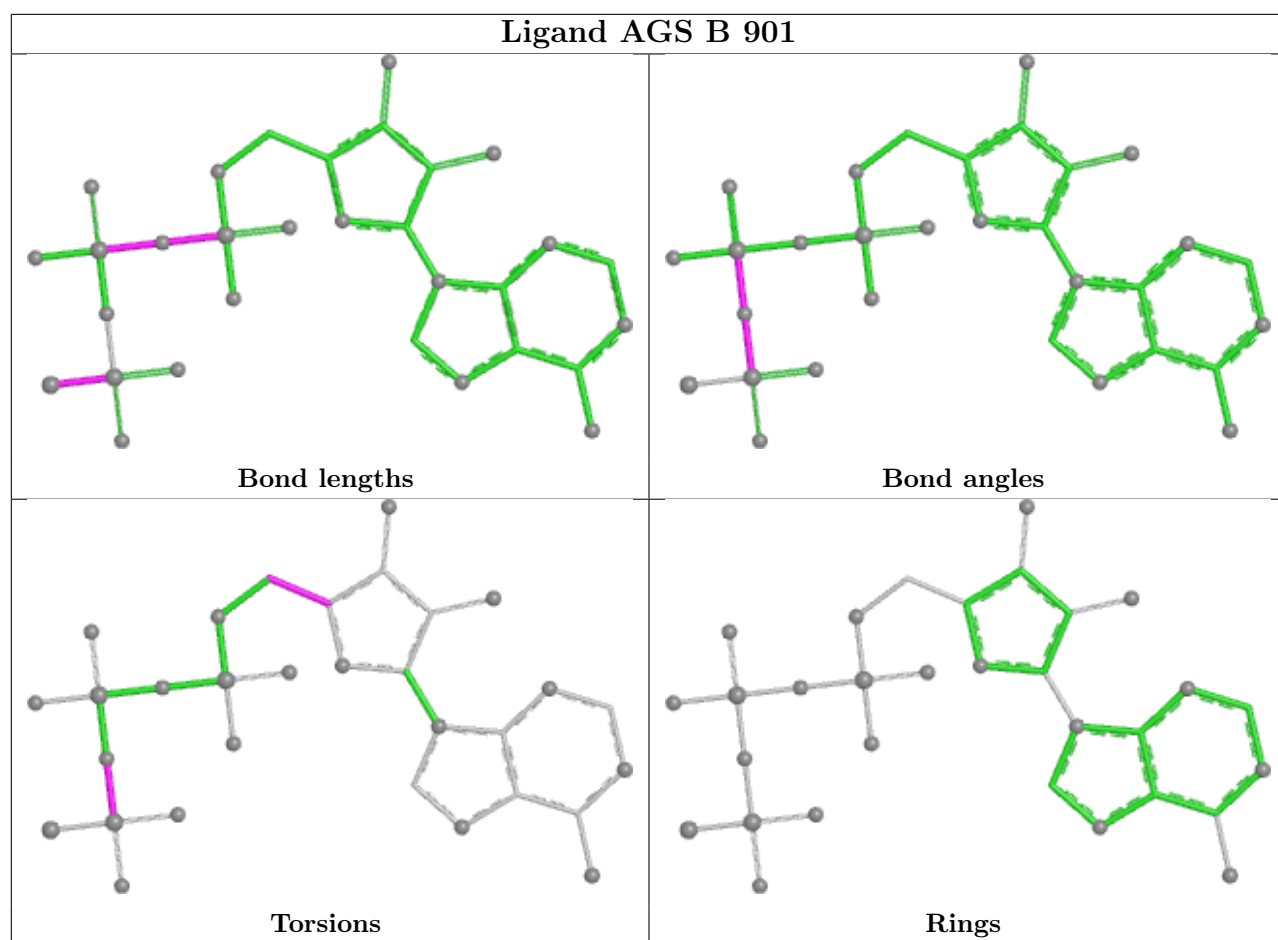
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | F     | 902 | ADP  | 2       | 0            |
| 4   | C     | 901 | AGS  | 6       | 0            |
| 4   | F     | 901 | AGS  | 3       | 0            |
| 4   | B     | 901 | AGS  | 3       | 0            |
| 4   | A     | 902 | AGS  | 4       | 0            |
| 4   | A     | 901 | AGS  | 3       | 0            |
| 4   | D     | 902 | AGS  | 9       | 0            |
| 4   | E     | 901 | AGS  | 14      | 0            |
| 4   | D     | 901 | AGS  | 4       | 0            |
| 5   | E     | 902 | ADP  | 3       | 0            |
| 4   | B     | 902 | AGS  | 4       | 0            |
| 4   | C     | 902 | AGS  | 4       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

