



## Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 05:35 AM UTC

PDB ID : 7V2A / pdb\_00007v2a  
EMDB ID : EMD-31639  
Title : SARS-CoV-2 Spike trimer in complex with XG014 Fab  
Authors : Wang, K.; Wang, X.; Pan, L.  
Deposited on : 2021-08-07  
Resolution : 3.40 Å (reported)  
Based on initial models : 6PZE, 6Z3P, 6VXX

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  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

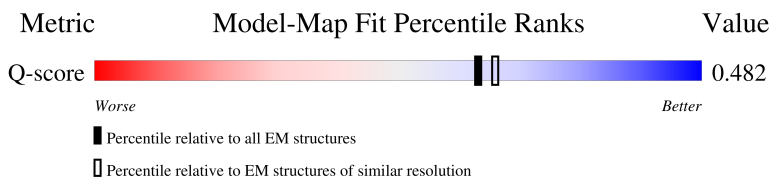
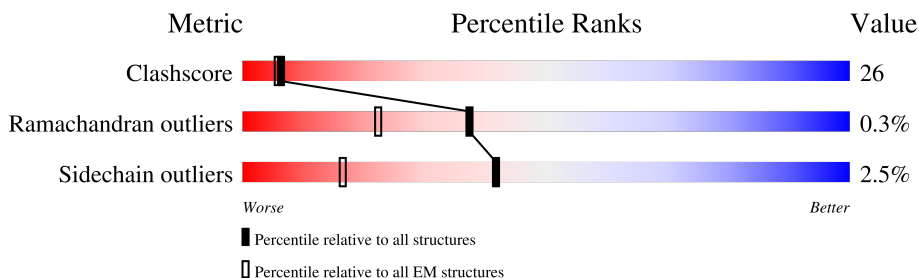
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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                       | 14717 ( 2.90 - 3.90 )                                    |

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     | 1208   |  |
| 1   | B     | 1208   |  |
| 1   | C     | 1208   |  |
| 2   | D     | 216    |  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain                                                            |
|-----|-------|--------|-----------------------------------------------------------------------------|
| 2   | F     | 216    | <div><div><div></div><div></div><div></div></div><div>26%24%49%</div></div> |
| 2   | H     | 216    | <div><div><div></div><div></div><div></div></div><div>25%24%49%</div></div> |
| 3   | E     | 237    | <div><div><div></div><div></div><div></div></div><div>23%27%49%</div></div> |
| 3   | G     | 237    | <div><div><div></div><div></div><div></div></div><div>23%27%49%</div></div> |
| 3   | I     | 237    | <div><div><div></div><div></div><div></div></div><div>24%27%49%</div></div> |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28017 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 Spike glycoprotein.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 988      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7464  | 4774 | 1240 | 1416 | 34 |         |       |
| 1   | B     | 988      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7464  | 4774 | 1240 | 1416 | 34 |         |       |
| 1   | C     | 988      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7464  | 4774 | 1240 | 1416 | 34 |         |       |

There are 15 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 682     | GLY      | ARG    | engineered mutation | UNP P0DTC2 |
| A     | 683     | SER      | ARG    | engineered mutation | UNP P0DTC2 |
| A     | 685     | SER      | ARG    | engineered mutation | UNP P0DTC2 |
| A     | 986     | PRO      | LYS    | engineered mutation | UNP P0DTC2 |
| A     | 987     | PRO      | VAL    | engineered mutation | UNP P0DTC2 |
| B     | 682     | GLY      | ARG    | engineered mutation | UNP P0DTC2 |
| B     | 683     | SER      | ARG    | engineered mutation | UNP P0DTC2 |
| B     | 685     | SER      | ARG    | engineered mutation | UNP P0DTC2 |
| B     | 986     | PRO      | LYS    | engineered mutation | UNP P0DTC2 |
| B     | 987     | PRO      | VAL    | engineered mutation | UNP P0DTC2 |
| C     | 682     | GLY      | ARG    | engineered mutation | UNP P0DTC2 |
| C     | 683     | SER      | ARG    | engineered mutation | UNP P0DTC2 |
| C     | 685     | SER      | ARG    | engineered mutation | UNP P0DTC2 |
| C     | 986     | PRO      | LYS    | engineered mutation | UNP P0DTC2 |
| C     | 987     | PRO      | VAL    | engineered mutation | UNP P0DTC2 |

- Molecule 2 is a protein called The light chain of XG014 Fab.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | D     | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 799   | 496 | 139 | 162 | 2 |         |       |
| 2   | F     | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 799   | 496 | 139 | 162 | 2 |         |       |

*Continued on next page...*

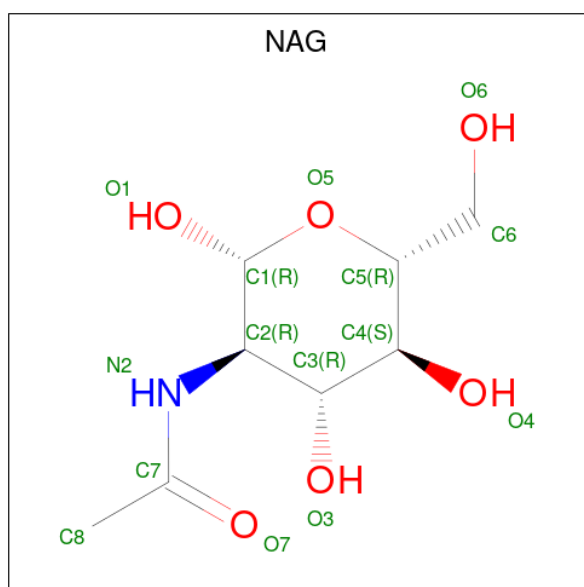
Continued from previous page...

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | H     | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 799   | 496 | 139 | 162 | 2 |         |       |

- Molecule 3 is a protein called The heavy chain of XG014.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | E     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 964   | 623 | 153 | 183 | 5 |         |       |
| 3   | G     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 964   | 623 | 153 | 183 | 5 |         |       |
| 3   | I     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 964   | 623 | 153 | 183 | 5 |         |       |

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 4   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 4   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

Continued on next page...