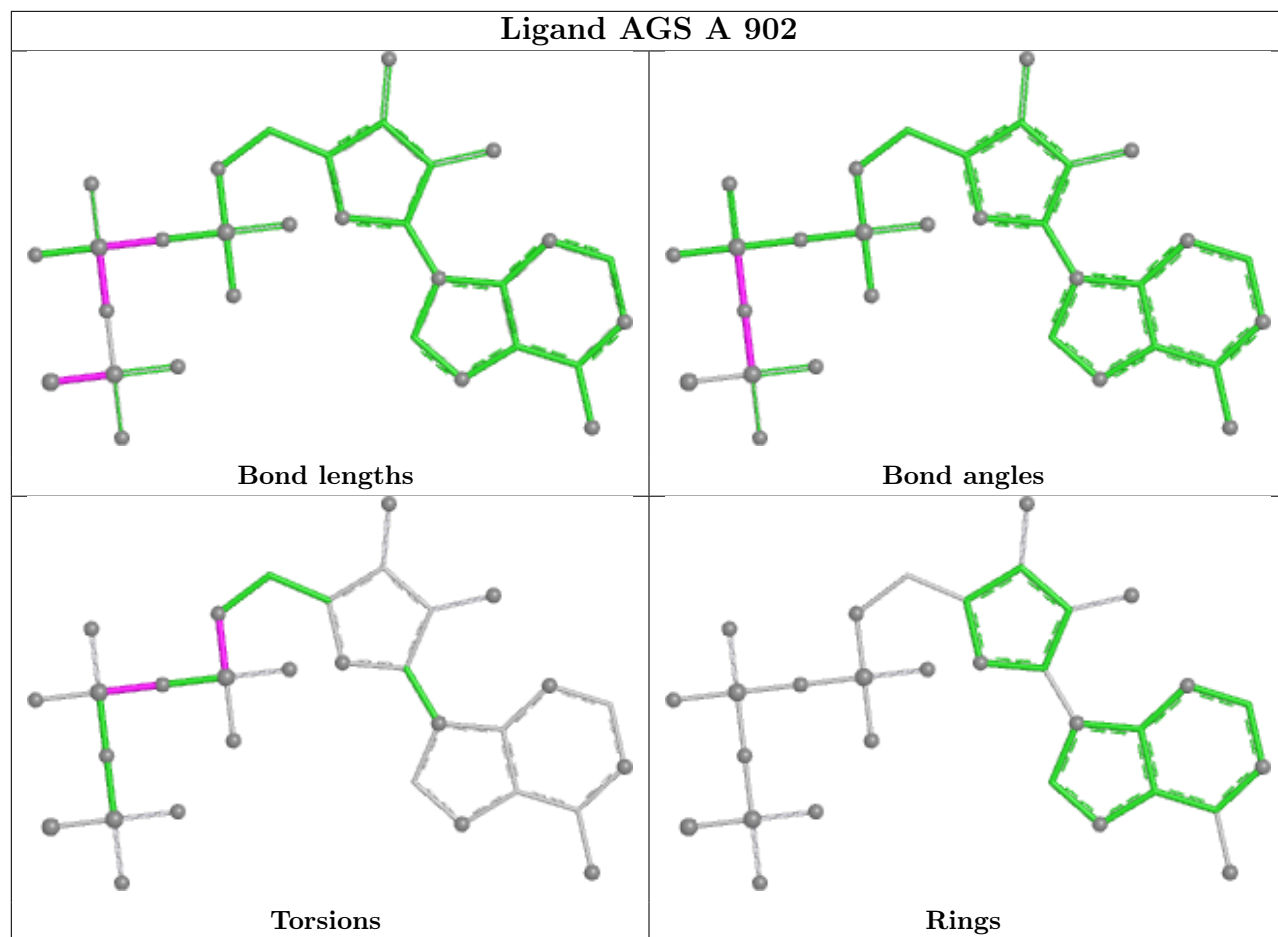


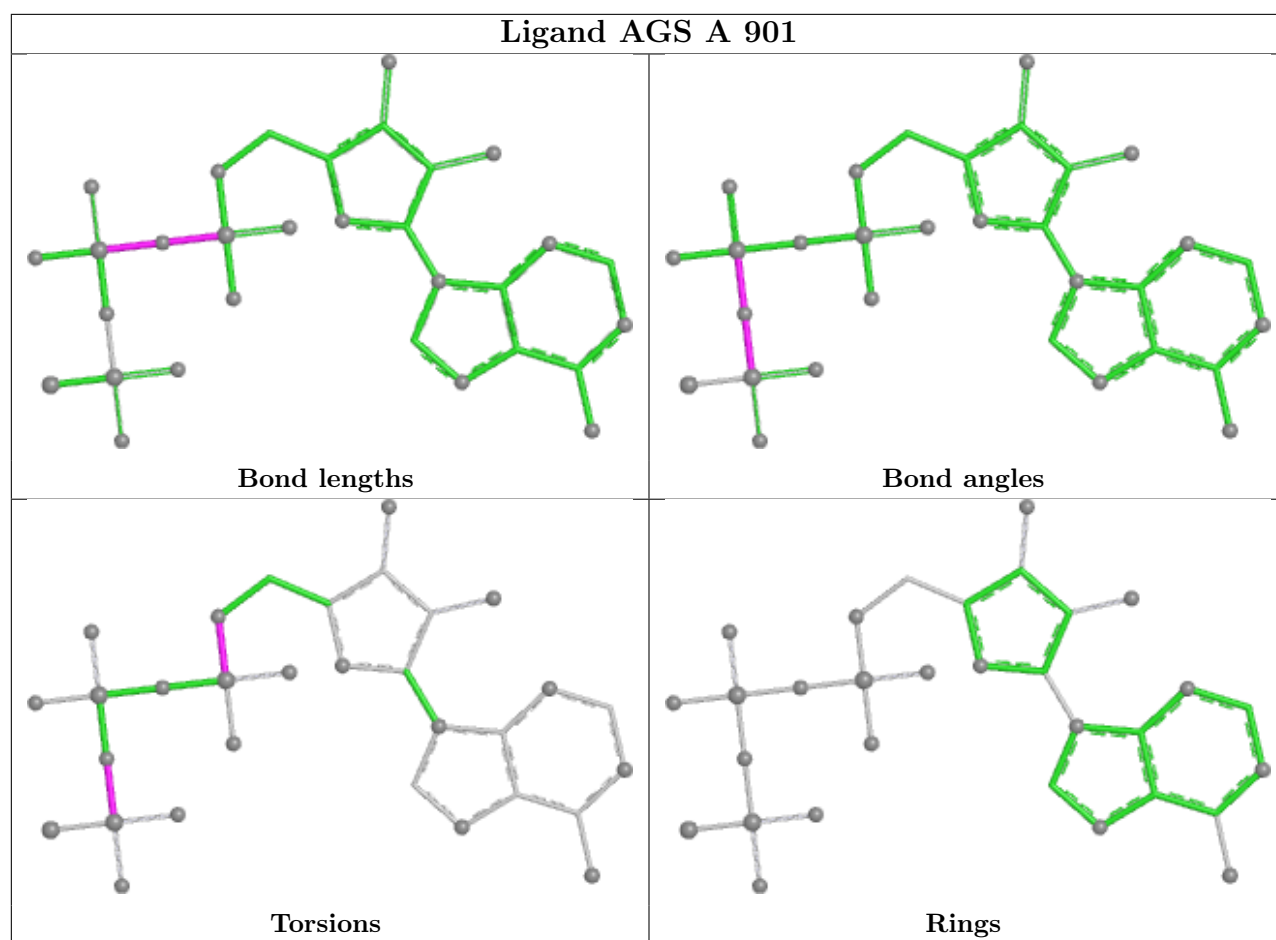
## Ligand AGS F 901

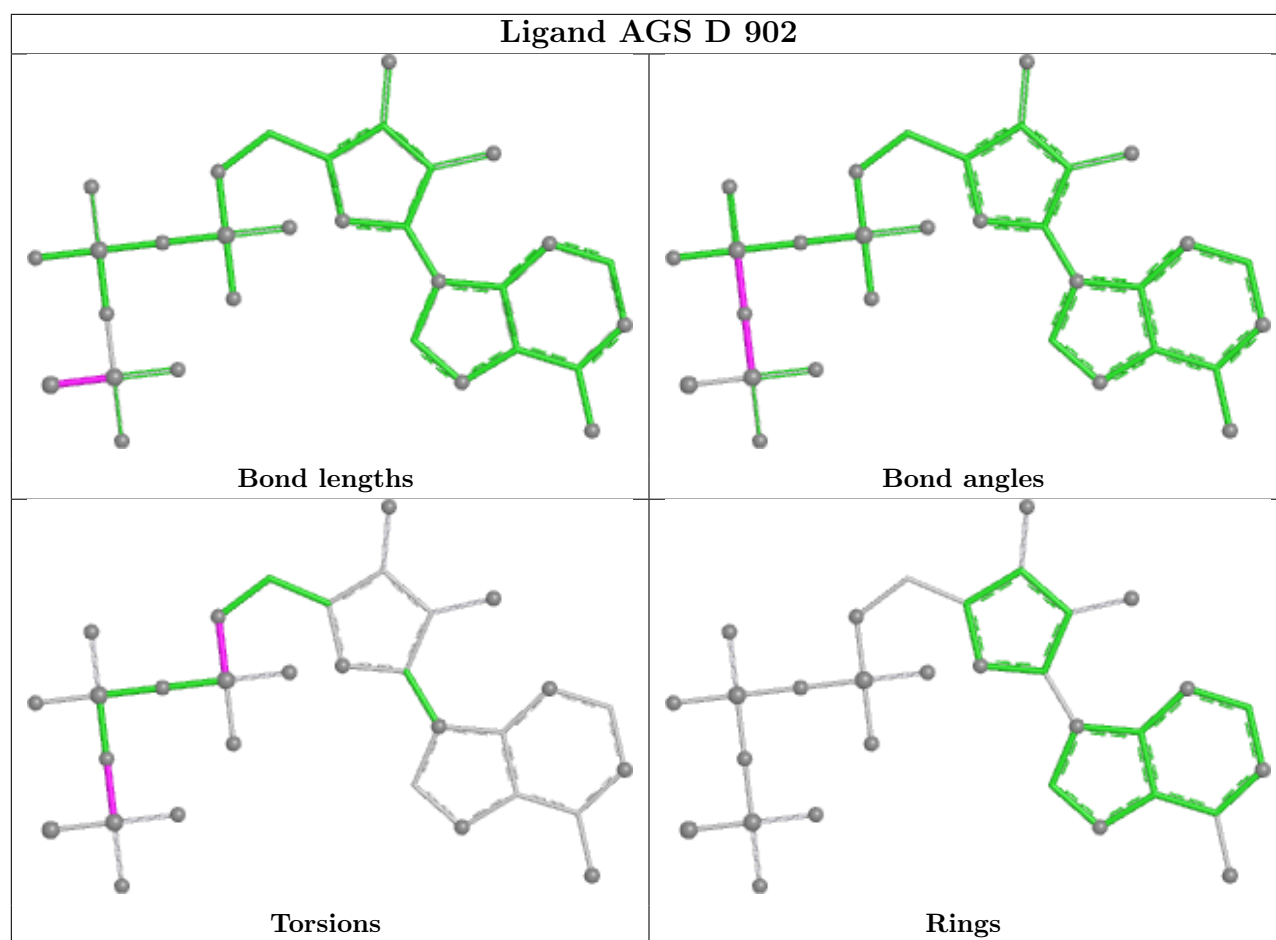




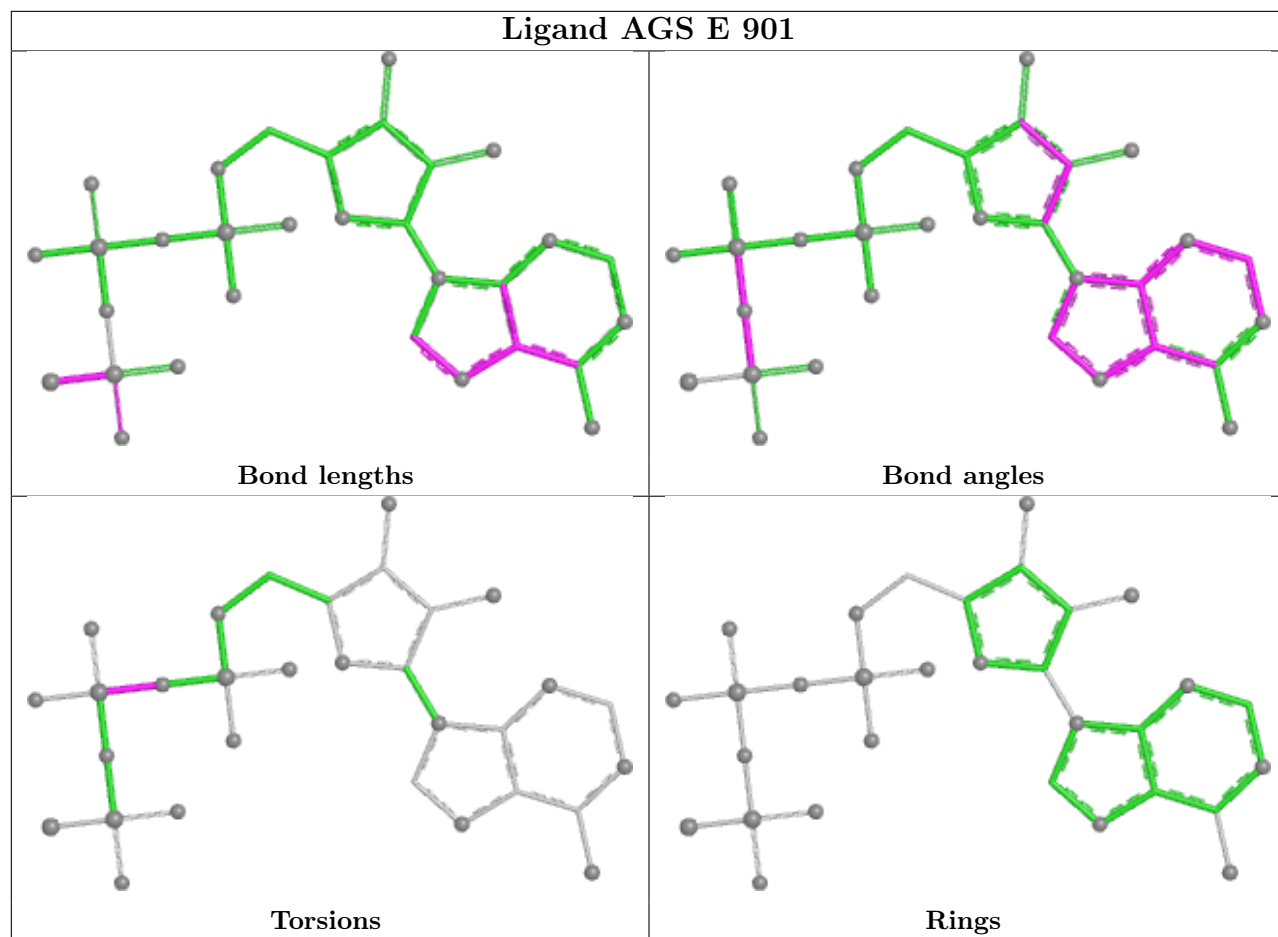




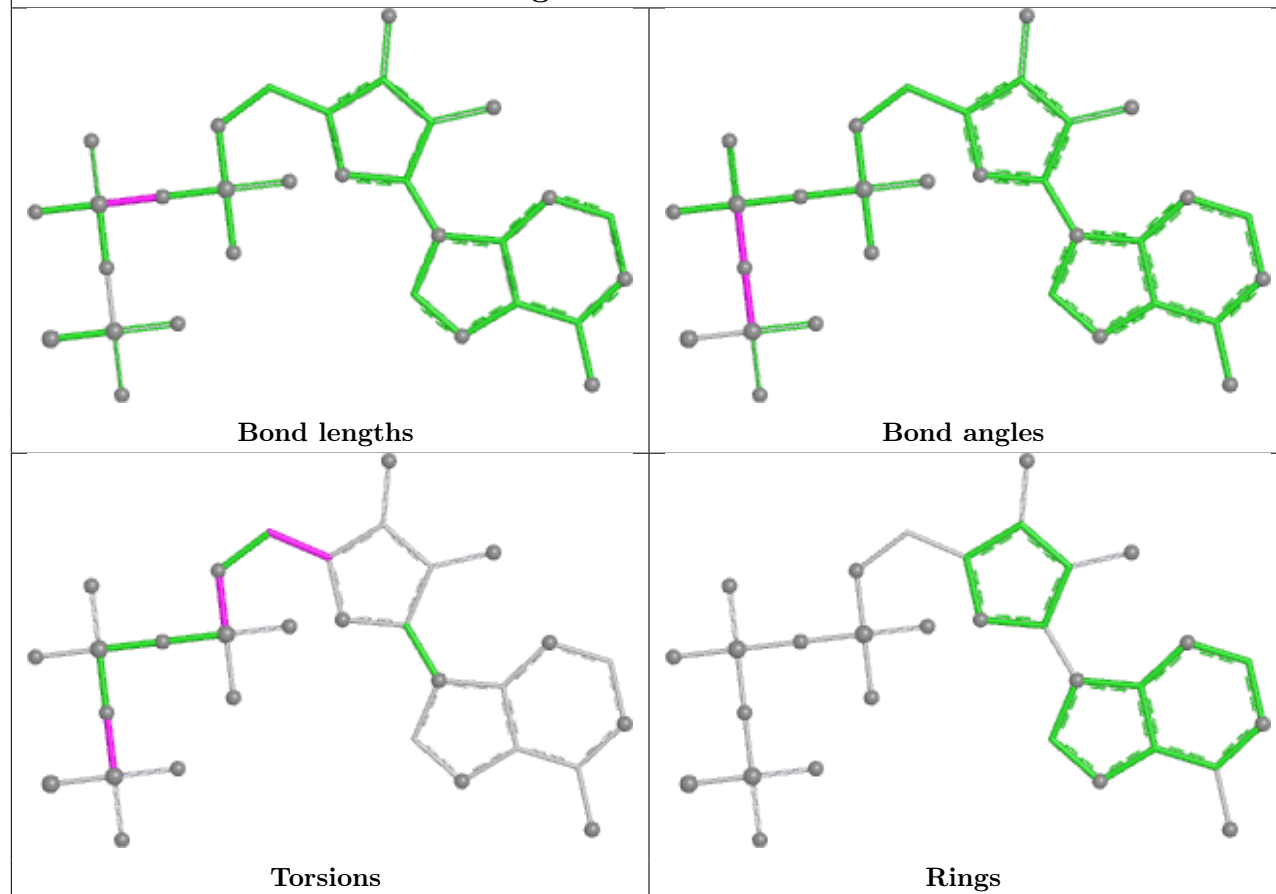




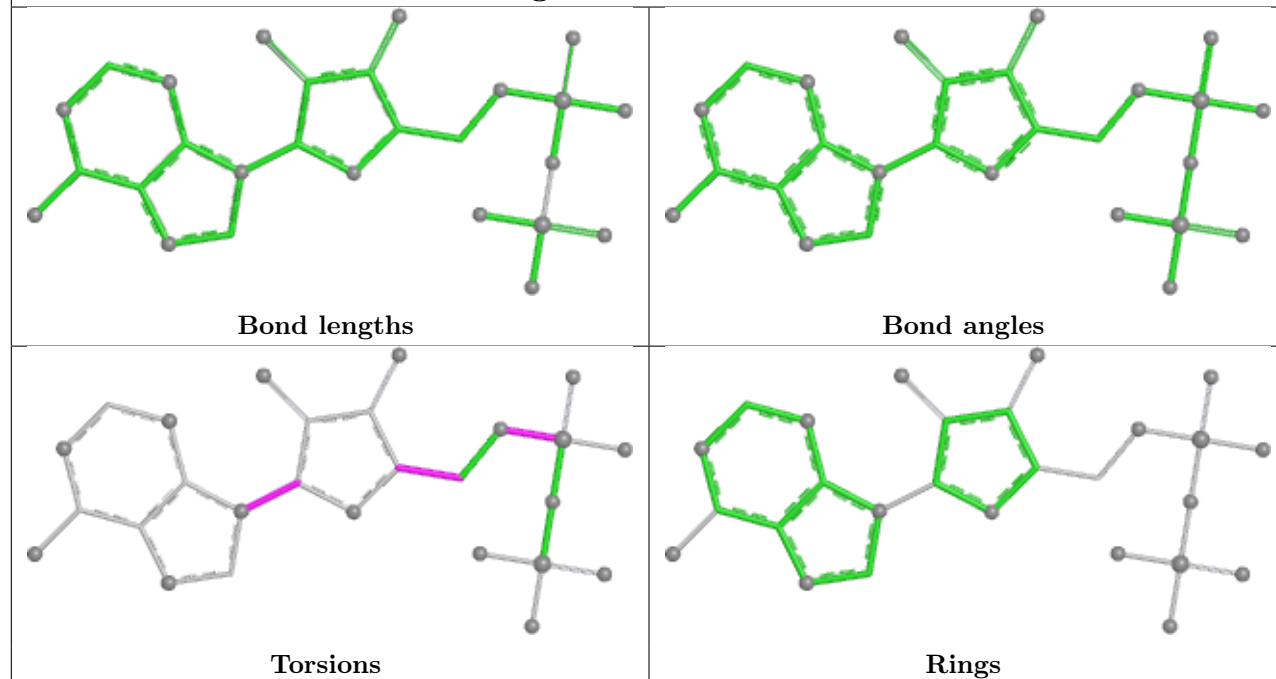
## Ligand AGS E 901

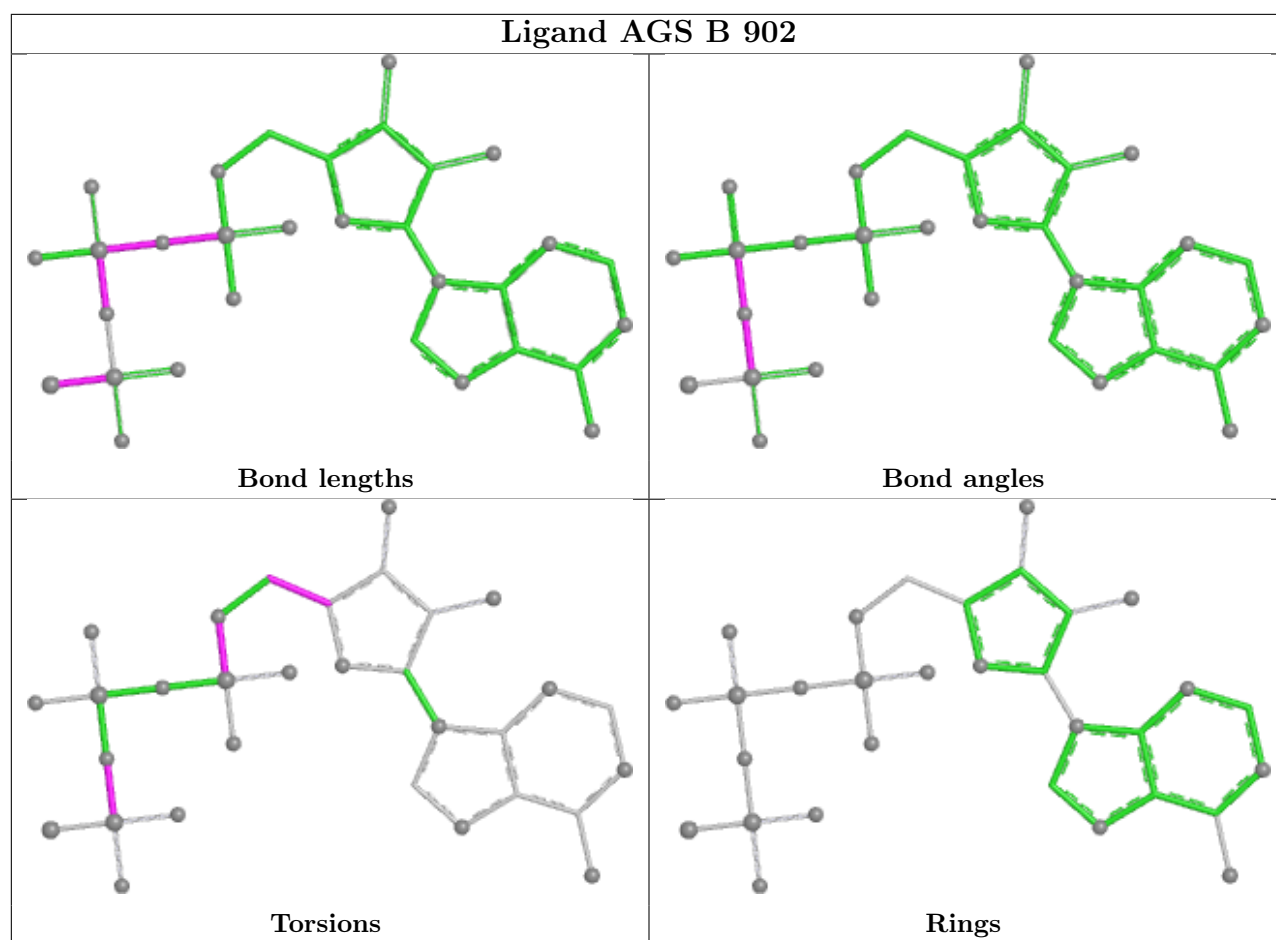


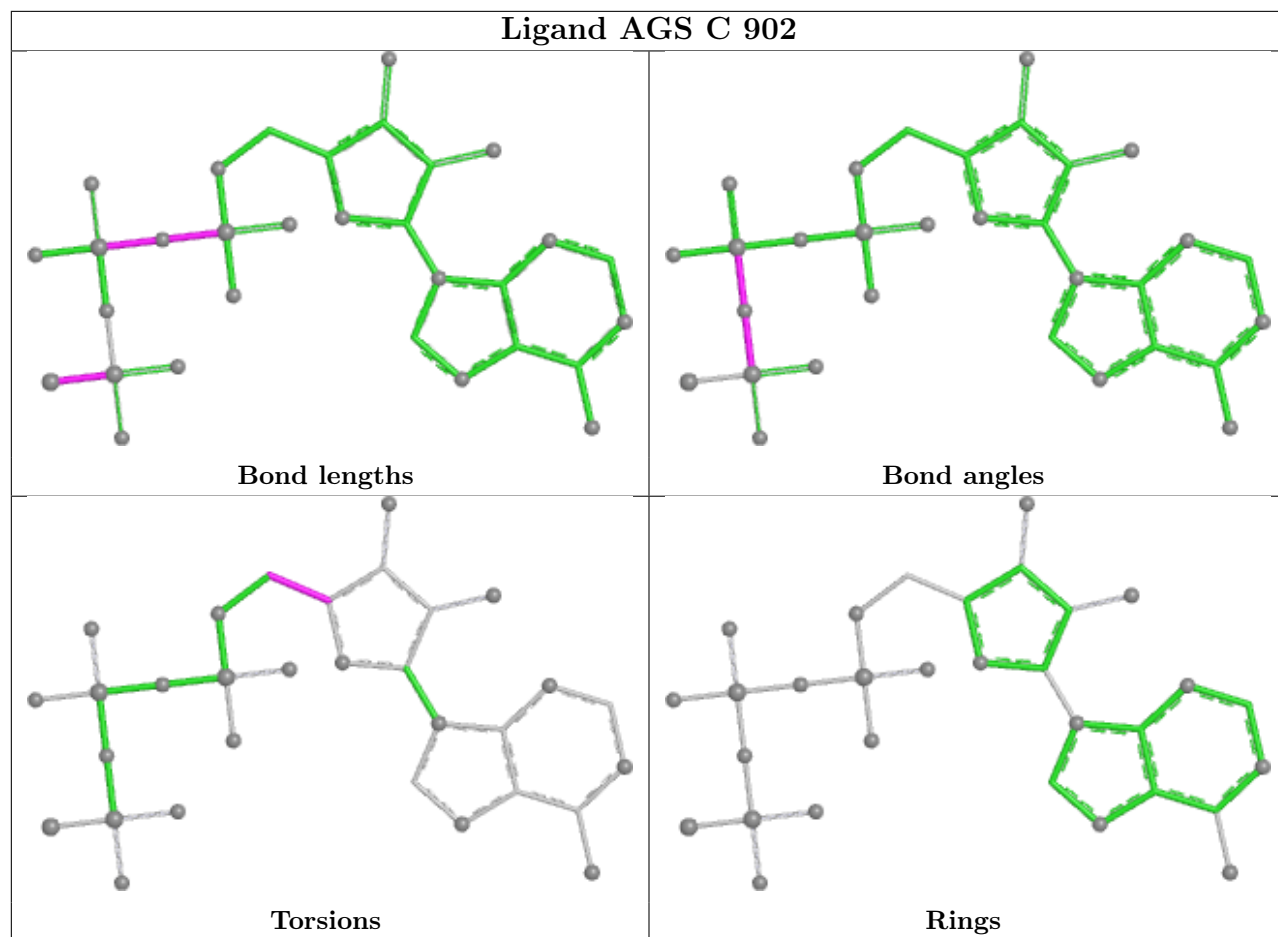