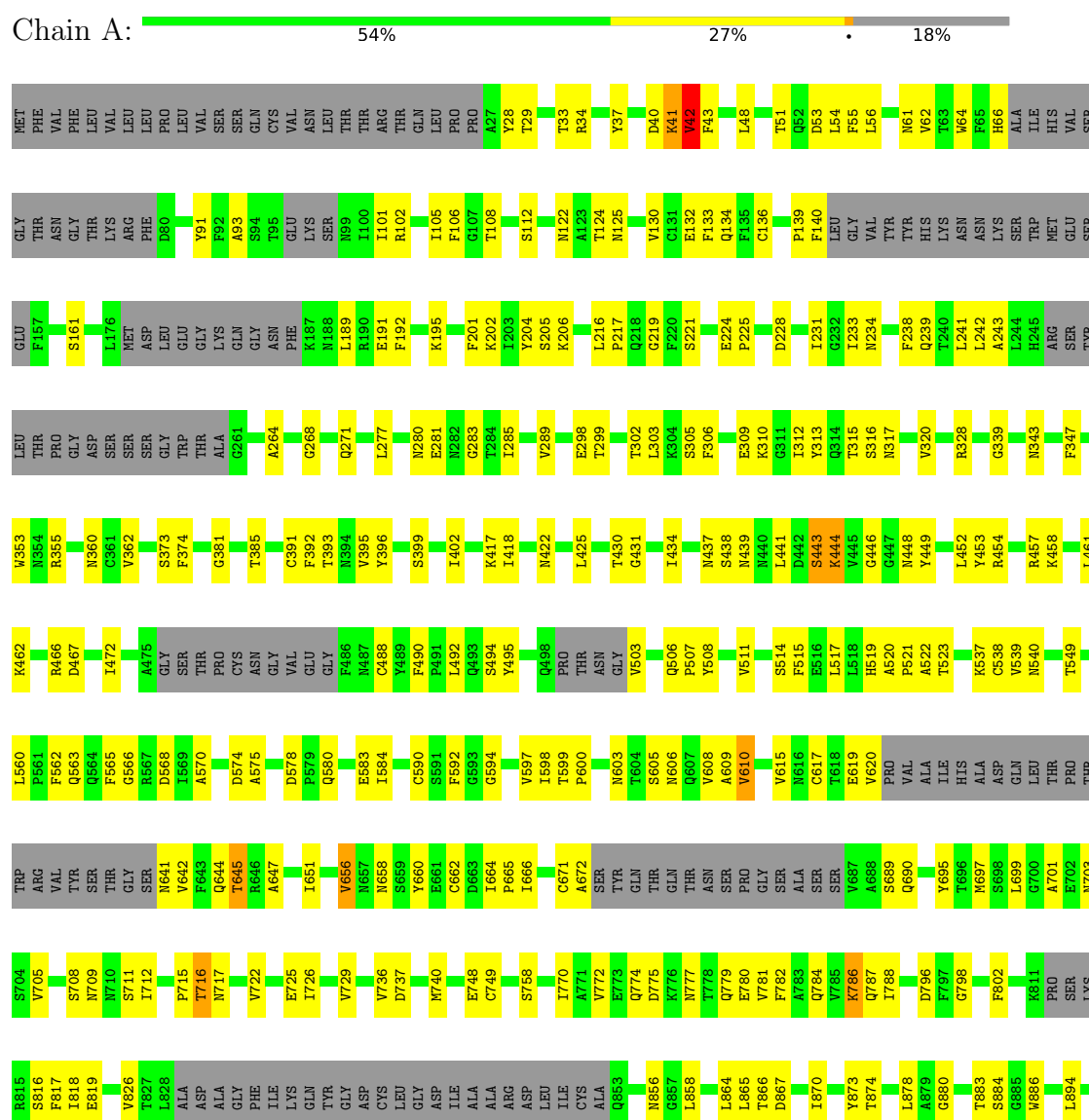
*Continued from previous page...*

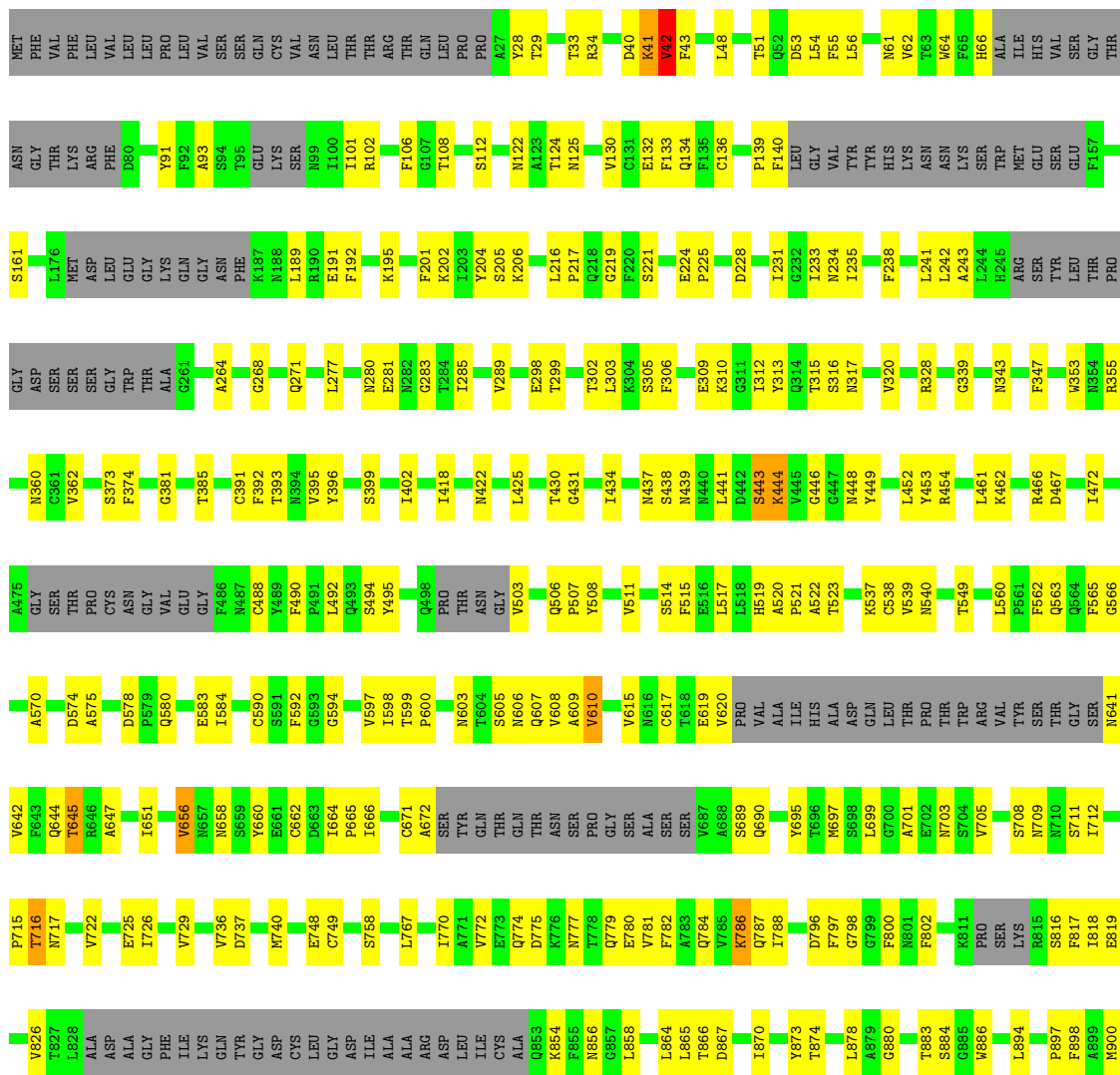
| Mol | Chain | Residues | Atoms       |        |        |        | AltConf |
|-----|-------|----------|-------------|--------|--------|--------|---------|
| 4   | A     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | A     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | A     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | B     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | B     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | B     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | B     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | B     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | B     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | B     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | B     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | C     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | C     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | C     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | C     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | C     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | C     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | C     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | C     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