## Ligand AGS D 901



## Ligand ADP E 902







## 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.

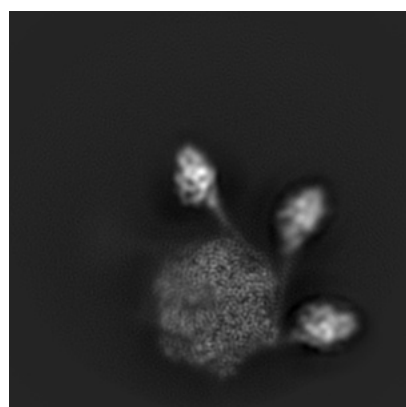
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23206. These allow visual inspection of the internal detail of the map and identification of artifacts.

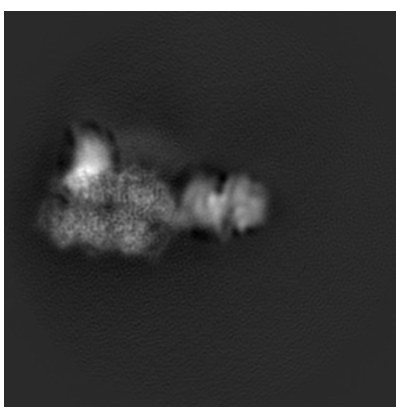
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

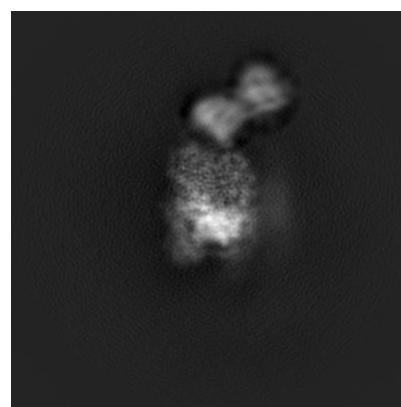
#### 6.1.1 Primary map



X



Y

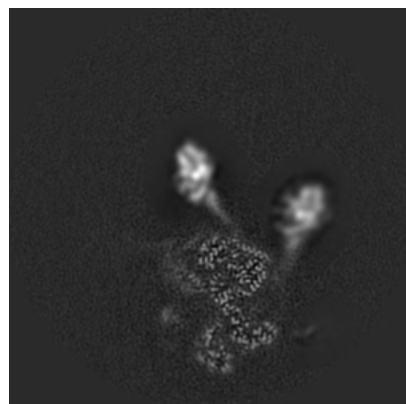


Z

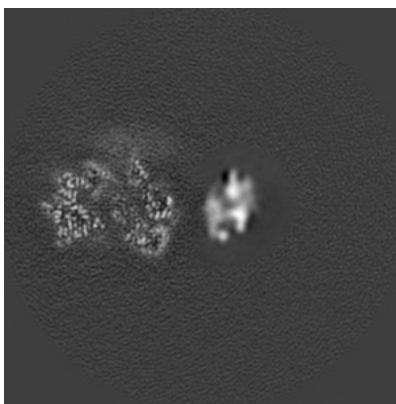
The images above show the map projected in three orthogonal directions.

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

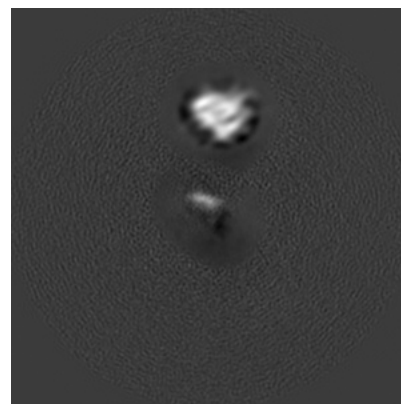
#### 6.2.1 Primary map



X Index: 180



Y Index: 180



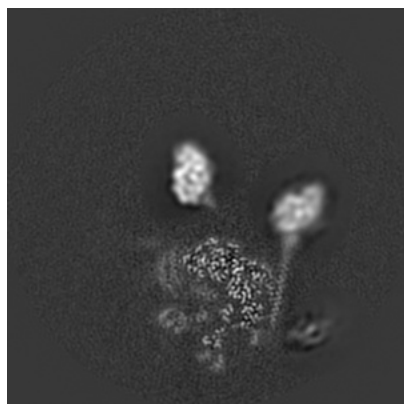
Z Index: 180



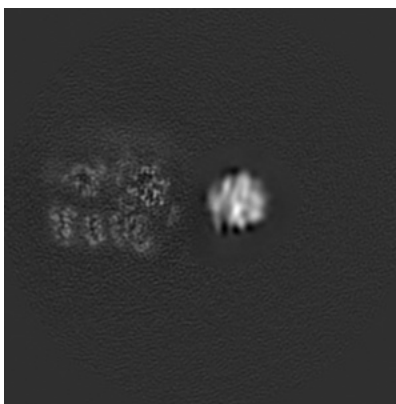