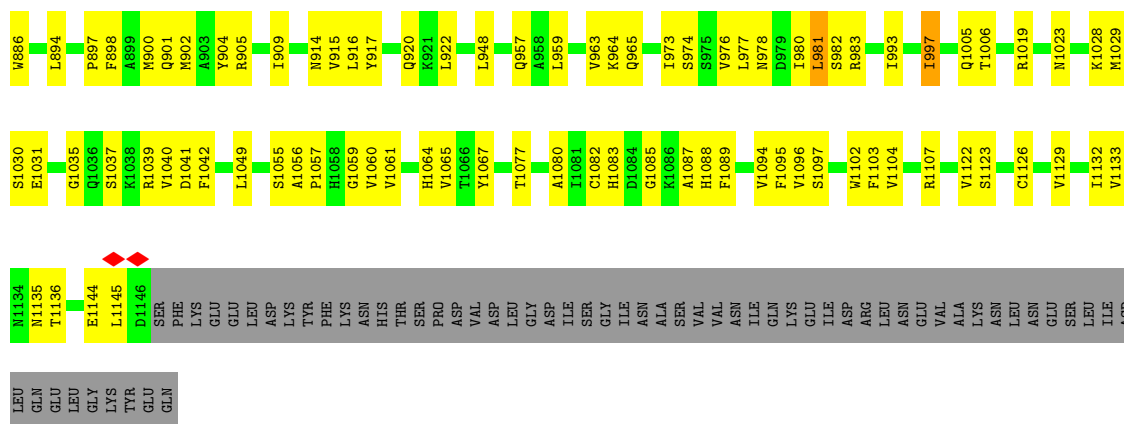
#### • Molecule 1: Spike glycoprotein



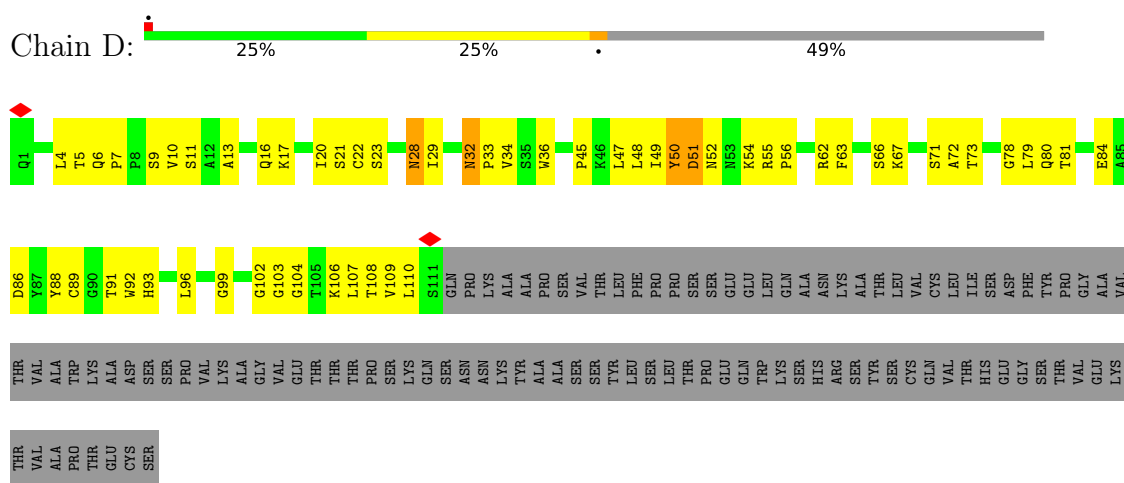




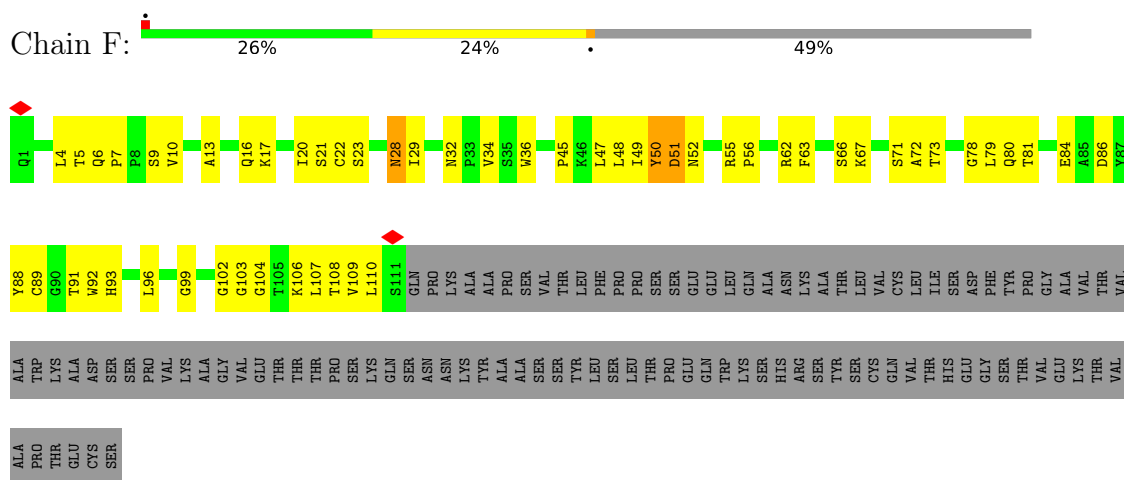




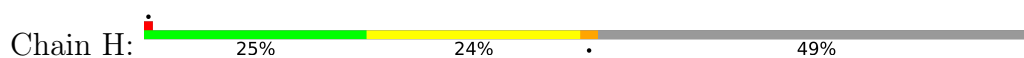
• Molecule 2: The light chain of XG014 Fab

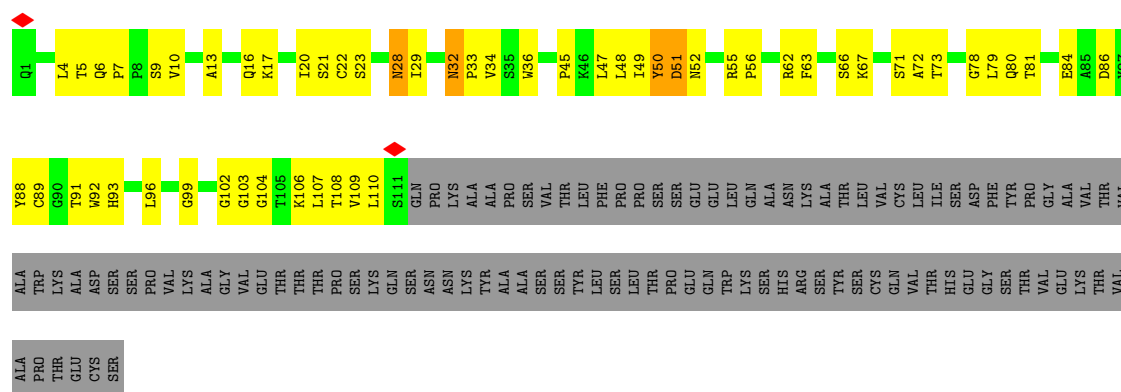


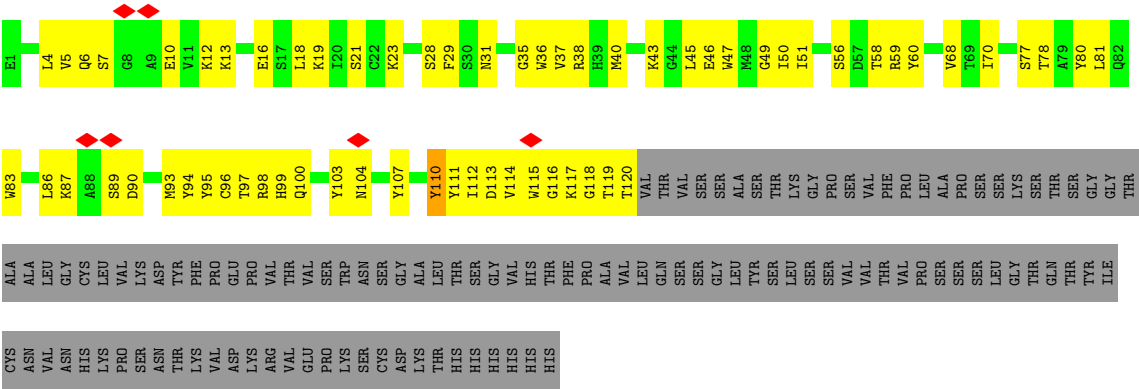
• Molecule 2: The light chain of XG014 Fab



• Molecule 2: The light chain of XG014 Fab







## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE           | Depositor |
| Imposed symmetry                     | POINT, Not provided       |           |
| Number of particles used             | 414922                    | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF         | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY       | Depositor |
| Microscope                           | FEI TITAN KRIOS           | Depositor |
| Voltage (kV)                         | 300                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                        | Depositor |
| Minimum defocus (nm)                 | 1200                      | Depositor |
| Maximum defocus (nm)                 | 2500                      | Depositor |
| Magnification                        | Not provided              |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value                    | 0.071                     | Depositor |
| Minimum map value                    | -0.034                    | Depositor |
| Average map value                    | 0.000                     | Depositor |
| Map value standard deviation         | 0.002                     | Depositor |
| Recommended contour level            | 0.01                      | Depositor |
| Map size (Å)                         | 416.0, 416.0, 416.0       | wwPDB     |
| Map dimensions                       | 400, 400, 400             | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0          | wwPDB     |
| Pixel spacing (Å)                    | 1.04, 1.04, 1.04          | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.54         | 1/7625 (0.0%)  | 0.58        | 1/10400 (0.0%) |
| 1   | B     | 0.54         | 1/7625 (0.0%)  | 0.57        | 1/10400 (0.0%) |
| 1   | C     | 0.54         | 1/7625 (0.0%)  | 0.58        | 2/10400 (0.0%) |
| 2   | D     | 0.40         | 0/817          | 0.61        | 1/1113 (0.1%)  |
| 2   | F     | 0.40         | 0/817          | 0.61        | 1/1113 (0.1%)  |
| 2   | H     | 0.41         | 0/817          | 0.62        | 1/1113 (0.1%)  |
| 3   | E     | 0.43         | 0/996          | 0.60        | 0/1352         |
| 3   | G     | 0.42         | 0/996          | 0.65        | 1/1352 (0.1%)  |
| 3   | I     | 0.45         | 0/996          | 0.67        | 1/1352 (0.1%)  |
| All | All   | 0.52         | 3/28314 (0.0%) | 0.59        | 9/38595 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | B     | 0                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 2   | D     | 0                   | 1                   |
| 2   | F     | 0                   | 1                   |
| 2   | H     | 0                   | 1                   |
| 3   | E     | 0                   | 1                   |
| 3   | G     | 0                   | 1                   |
| All | All   | 0                   | 8                   |

All (3) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | C     | 1088 | HIS  | C-N   | -5.80 | 1.21        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 1088 | HIS  | C-N   | -5.78 | 1.21        | 1.33     |
| 1   | B     | 1088 | HIS  | C-N   | -5.77 | 1.21        | 1.33     |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | G     | 110 | TYR  | CB-CA-C | -8.09 | 95.26       | 112.82   |
| 3   | I     | 110 | TYR  | CB-CA-C | -8.03 | 95.39       | 112.82   |
| 1   | B     | 41  | LYS  | N-CA-C  | -5.48 | 107.59      | 114.56   |
| 1   | A     | 41  | LYS  | N-CA-C  | -5.42 | 106.60      | 113.43   |
| 1   | C     | 324 | GLU  | CB-CA-C | -5.38 | 100.98      | 114.11   |
| 2   | H     | 32  | ASN  | CB-CA-C | 5.14  | 115.53      | 109.47   |
| 1   | C     | 41  | LYS  | N-CA-C  | -5.11 | 106.38      | 113.18   |
| 2   | F     | 32  | ASN  | CB-CA-C | 5.08  | 115.46      | 109.47   |
| 2   | D     | 32  | ASN  | CB-CA-C | 5.06  | 115.54      | 109.31   |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 443 | SER  | Peptide |
| 1   | B     | 443 | SER  | Peptide |
| 1   | C     | 443 | SER  | Peptide |
| 2   | D     | 50  | TYR  | Peptide |
| 3   | E     | 104 | ASN  | Peptide |
| 2   | F     | 50  | TYR  | Peptide |
| 3   | G     | 104 | ASN  | Peptide |
| 2   | H     | 50  | TYR  | Peptide |

## 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     | 7464  | 0        | 7087     | 422     | 0            |
| 1   | B     | 7464  | 0        | 7087     | 423     | 0            |
| 1   | C     | 7464  | 0        | 7087     | 431     | 0            |
| 2   | D     | 799   | 0        | 782      | 58      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | F     | 799   | 0        | 782      | 56      | 0            |
| 2   | H     | 799   | 0        | 782      | 50      | 0            |
| 3   | E     | 964   | 0        | 904      | 64      | 0            |
| 3   | G     | 964   | 0        | 904      | 69      | 0            |
| 3   | I     | 964   | 0        | 904      | 63      | 0            |
| 4   | A     | 112   | 0        | 104      | 3       | 0            |
| 4   | B     | 112   | 0        | 104      | 3       | 0            |
| 4   | C     | 112   | 0        | 104      | 4       | 0            |
| All | All   | 28017 | 0        | 26631    | 1394    | 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 26.