The images above show central slices of the map in three orthogonal directions.

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

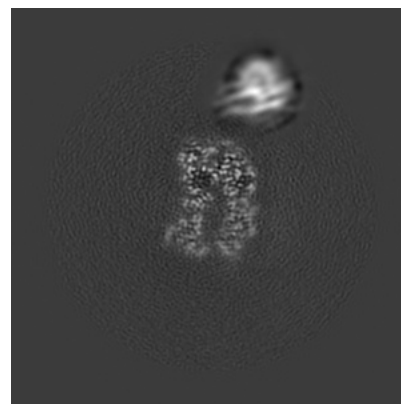
### 6.3.1 Primary map



X Index: 189



Y Index: 169

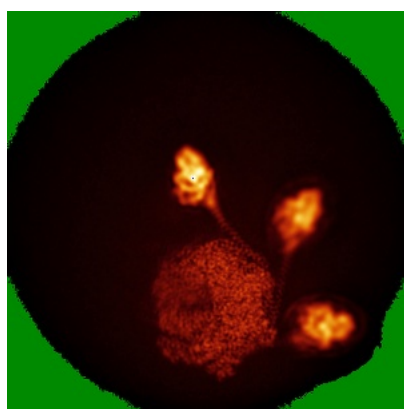


Z Index: 75

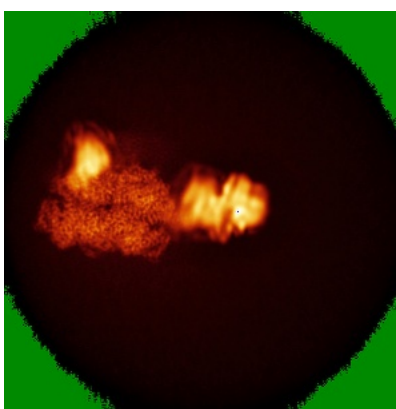
The images above show the largest variance slices of the map in three orthogonal directions.