All (1394) 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:B:697:MET:CE   | 1:C:864:LEU:HD11  | 1.11                     | 1.56              |
| 1:A:697:MET:CE   | 1:B:864:LEU:HD11  | 1.13                     | 1.54              |
| 1:A:864:LEU:HD11 | 1:C:697:MET:CE    | 1.11                     | 1.51              |
| 1:A:864:LEU:CD1  | 1:C:697:MET:CE    | 1.90                     | 1.48              |
| 1:B:697:MET:CE   | 1:C:864:LEU:CD1   | 1.90                     | 1.46              |
| 1:A:697:MET:CE   | 1:B:864:LEU:CD1   | 1.92                     | 1.45              |
| 1:A:560:LEU:CD2  | 1:B:224:GLU:OE2   | 1.73                     | 1.37              |
| 1:B:560:LEU:CD2  | 1:C:224:GLU:OE2   | 1.71                     | 1.37              |
| 1:A:224:GLU:OE2  | 1:C:560:LEU:CD2   | 1.71                     | 1.36              |
| 1:C:1031:GLU:OE2 | 1:C:1039:ARG:CD   | 1.84                     | 1.25              |
| 1:A:904:TYR:CD1  | 1:C:1107:ARG:NH1  | 1.83                     | 1.25              |
| 1:A:1031:GLU:OE2 | 1:A:1039:ARG:CD   | 1.84                     | 1.24              |
| 1:B:1031:GLU:OE2 | 1:B:1039:ARG:CD   | 1.84                     | 1.24              |
| 1:A:1129:VAL:CG2 | 1:B:917:TYR:HB3   | 1.69                     | 1.22              |
| 1:B:1107:ARG:NH1 | 1:C:904:TYR:CD1   | 1.85                     | 1.22              |
| 1:A:779:GLN:OE1  | 1:A:865:LEU:CD1   | 1.88                     | 1.21              |
| 1:B:779:GLN:OE1  | 1:B:865:LEU:CD1   | 1.88                     | 1.21              |
| 1:B:1129:VAL:CG2 | 1:C:917:TYR:HB3   | 1.70                     | 1.20              |
| 1:C:779:GLN:OE1  | 1:C:865:LEU:CD1   | 1.88                     | 1.20              |
| 1:A:1107:ARG:NH1 | 1:B:904:TYR:CD1   | 1.84                     | 1.20              |
| 1:A:917:TYR:HB3  | 1:C:1129:VAL:CG2  | 1.71                     | 1.18              |
| 1:A:712:ILE:HB   | 1:A:1077:THR:HG21 | 1.24                     | 1.18              |
| 1:C:101:ILE:HD12 | 1:C:242:LEU:CD2   | 1.74                     | 1.17              |
| 1:C:101:ILE:CD1  | 1:C:242:LEU:HD21  | 1.74                     | 1.17              |
| 1:A:101:ILE:HD12 | 1:A:242:LEU:CD2   | 1.74                     | 1.16              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:697:MET:HE1  | 1:C:864:LEU:CD1   | 1.74                     | 1.16              |
| 1:B:101:ILE:HD12 | 1:B:242:LEU:CD2   | 1.74                     | 1.15              |
| 1:B:101:ILE:CD1  | 1:B:242:LEU:HD21  | 1.74                     | 1.15              |
| 1:A:779:GLN:OE1  | 1:A:865:LEU:HD11  | 1.45                     | 1.15              |
| 1:B:712:ILE:HB   | 1:B:1077:THR:HG21 | 1.24                     | 1.15              |
| 1:A:101:ILE:CD1  | 1:A:242:LEU:HD21  | 1.74                     | 1.14              |
| 1:A:697:MET:HE1  | 1:B:864:LEU:CG    | 1.79                     | 1.12              |
| 1:B:697:MET:HE1  | 1:C:864:LEU:CG    | 1.77                     | 1.12              |
| 1:A:130:VAL:CG1  | 1:A:233:ILE:HD11  | 1.80                     | 1.12              |
| 1:B:130:VAL:CG1  | 1:B:233:ILE:HD11  | 1.80                     | 1.12              |
| 1:B:779:GLN:OE1  | 1:B:865:LEU:HD11  | 1.45                     | 1.12              |
| 1:C:779:GLN:OE1  | 1:C:865:LEU:HD11  | 1.45                     | 1.12              |
| 1:A:864:LEU:CG   | 1:C:697:MET:HE1   | 1.77                     | 1.12              |
| 1:A:864:LEU:CD1  | 1:C:697:MET:HE1   | 1.74                     | 1.11              |
| 1:C:712:ILE:HB   | 1:C:1077:THR:HG21 | 1.24                     | 1.11              |
| 1:C:130:VAL:CG1  | 1:C:233:ILE:HD11  | 1.80                     | 1.10              |
| 1:A:599:THR:HG22 | 1:A:608:VAL:HG12  | 1.37                     | 1.07              |
| 1:C:1031:GLU:OE2 | 1:C:1039:ARG:HD2  | 1.54                     | 1.06              |
| 1:A:560:LEU:HD22 | 1:B:224:GLU:OE2   | 1.56                     | 1.06              |
| 1:B:697:MET:HE3  | 1:C:864:LEU:CD1   | 1.85                     | 1.05              |
| 1:A:697:MET:HE1  | 1:B:864:LEU:HD11  | 1.32                     | 1.05              |
| 1:B:1031:GLU:OE2 | 1:B:1039:ARG:HD3  | 1.56                     | 1.05              |
| 2:F:22:CYS:SG    | 2:F:36:TRP:CH2    | 2.50                     | 1.05              |
| 2:D:22:CYS:SG    | 2:D:36:TRP:CH2    | 2.50                     | 1.05              |
| 1:B:560:LEU:HD22 | 1:C:224:GLU:OE2   | 1.54                     | 1.04              |
| 1:B:697:MET:HE1  | 1:C:864:LEU:HD11  | 1.30                     | 1.04              |
| 1:A:864:LEU:CD1  | 1:C:697:MET:HE3   | 1.85                     | 1.04              |
| 1:B:599:THR:HG22 | 1:B:608:VAL:HG12  | 1.37                     | 1.04              |
| 1:A:697:MET:HE3  | 1:B:864:LEU:HD11  | 1.40                     | 1.04              |
| 1:B:1031:GLU:OE2 | 1:B:1039:ARG:HD2  | 1.54                     | 1.04              |
| 1:A:224:GLU:OE2  | 1:C:560:LEU:HD22  | 1.54                     | 1.03              |
| 2:D:21:SER:OG    | 2:D:73:THR:HG22   | 1.58                     | 1.03              |
| 2:H:21:SER:OG    | 2:H:73:THR:HG22   | 1.58                     | 1.03              |
| 2:D:92:TRP:CD1   | 3:E:107:TYR:HH    | 1.76                     | 1.03              |
| 1:C:599:THR:HG22 | 1:C:608:VAL:HG12  | 1.37                     | 1.03              |
| 1:A:864:LEU:HD11 | 1:C:697:MET:HE1   | 1.30                     | 1.02              |
| 1:A:1031:GLU:OE2 | 1:A:1039:ARG:HD2  | 1.54                     | 1.02              |
| 2:F:92:TRP:CD1   | 3:G:107:TYR:HH    | 1.76                     | 1.02              |
| 1:A:130:VAL:HG11 | 1:A:233:ILE:HD11  | 1.39                     | 1.02              |
| 1:B:697:MET:HE3  | 1:C:864:LEU:HD11  | 1.39                     | 1.01              |
| 1:C:130:VAL:HG11 | 1:C:233:ILE:HD11  | 1.39                     | 1.01              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:697:MET:HE3   | 1:B:864:LEU:CD1   | 1.86                     | 1.01              |
| 1:B:130:VAL:HG11  | 1:B:233:ILE:HD11  | 1.39                     | 1.01              |
| 2:F:21:SER:OG     | 2:F:73:THR:HG22   | 1.58                     | 1.01              |
| 1:A:1129:VAL:HG21 | 1:B:917:TYR:HB3   | 1.42                     | 1.00              |
| 1:A:1031:GLU:OE2  | 1:A:1039:ARG:HD3  | 1.56                     | 1.00              |
| 1:B:560:LEU:HD21  | 1:C:224:GLU:OE2   | 1.62                     | 1.00              |
| 1:A:224:GLU:OE2   | 1:C:560:LEU:HD21  | 1.61                     | 0.98              |
| 1:A:864:LEU:HD11  | 1:C:697:MET:HE3   | 1.40                     | 0.98              |
| 1:B:472:ILE:HG23  | 1:B:488:CYS:O     | 1.64                     | 0.98              |
| 1:C:1031:GLU:OE2  | 1:C:1039:ARG:HD3  | 1.56                     | 0.98              |
| 1:A:472:ILE:HG23  | 1:A:488:CYS:O     | 1.64                     | 0.98              |
| 1:A:917:TYR:CD2   | 1:C:1089:PHE:HE2  | 1.81                     | 0.98              |
| 1:A:712:ILE:HB    | 1:A:1077:THR:CG2  | 1.95                     | 0.97              |
| 1:C:472:ILE:HG23  | 1:C:488:CYS:O     | 1.64                     | 0.97              |
| 1:C:712:ILE:HB    | 1:C:1077:THR:CG2  | 1.95                     | 0.97              |
| 1:B:355:ARG:NH2   | 1:B:396:TYR:CD2   | 2.34                     | 0.96              |
| 1:A:894:LEU:CD1   | 1:C:715:PRO:HD3   | 1.94                     | 0.96              |
| 1:A:917:TYR:HB3   | 1:C:1129:VAL:HG21 | 1.42                     | 0.96              |
| 1:B:712:ILE:HB    | 1:B:1077:THR:CG2  | 1.95                     | 0.96              |
| 1:B:1089:PHE:HE2  | 1:C:917:TYR:CD2   | 1.82                     | 0.96              |
| 1:B:715:PRO:HD3   | 1:C:894:LEU:CD1   | 1.96                     | 0.95              |
| 1:A:1089:PHE:HE2  | 1:B:917:TYR:CD2   | 1.84                     | 0.95              |
| 1:A:904:TYR:HD1   | 1:C:1107:ARG:HH12 | 1.13                     | 0.95              |
| 1:B:1129:VAL:HG21 | 1:C:917:TYR:HB3   | 1.44                     | 0.95              |
| 1:A:355:ARG:NH2   | 1:A:396:TYR:CD2   | 2.34                     | 0.95              |
| 1:A:715:PRO:HD3   | 1:B:894:LEU:CD1   | 1.96                     | 0.95              |
| 1:C:355:ARG:NH2   | 1:C:396:TYR:CD2   | 2.34                     | 0.95              |
| 1:A:779:GLN:OE1   | 1:A:865:LEU:HD13  | 1.67                     | 0.94              |
| 3:I:90:ASP:OD1    | 3:I:94:TYR:OH     | 1.85                     | 0.94              |
| 3:G:90:ASP:OD1    | 3:G:94:TYR:OH     | 1.85                     | 0.94              |
| 1:A:917:TYR:HD2   | 1:C:1089:PHE:CE2  | 1.86                     | 0.93              |
| 3:E:90:ASP:OD1    | 3:E:94:TYR:OH     | 1.85                     | 0.93              |
| 1:A:560:LEU:HD21  | 1:B:224:GLU:OE2   | 1.63                     | 0.93              |
| 1:A:1107:ARG:HH12 | 1:B:904:TYR:HD1   | 1.13                     | 0.93              |
| 1:B:560:LEU:CD2   | 1:C:224:GLU:CD    | 2.42                     | 0.93              |
| 1:A:224:GLU:CD    | 1:C:560:LEU:CD2   | 2.41                     | 0.93              |
| 1:B:779:GLN:OE1   | 1:B:865:LEU:HD13  | 1.68                     | 0.93              |
| 1:C:779:GLN:OE1   | 1:C:865:LEU:HD13  | 1.67                     | 0.93              |
| 1:A:697:MET:HE2   | 1:B:864:LEU:HD11  | 0.92                     | 0.92              |
| 1:B:562:PHE:CE2   | 1:C:225:PRO:HD2   | 2.05                     | 0.92              |
| 1:B:1089:PHE:CE2  | 1:C:917:TYR:HD2   | 1.88                     | 0.91              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:560:LEU:CD2   | 1:B:224:GLU:CD   | 2.44                     | 0.91              |
| 1:A:689:SER:C     | 1:A:690:GLN:OE1  | 2.14                     | 0.91              |
| 1:A:697:MET:HE1   | 1:B:864:LEU:CD1  | 1.76                     | 0.91              |
| 1:A:225:PRO:HD2   | 1:C:562:PHE:CE2  | 2.05                     | 0.91              |
| 1:A:599:THR:HG22  | 1:A:608:VAL:CG1  | 2.01                     | 0.90              |
| 1:C:689:SER:C     | 1:C:690:GLN:OE1  | 2.14                     | 0.90              |
| 1:A:562:PHE:CE2   | 1:B:225:PRO:HD2  | 2.07                     | 0.90              |
| 1:A:965:GLN:HE22  | 1:B:758:SER:H    | 1.17                     | 0.90              |
| 1:B:689:SER:C     | 1:B:690:GLN:OE1  | 2.14                     | 0.90              |
| 1:C:599:THR:HG22  | 1:C:608:VAL:CG1  | 2.01                     | 0.90              |
| 1:A:864:LEU:HG    | 1:C:697:MET:HE1  | 1.53                     | 0.90              |
| 1:B:697:MET:HE1   | 1:C:864:LEU:HG   | 1.54                     | 0.90              |
| 1:B:697:MET:HE2   | 1:C:864:LEU:HD11 | 0.91                     | 0.90              |
| 2:D:92:TRP:CZ2    | 3:E:101:TYR:OH   | 2.25                     | 0.90              |
| 1:C:130:VAL:HG13  | 1:C:233:ILE:CD1  | 2.03                     | 0.89              |
| 1:B:560:LEU:HD23  | 1:C:224:GLU:CD   | 1.97                     | 0.89              |
| 1:A:1089:PHE:CE2  | 1:B:917:TYR:HD2  | 1.89                     | 0.89              |
| 1:B:599:THR:HG22  | 1:B:608:VAL:CG1  | 2.01                     | 0.89              |
| 1:B:1089:PHE:HE2  | 1:C:917:TYR:HD2  | 0.95                     | 0.89              |
| 1:A:224:GLU:CD    | 1:C:560:LEU:HD23 | 1.97                     | 0.89              |
| 1:A:864:LEU:HD11  | 1:C:697:MET:HE2  | 0.91                     | 0.89              |
| 1:B:130:VAL:HG13  | 1:B:233:ILE:CD1  | 2.03                     | 0.88              |
| 2:F:92:TRP:CZ2    | 3:G:101:TYR:OH   | 2.25                     | 0.88              |
| 1:A:560:LEU:HD23  | 1:B:224:GLU:CD   | 1.99                     | 0.88              |
| 1:A:917:TYR:HD2   | 1:C:1089:PHE:HE2 | 0.93                     | 0.88              |
| 1:A:130:VAL:HG13  | 1:A:233:ILE:CD1  | 2.03                     | 0.88              |
| 1:B:1107:ARG:HH12 | 1:C:904:TYR:HD1  | 1.15                     | 0.88              |
| 1:C:355:ARG:NH2   | 1:C:396:TYR:CG   | 2.42                     | 0.87              |
| 3:G:40:MET:HB2    | 3:G:43:LYS:HB2   | 1.56                     | 0.87              |
| 1:B:231:ILE:HG22  | 1:B:233:ILE:HG13 | 1.57                     | 0.87              |
| 3:E:40:MET:HB2    | 3:E:43:LYS:HB2   | 1.57                     | 0.87              |
| 1:B:355:ARG:NH2   | 1:B:396:TYR:CG   | 2.42                     | 0.87              |
| 3:I:40:MET:HB2    | 3:I:43:LYS:HB2   | 1.56                     | 0.87              |
| 1:A:540:ASN:OD1   | 1:A:549:THR:HG22 | 1.75                     | 0.87              |
| 1:B:965:GLN:HE22  | 1:C:758:SER:H    | 1.18                     | 0.87              |
| 1:A:130:VAL:HG13  | 1:A:233:ILE:HD11 | 1.56                     | 0.87              |
| 1:B:101:ILE:HD12  | 1:B:242:LEU:HD21 | 0.89                     | 0.87              |
| 1:B:540:ASN:OD1   | 1:B:549:THR:HG22 | 1.75                     | 0.86              |
| 1:A:705:VAL:CG1   | 1:B:883:THR:HG21 | 2.06                     | 0.86              |
| 1:B:715:PRO:HD3   | 1:C:894:LEU:HD11 | 1.57                     | 0.86              |
| 1:C:231:ILE:HG22  | 1:C:233:ILE:HG13 | 1.57                     | 0.86              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:758:SER:H     | 1:C:965:GLN:HE22  | 1.18                     | 0.86              |
| 1:B:1129:VAL:HG23 | 1:C:917:TYR:HB3   | 1.57                     | 0.86              |
| 1:A:101:ILE:HD12  | 1:A:242:LEU:HD21  | 0.89                     | 0.86              |
| 1:A:231:ILE:HG22  | 1:A:233:ILE:HG13  | 1.57                     | 0.86              |
| 1:A:355:ARG:NH2   | 1:A:396:TYR:CG    | 2.42                     | 0.86              |
| 1:C:540:ASN:OD1   | 1:C:549:THR:HG22  | 1.75                     | 0.85              |