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

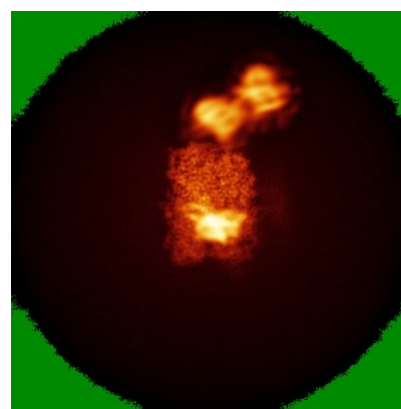
### 6.4.1 Primary map



X



Y

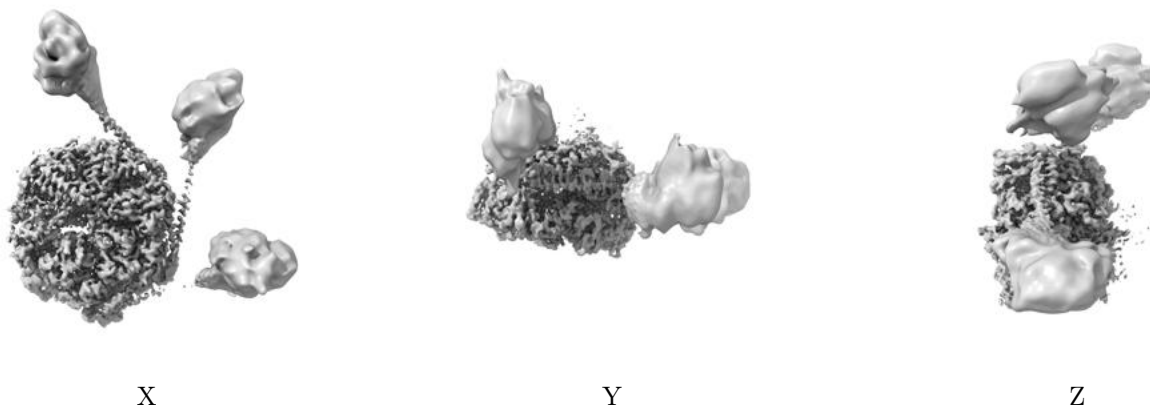


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 7.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

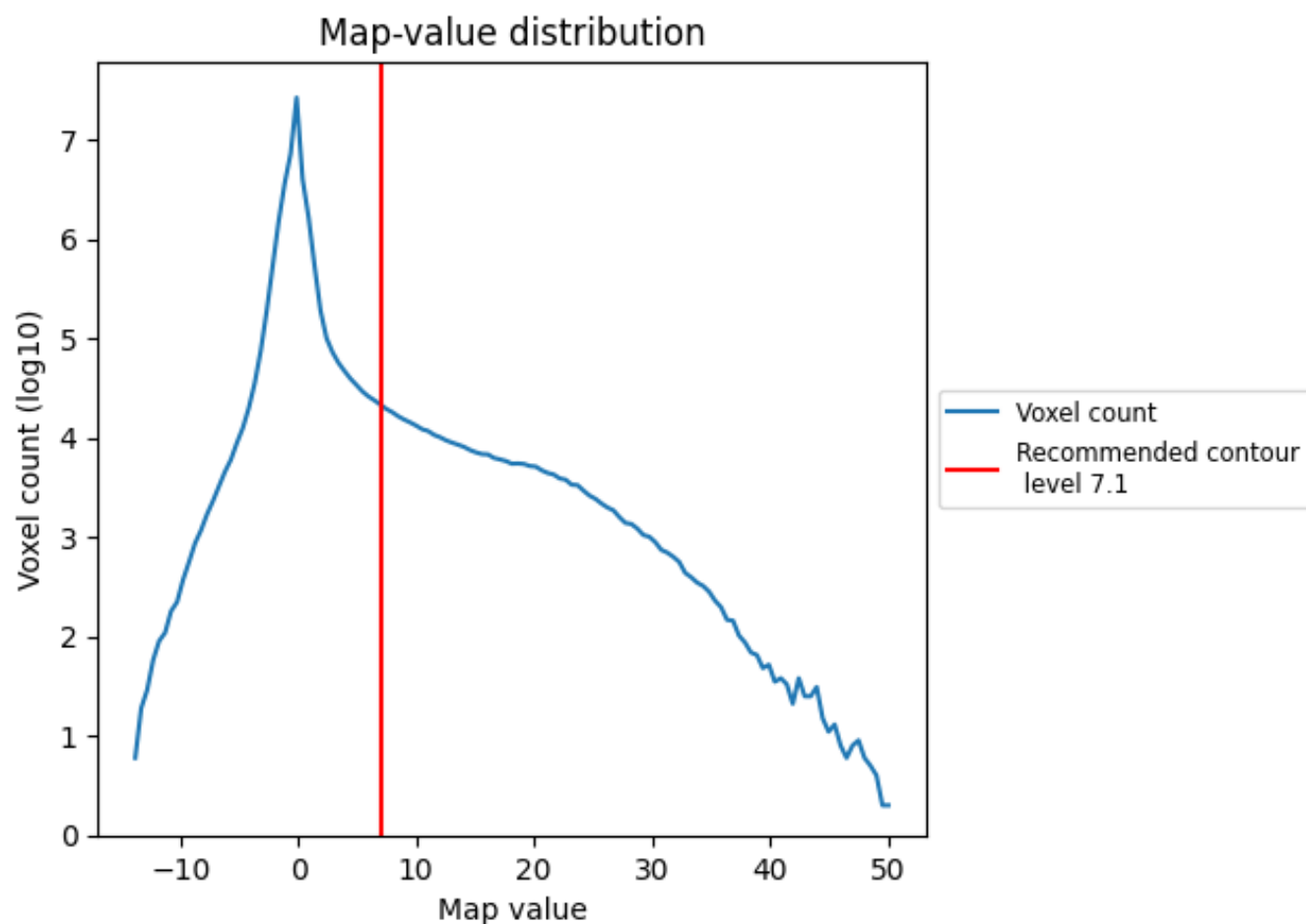
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