| 1:A:538:CYS:HB3   | 1:A:590:CYS:HB3   | 1.58                     | 0.85              |
| 1:C:101:ILE:HD12  | 1:C:242:LEU:HD21  | 0.89                     | 0.85              |
| 1:B:130:VAL:HG13  | 1:B:233:ILE:HD11  | 1.56                     | 0.85              |
| 1:A:699:LEU:HB3   | 1:B:788:ILE:HD11  | 1.56                     | 0.85              |
| 1:A:697:MET:HE1   | 1:B:864:LEU:HG    | 1.54                     | 0.85              |
| 1:A:917:TYR:HB3   | 1:C:1129:VAL:HG23 | 1.59                     | 0.85              |
| 1:A:1129:VAL:HG23 | 1:B:917:TYR:HB3   | 1.56                     | 0.85              |
| 1:C:538:CYS:HB3   | 1:C:590:CYS:HB3   | 1.59                     | 0.85              |
| 1:A:715:PRO:HD3   | 1:B:894:LEU:HD11  | 1.58                     | 0.85              |
| 1:A:788:ILE:HD11  | 1:C:699:LEU:HB3   | 1.59                     | 0.85              |
| 1:A:904:TYR:OH    | 1:C:1094:VAL:HG12 | 1.76                     | 0.85              |
| 1:B:775:ASP:O     | 1:B:779:GLN:HG2   | 1.77                     | 0.84              |
| 1:A:775:ASP:O     | 1:A:779:GLN:HG2   | 1.77                     | 0.84              |
| 1:B:699:LEU:HB3   | 1:C:788:ILE:HD11  | 1.58                     | 0.84              |
| 1:A:894:LEU:HD11  | 1:C:715:PRO:HD3   | 1.56                     | 0.84              |
| 1:C:775:ASP:O     | 1:C:779:GLN:HG2   | 1.77                     | 0.84              |
| 1:A:883:THR:HG21  | 1:C:705:VAL:CG1   | 2.07                     | 0.84              |
| 1:B:705:VAL:CG1   | 1:C:883:THR:HG21  | 2.08                     | 0.84              |
| 1:A:1094:VAL:HG12 | 1:B:904:TYR:OH    | 1.78                     | 0.83              |
| 1:B:540:ASN:OD1   | 1:B:549:THR:CG2   | 2.26                     | 0.83              |
| 1:A:540:ASN:OD1   | 1:A:549:THR:CG2   | 2.26                     | 0.83              |
| 1:A:1107:ARG:CZ   | 1:B:904:TYR:CE1   | 2.29                     | 0.83              |
| 1:A:1089:PHE:HE2  | 1:B:917:TYR:HD2   | 0.96                     | 0.83              |
| 1:A:701:ALA:O     | 1:B:787:GLN:HB3   | 1.78                     | 0.83              |
| 3:E:35:GLY:HA3    | 3:E:50:ILE:HG22   | 1.61                     | 0.82              |
| 1:B:538:CYS:HB3   | 1:B:590:CYS:HB3   | 1.58                     | 0.82              |
| 2:F:22:CYS:SG     | 2:F:36:TRP:CZ2    | 2.73                     | 0.82              |
| 1:C:540:ASN:OD1   | 1:C:549:THR:CG2   | 2.26                     | 0.82              |
| 3:G:35:GLY:HA3    | 3:G:50:ILE:HG22   | 1.61                     | 0.82              |
| 1:A:130:VAL:CG1   | 1:A:233:ILE:CD1   | 2.58                     | 0.82              |
| 1:A:904:TYR:CE1   | 1:C:1107:ARG:CZ   | 2.29                     | 0.82              |
| 1:B:130:VAL:CG1   | 1:B:233:ILE:CD1   | 2.58                     | 0.81              |
| 1:B:216:LEU:HD12  | 1:B:217:PRO:HD2   | 1.62                     | 0.81              |
| 1:B:701:ALA:O     | 1:C:787:GLN:HB3   | 1.80                     | 0.81              |
| 3:I:35:GLY:HA3    | 3:I:50:ILE:HG22   | 1.60                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:725:GLU:OE1   | 1:B:1064:HIS:NE2  | 2.14                     | 0.81              |
| 1:B:1094:VAL:HG12 | 1:C:904:TYR:OH    | 1.79                     | 0.81              |
| 1:C:130:VAL:CG1   | 1:C:233:ILE:CD1   | 2.58                     | 0.81              |
| 1:A:216:LEU:HD12  | 1:A:217:PRO:HD2   | 1.62                     | 0.81              |
| 1:A:894:LEU:HD13  | 1:C:715:PRO:HD3   | 1.63                     | 0.81              |
| 2:D:22:CYS:SG     | 2:D:36:TRP:CZ2    | 2.73                     | 0.81              |
| 1:A:725:GLU:OE1   | 1:A:1064:HIS:NE2  | 2.14                     | 0.80              |
| 1:C:216:LEU:HD12  | 1:C:217:PRO:HD2   | 1.62                     | 0.80              |
| 1:C:900:MET:CE    | 1:C:904:TYR:OH    | 2.30                     | 0.80              |
| 1:A:355:ARG:NE    | 1:A:396:TYR:CD1   | 2.50                     | 0.80              |
| 3:E:104:ASN:H     | 3:E:108:PHE:HE2   | 1.27                     | 0.80              |
| 1:A:787:GLN:HB3   | 1:C:701:ALA:O     | 1.81                     | 0.80              |
| 1:C:64:TRP:HE1    | 1:C:264:ALA:HB1   | 1.47                     | 0.79              |
| 1:A:900:MET:CE    | 1:A:904:TYR:OH    | 2.30                     | 0.79              |
| 1:B:355:ARG:NE    | 1:B:396:TYR:CD1   | 2.50                     | 0.79              |
| 1:B:64:TRP:HE1    | 1:B:264:ALA:HB1   | 1.47                     | 0.79              |
| 1:C:130:VAL:HG13  | 1:C:233:ILE:HD11  | 1.56                     | 0.79              |
| 1:A:917:TYR:CB    | 1:C:1129:VAL:HG21 | 2.13                     | 0.79              |
| 1:C:355:ARG:NE    | 1:C:396:TYR:CD1   | 2.50                     | 0.79              |
| 1:B:900:MET:CE    | 1:B:904:TYR:OH    | 2.30                     | 0.79              |
| 1:C:725:GLU:OE1   | 1:C:1064:HIS:NE2  | 2.14                     | 0.79              |
| 1:A:1129:VAL:HG21 | 1:B:917:TYR:CB    | 2.12                     | 0.79              |
| 1:A:699:LEU:HD22  | 1:B:873:TYR:CZ    | 2.18                     | 0.79              |
| 1:A:64:TRP:HE1    | 1:A:264:ALA:HB1   | 1.47                     | 0.78              |
| 1:B:1107:ARG:NH1  | 1:C:904:TYR:HD1   | 1.74                     | 0.78              |
| 2:F:22:CYS:HG     | 2:F:36:TRP:HH2    | 1.27                     | 0.78              |
| 1:A:28:TYR:HA     | 1:A:62:VAL:O      | 1.84                     | 0.78              |
| 1:A:715:PRO:HD3   | 1:B:894:LEU:HD13  | 1.65                     | 0.78              |
| 1:B:1129:VAL:HG21 | 1:C:917:TYR:CB    | 2.13                     | 0.78              |
| 1:B:28:TYR:HA     | 1:B:62:VAL:O      | 1.84                     | 0.78              |
| 3:G:104:ASN:H     | 3:G:108:PHE:HE2   | 1.28                     | 0.78              |
| 1:A:597:VAL:HG22  | 1:A:610:VAL:HG22  | 1.66                     | 0.77              |
| 1:B:699:LEU:HD22  | 1:C:873:TYR:CZ    | 2.19                     | 0.77              |
| 1:C:597:VAL:HG22  | 1:C:610:VAL:HG22  | 1.66                     | 0.77              |
| 1:A:328:ARG:HH21  | 1:A:580:GLN:HB2   | 1.50                     | 0.77              |
| 1:A:905:ARG:NH1   | 1:A:1049:LEU:O    | 2.18                     | 0.77              |
| 2:D:22:CYS:HG     | 2:D:36:TRP:HH2    | 1.26                     | 0.77              |
| 1:C:28:TYR:HA     | 1:C:62:VAL:O      | 1.83                     | 0.77              |
| 1:A:864:LEU:CD1   | 1:C:697:MET:HE2   | 1.87                     | 0.76              |
| 1:A:873:TYR:CZ    | 1:C:699:LEU:HD22  | 2.20                     | 0.76              |
| 1:A:43:PHE:N      | 1:C:565:PHE:O     | 2.18                     | 0.76              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:328:ARG:HH21 | 1:C:580:GLN:HB2  | 1.50                     | 0.76              |
| 1:C:905:ARG:NH1  | 1:C:1049:LEU:O   | 2.18                     | 0.76              |
| 1:B:565:PHE:O    | 1:C:43:PHE:N     | 2.17                     | 0.76              |
| 1:B:1031:GLU:OE1 | 1:B:1042:PHE:CE2 | 2.39                     | 0.76              |
| 1:A:1031:GLU:OE1 | 1:A:1042:PHE:CE2 | 2.39                     | 0.76              |
| 1:B:597:VAL:HG22 | 1:B:610:VAL:HG22 | 1.66                     | 0.75              |
| 1:B:328:ARG:HH21 | 1:B:580:GLN:HB2  | 1.50                     | 0.75              |
| 1:B:538:CYS:CB   | 1:B:590:CYS:HB3  | 2.16                     | 0.75              |
| 3:E:104:ASN:N    | 3:E:108:PHE:HE2  | 1.84                     | 0.75              |
| 1:B:715:PRO:HD3  | 1:C:894:LEU:HD13 | 1.66                     | 0.75              |
| 1:C:1031:GLU:OE1 | 1:C:1042:PHE:CE2 | 2.39                     | 0.75              |
| 3:G:104:ASN:N    | 3:G:108:PHE:HE2  | 1.84                     | 0.75              |
| 1:A:33:THR:OG1   | 1:A:219:GLY:O    | 2.04                     | 0.75              |
| 1:C:538:CYS:CB   | 1:C:590:CYS:HB3  | 2.16                     | 0.75              |
| 1:A:617:CYS:SG   | 1:A:644:GLN:NE2  | 2.61                     | 0.74              |
| 1:B:905:ARG:NH1  | 1:B:1049:LEU:O   | 2.18                     | 0.74              |
| 1:B:33:THR:OG1   | 1:B:219:GLY:O    | 2.04                     | 0.74              |
| 1:B:461:LEU:HD12 | 1:B:461:LEU:C    | 2.13                     | 0.74              |
| 1:B:617:CYS:SG   | 1:B:644:GLN:NE2  | 2.60                     | 0.74              |
| 1:C:461:LEU:C    | 1:C:461:LEU:HD12 | 2.13                     | 0.74              |
| 2:F:81:THR:HA    | 2:F:109:VAL:HG21 | 1.70                     | 0.74              |
| 1:A:538:CYS:CB   | 1:A:590:CYS:HB3  | 2.16                     | 0.74              |
| 2:H:81:THR:HA    | 2:H:109:VAL:HG21 | 1.70                     | 0.74              |
| 1:A:461:LEU:C    | 1:A:461:LEU:HD12 | 2.13                     | 0.74              |
| 2:D:92:TRP:CD1   | 3:E:107:TYR:OH   | 2.41                     | 0.74              |
| 1:C:617:CYS:SG   | 1:C:644:GLN:NE2  | 2.60                     | 0.74              |
| 1:A:864:LEU:HD12 | 1:C:697:MET:HE3  | 1.69                     | 0.74              |
| 1:B:965:GLN:NE2  | 1:C:758:SER:H    | 1.86                     | 0.73              |
| 1:A:538:CYS:SG   | 1:A:590:CYS:CB   | 2.77                     | 0.73              |
| 1:B:642:VAL:HG13 | 1:B:651:ILE:HG22 | 1.71                     | 0.73              |
| 1:A:965:GLN:NE2  | 1:B:758:SER:H    | 1.86                     | 0.73              |
| 2:D:81:THR:HA    | 2:D:109:VAL:HG21 | 1.70                     | 0.73              |
| 1:C:472:ILE:HA   | 1:C:490:PHE:HA   | 1.70                     | 0.73              |
| 1:A:565:PHE:O    | 1:B:43:PHE:N     | 2.18                     | 0.73              |
| 1:A:503:VAL:HA   | 1:A:506:GLN:HG2  | 1.71                     | 0.72              |
| 1:B:538:CYS:SG   | 1:B:590:CYS:CB   | 2.77                     | 0.72              |
| 1:A:360:ASN:H    | 1:A:523:THR:HG22 | 1.54                     | 0.72              |
| 1:B:503:VAL:HA   | 1:B:506:GLN:HG2  | 1.71                     | 0.72              |
| 1:B:1107:ARG:CZ  | 1:C:904:TYR:CE1  | 2.31                     | 0.72              |
| 1:C:538:CYS:SG   | 1:C:590:CYS:CB   | 2.77                     | 0.72              |
| 1:A:1135:ASN:OD1 | 1:A:1136:THR:N   | 2.22                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:758:SER:H    | 1:C:965:GLN:NE2  | 1.86                     | 0.72              |
| 1:A:917:TYR:CB   | 1:C:1129:VAL:CG2 | 2.61                     | 0.72              |
| 1:A:224:GLU:OE1  | 1:C:560:LEU:HD23 | 1.90                     | 0.72              |
| 1:A:917:TYR:CD2  | 1:C:1089:PHE:CE2 | 2.70                     | 0.72              |
| 2:F:92:TRP:CD1   | 3:G:107:TYR:OH   | 2.41                     | 0.72              |
| 3:G:98:ARG:HH21  | 3:G:112:ILE:HG13 | 1.55                     | 0.72              |
| 1:A:642:VAL:HG13 | 1:A:651:ILE:HG22 | 1.71                     | 0.72              |
| 1:C:503:VAL:HA   | 1:C:506:GLN:HG2  | 1.71                     | 0.72              |
| 1:A:538:CYS:HG   | 1:A:590:CYS:HG   | 0.98                     | 0.71              |
| 2:D:66:SER:OG    | 2:D:73:THR:OG1   | 2.08                     | 0.71              |
| 1:A:697:MET:HE3  | 1:B:864:LEU:HD12 | 1.71                     | 0.71              |
| 3:E:98:ARG:HH21  | 3:E:112:ILE:HG13 | 1.55                     | 0.71              |
| 1:B:1135:ASN:OD1 | 1:B:1136:THR:N   | 2.22                     | 0.71              |
| 1:C:360:ASN:H    | 1:C:523:THR:HG22 | 1.55                     | 0.71              |
| 3:I:23:LYS:HG2   | 3:I:78:THR:HG22  | 1.72                     | 0.71              |
| 3:G:23:LYS:HG2   | 3:G:78:THR:HG22  | 1.72                     | 0.71              |
| 1:A:472:ILE:HA   | 1:A:490:PHE:HA   | 1.70                     | 0.71              |
| 1:A:563:GLN:HA   | 1:B:41:LYS:HB2   | 1.71                     | 0.71              |
| 1:B:360:ASN:H    | 1:B:523:THR:HG22 | 1.55                     | 0.71              |
| 1:B:697:MET:HE3  | 1:C:864:LEU:HD12 | 1.69                     | 0.71              |
| 1:C:642:VAL:HG13 | 1:C:651:ILE:HG22 | 1.70                     | 0.71              |
| 3:I:98:ARG:HH21  | 3:I:112:ILE:HG13 | 1.56                     | 0.71              |
| 1:B:560:LEU:HD23 | 1:C:224:GLU:OE1  | 1.90                     | 0.70              |
| 1:B:472:ILE:HA   | 1:B:490:PHE:HA   | 1.70                     | 0.70              |
| 1:A:1041:ASP:OD1 | 1:A:1041:ASP:O   | 2.10                     | 0.70              |
| 3:E:23:LYS:HG2   | 3:E:78:THR:HG22  | 1.72                     | 0.70              |
| 1:B:1089:PHE:CE2 | 1:C:917:TYR:CD2  | 2.72                     | 0.70              |
| 1:B:316:SER:OG   | 1:B:317:ASN:N    | 2.25                     | 0.69              |
| 1:B:1041:ASP:OD1 | 1:B:1041:ASP:O   | 2.10                     | 0.69              |
| 3:E:100:GLN:HB2  | 3:E:110:TYR:HB2  | 1.72                     | 0.69              |
| 1:A:316:SER:OG   | 1:A:317:ASN:N    | 2.26                     | 0.69              |
| 1:B:425:LEU:HD22 | 1:B:430:THR:HG21 | 1.74                     | 0.69              |
| 1:C:461:LEU:CD1  | 1:C:462:LYS:O    | 2.41                     | 0.69              |
| 1:C:1135:ASN:OD1 | 1:C:1136:THR:N   | 2.22                     | 0.69              |
| 1:C:425:LEU:HD22 | 1:C:430:THR:HG21 | 1.74                     | 0.69              |
| 1:A:779:GLN:CD   | 1:A:865:LEU:HD11 | 2.18                     | 0.69              |
| 1:A:560:LEU:HD23 | 1:B:224:GLU:OE1  | 1.92                     | 0.69              |
| 1:C:1041:ASP:OD1 | 1:C:1041:ASP:O   | 2.10                     | 0.69              |
| 1:B:1129:VAL:CG2 | 1:C:917:TYR:CB   | 2.61                     | 0.69              |