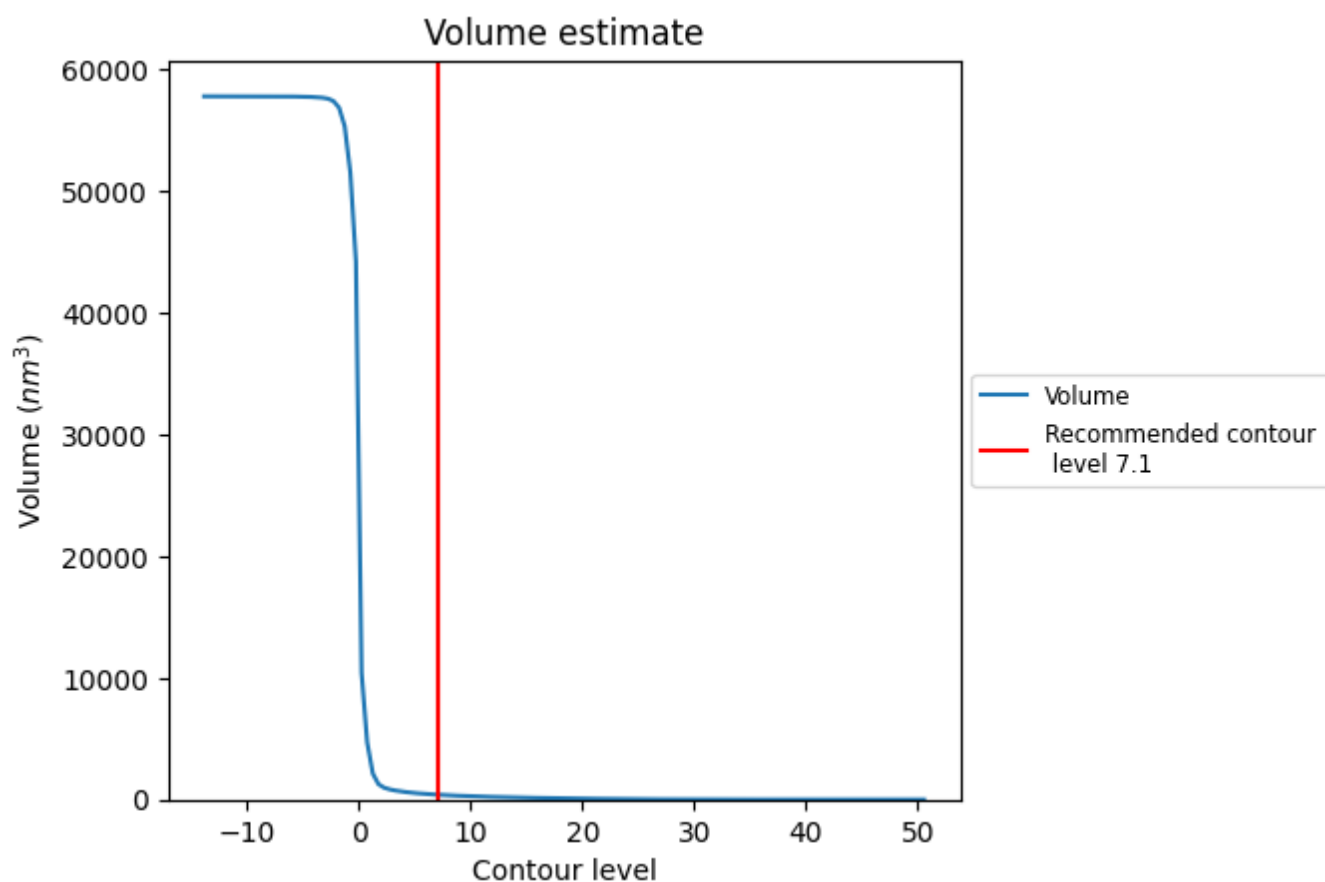
This section contains the results of statistical analysis of the map.

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



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

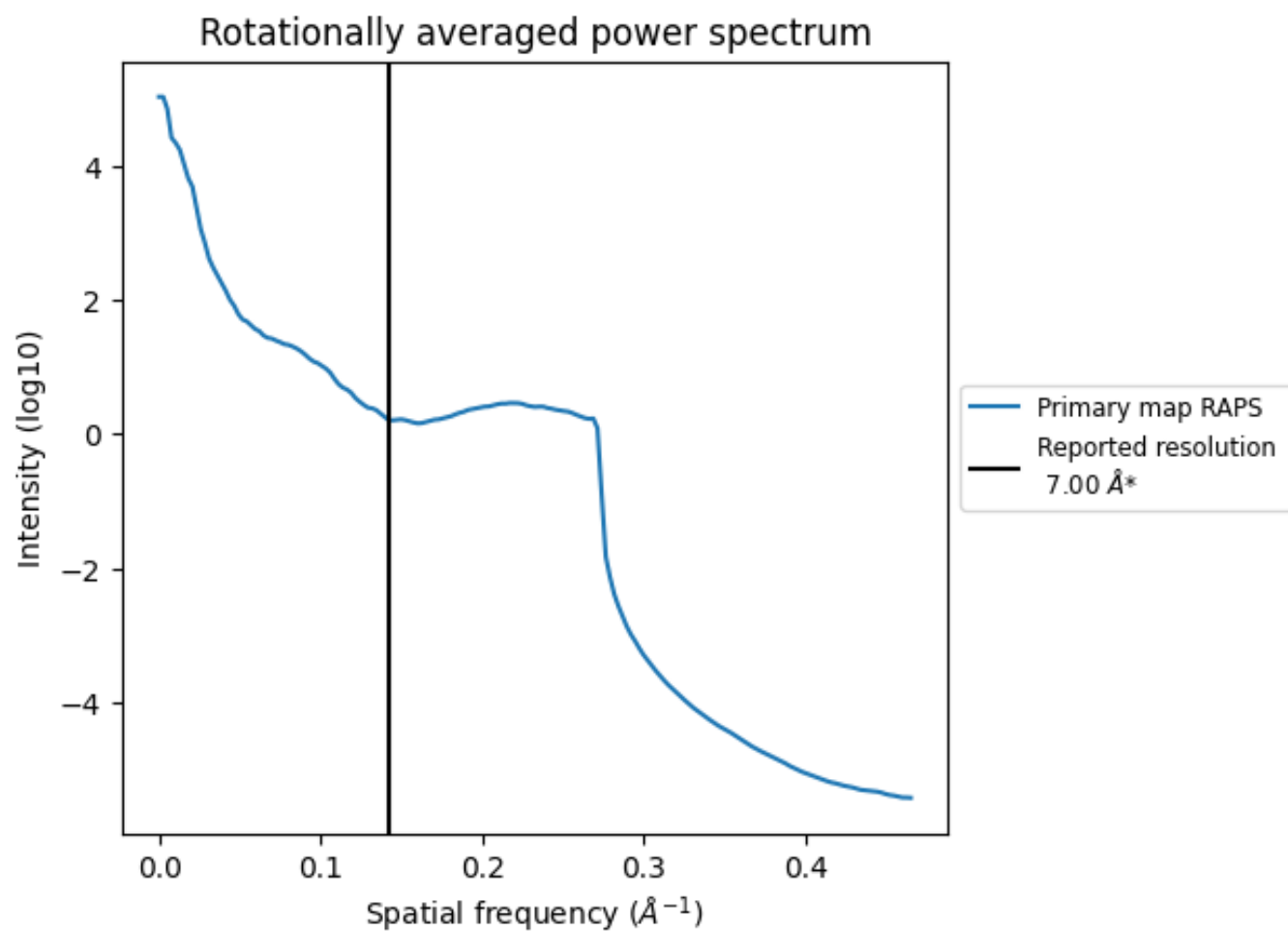
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 397 nm<sup>3</sup>; this corresponds to an approximate mass of 359 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 0.143 Å<sup>-1</sup>

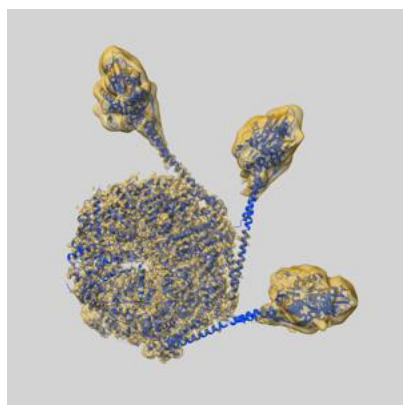
## 8 Fourier-Shell correlation ⓘ

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

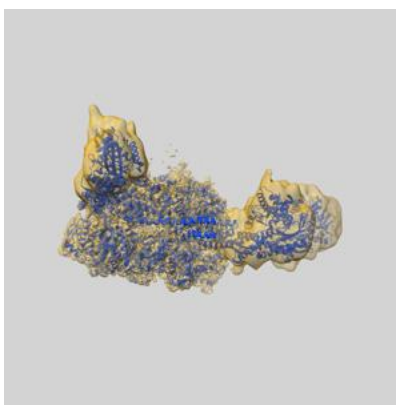
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23206 and PDB model 7L6N. Per-residue inclusion information can be found in section [3](#) on page [7](#).

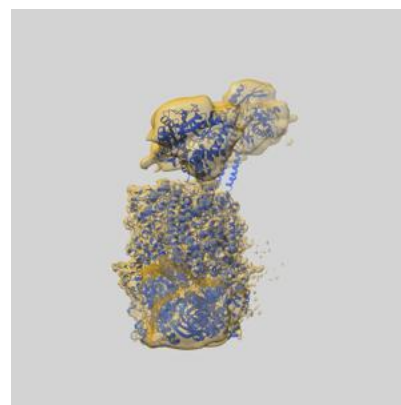
### 9.1 Map-model overlay [i](#)



X



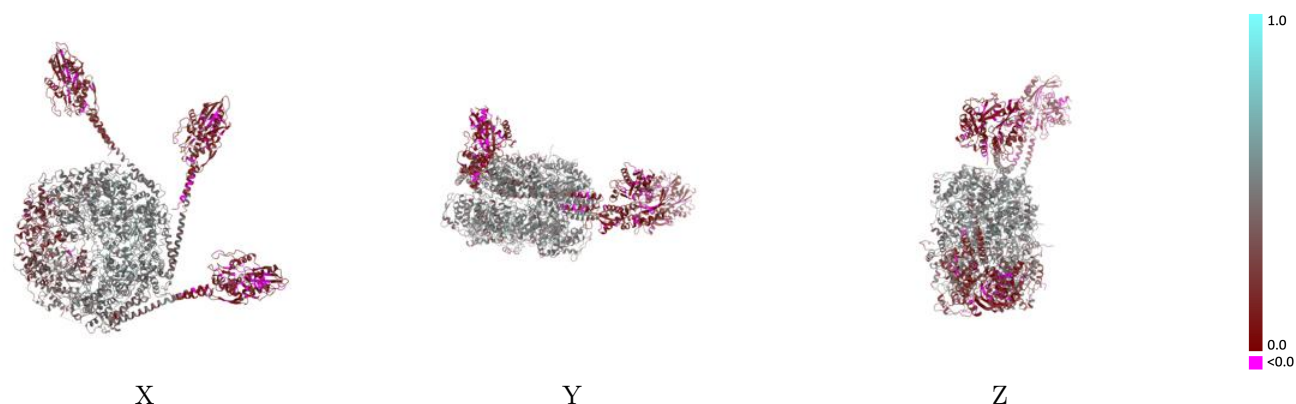
Y



Z

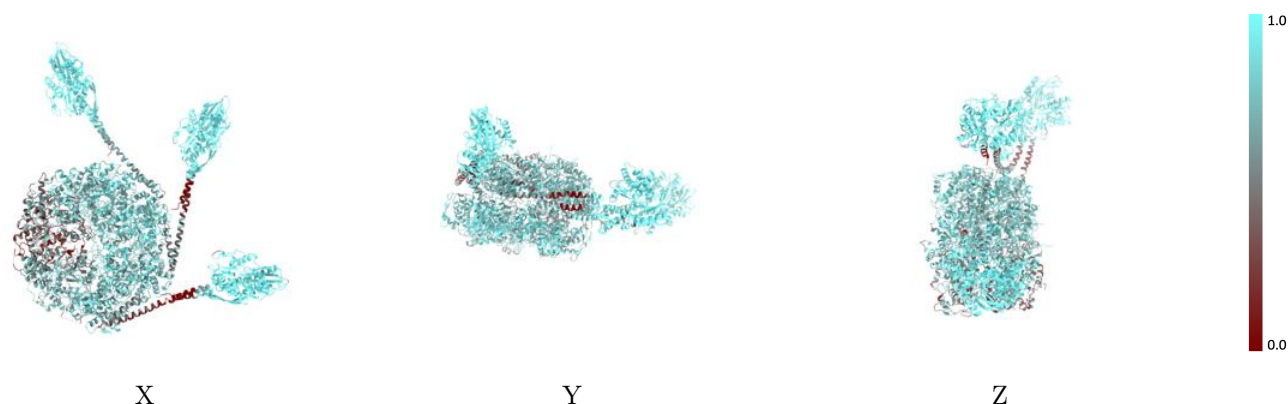
The images above show the 3D surface view of the map at the recommended contour level 7.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according 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.

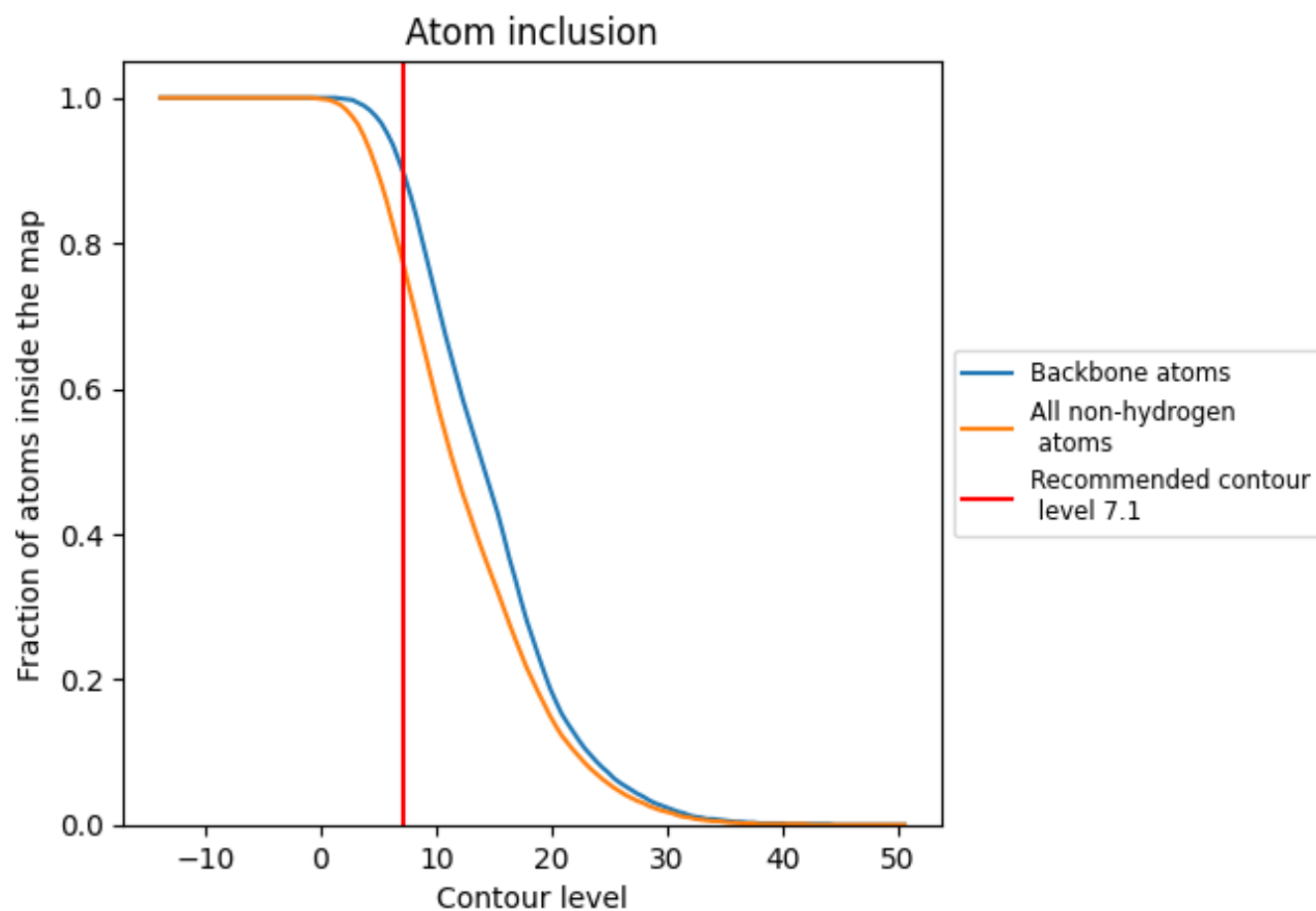
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (7.1).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (7.1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.7760 | <div></div> 0.3550 |
| A     | <div></div> 0.8010 | <div></div> 0.4420 |
| B     | <div></div> 0.7820 | <div></div> 0.4530 |
| C     | <div></div> 0.7610 | <div></div> 0.4530 |
| D     | <div></div> 0.8000 | <div></div> 0.4560 |
| E     | <div></div> 0.6270 | <div></div> 0.3510 |
| F     | <div></div> 0.5040 | <div></div> 0.3330 |
| I     | <div></div> 0.9860 | <div></div> 0.1440 |
| J     | <div></div> 0.9640 | <div></div> 0.1230 |
| K     | <div></div> 0.9660 | <div></div> 0.1140 |
| N     | <div></div> 0.8540 | <div></div> 0.4860 |

1.0

0.0

<0.0