| 2:H:66:SER:OG    | 2:H:73:THR:OG1   | 2.08                     | 0.69              |
| 1:B:974:SER:O    | 1:B:980:ILE:HD11 | 1.93                     | 0.69              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:461:LEU:CD1  | 1:A:462:LYS:O     | 2.41                     | 0.68              |
| 2:H:93:HIS:CE1   | 2:H:96:LEU:HG     | 2.28                     | 0.68              |
| 1:C:61:ASN:OD1   | 1:C:61:ASN:O      | 2.11                     | 0.68              |
| 1:C:779:GLN:CD   | 1:C:865:LEU:HD11  | 2.18                     | 0.68              |
| 1:A:425:LEU:HD22 | 1:A:430:THR:HG21  | 1.74                     | 0.68              |
| 1:C:900:MET:HE3  | 1:C:904:TYR:OH    | 1.94                     | 0.68              |
| 2:F:93:HIS:CE1   | 2:F:96:LEU:HG     | 2.28                     | 0.68              |
| 1:A:974:SER:O    | 1:A:980:ILE:HD11  | 1.93                     | 0.68              |
| 1:A:61:ASN:OD1   | 1:A:61:ASN:O      | 2.11                     | 0.68              |
| 2:F:66:SER:HG    | 2:F:73:THR:HG1    | 1.38                     | 0.68              |
| 1:B:461:LEU:CD1  | 1:B:462:LYS:O     | 2.41                     | 0.68              |
| 3:I:86:LEU:HD11  | 3:I:120:THR:HB    | 1.75                     | 0.68              |
| 1:B:61:ASN:OD1   | 1:B:61:ASN:O      | 2.11                     | 0.68              |
| 1:A:697:MET:HE2  | 1:B:864:LEU:CD1   | 1.89                     | 0.67              |
| 1:A:904:TYR:HD1  | 1:C:1107:ARG:NH1  | 1.72                     | 0.67              |
| 1:B:441:LEU:O    | 3:G:59:ARG:NH2    | 2.28                     | 0.67              |
| 1:B:697:MET:HE2  | 1:C:864:LEU:CD1   | 1.88                     | 0.67              |
| 1:B:779:GLN:CD   | 1:B:865:LEU:HD11  | 2.18                     | 0.67              |
| 3:G:86:LEU:HD11  | 3:G:120:THR:HB    | 1.75                     | 0.67              |
| 2:D:93:HIS:CE1   | 2:D:96:LEU:HG     | 2.29                     | 0.67              |
| 1:B:43:PHE:HE1   | 1:B:283:GLY:HA3   | 1.59                     | 0.67              |
| 1:C:43:PHE:HE1   | 1:C:283:GLY:HA3   | 1.59                     | 0.67              |
| 1:C:974:SER:O    | 1:C:980:ILE:HD11  | 1.93                     | 0.67              |
| 1:B:439:ASN:ND2  | 1:B:506:GLN:OE1   | 2.28                     | 0.67              |
| 1:C:316:SER:OG   | 1:C:317:ASN:N     | 2.25                     | 0.67              |
| 2:F:66:SER:OG    | 2:F:73:THR:OG1    | 2.08                     | 0.67              |
| 1:C:439:ASN:ND2  | 1:C:506:GLN:OE1   | 2.28                     | 0.67              |
| 2:F:22:CYS:SG    | 2:F:89:CYS:CB     | 2.83                     | 0.67              |
| 1:B:563:GLN:HA   | 1:C:41:LYS:HB3    | 1.75                     | 0.67              |
| 3:I:18:LEU:HB2   | 3:I:83:TRP:CD1    | 2.30                     | 0.67              |
| 1:A:91:TYR:N     | 1:A:268:GLY:O     | 2.26                     | 0.67              |
| 1:C:441:LEU:O    | 3:I:59:ARG:NH2    | 2.28                     | 0.67              |
| 1:A:439:ASN:ND2  | 1:A:506:GLN:OE1   | 2.28                     | 0.66              |
| 1:A:917:TYR:CG   | 1:C:1129:VAL:HG21 | 2.31                     | 0.66              |
| 1:B:355:ARG:NH2  | 1:B:396:TYR:CE2   | 2.63                     | 0.66              |
| 3:E:18:LEU:HB2   | 3:E:83:TRP:CD1    | 2.30                     | 0.66              |
| 1:A:900:MET:HE3  | 1:A:904:TYR:OH    | 1.94                     | 0.66              |
| 3:E:86:LEU:HD11  | 3:E:120:THR:HB    | 1.76                     | 0.66              |
| 1:B:93:ALA:HB1   | 1:B:189:LEU:HD21  | 1.78                     | 0.66              |
| 1:C:91:TYR:N     | 1:C:268:GLY:O     | 2.26                     | 0.66              |
| 1:A:441:LEU:O    | 3:E:59:ARG:NH2    | 2.28                     | 0.66              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1129:VAL:HG21 | 1:B:917:TYR:CG    | 2.30                     | 0.66              |
| 1:B:722:VAL:HG22  | 1:B:1065:VAL:HG22 | 1.78                     | 0.66              |
| 1:C:722:VAL:HG22  | 1:C:1065:VAL:HG22 | 1.78                     | 0.66              |
| 1:A:43:PHE:HE1    | 1:A:283:GLY:HA3   | 1.59                     | 0.66              |
| 1:A:93:ALA:HB1    | 1:A:189:LEU:HD21  | 1.78                     | 0.66              |
| 2:F:6:GLN:HG3     | 2:F:103:GLY:H     | 1.61                     | 0.66              |
| 1:B:1129:VAL:HG21 | 1:C:917:TYR:CG    | 2.30                     | 0.66              |
| 1:A:705:VAL:HG13  | 1:B:883:THR:HG21  | 1.76                     | 0.66              |
| 1:A:883:THR:HG21  | 1:C:705:VAL:HG13  | 1.77                     | 0.66              |
| 1:B:900:MET:HE3   | 1:B:904:TYR:OH    | 1.93                     | 0.66              |
| 2:H:22:CYS:SG     | 2:H:89:CYS:CB     | 2.83                     | 0.66              |
| 2:H:92:TRP:HA     | 2:H:99:GLY:HA2    | 1.77                     | 0.66              |
| 3:G:18:LEU:HB2    | 3:G:83:TRP:CD1    | 2.30                     | 0.66              |
| 2:F:92:TRP:HA     | 2:F:99:GLY:HA2    | 1.77                     | 0.65              |
| 2:D:22:CYS:SG     | 2:D:89:CYS:CB     | 2.83                     | 0.65              |
| 1:B:538:CYS:HG    | 1:B:590:CYS:CB    | 2.09                     | 0.65              |
| 1:B:1006:THR:OG1  | 1:C:1005:GLN:NE2  | 2.29                     | 0.65              |
| 2:D:92:TRP:HA     | 2:D:99:GLY:HA2    | 1.77                     | 0.65              |
| 1:A:722:VAL:HG22  | 1:A:1065:VAL:HG22 | 1.78                     | 0.65              |
| 2:H:6:GLN:HG3     | 2:H:103:GLY:H     | 1.61                     | 0.65              |
| 1:A:41:LYS:HB3    | 1:C:563:GLN:HA    | 1.79                     | 0.65              |
| 1:B:689:SER:O     | 1:B:690:GLN:CD    | 2.40                     | 0.65              |
| 1:C:93:ALA:HB1    | 1:C:189:LEU:HD21  | 1.78                     | 0.65              |
| 1:C:355:ARG:NH2   | 1:C:396:TYR:CE2   | 2.63                     | 0.65              |
| 1:C:689:SER:O     | 1:C:690:GLN:CD    | 2.40                     | 0.65              |
| 3:I:7:SER:OG      | 3:I:21:SER:OG     | 2.15                     | 0.65              |
| 2:H:6:GLN:OE1     | 2:H:104:GLY:N     | 2.30                     | 0.65              |
| 1:B:91:TYR:N      | 1:B:268:GLY:O     | 2.26                     | 0.64              |
| 1:B:880:GLY:O     | 1:B:884:SER:OG    | 2.14                     | 0.64              |
| 1:A:1005:GLN:NE2  | 1:C:1006:THR:OG1  | 2.30                     | 0.64              |
| 1:C:1085:GLY:O    | 1:C:1126:CYS:N    | 2.30                     | 0.64              |
| 1:A:689:SER:O     | 1:A:690:GLN:CD    | 2.40                     | 0.64              |
| 1:B:461:LEU:HD12  | 1:B:461:LEU:O     | 1.98                     | 0.64              |
| 1:A:1085:GLY:O    | 1:A:1126:CYS:N    | 2.30                     | 0.64              |
| 1:B:1085:GLY:O    | 1:B:1126:CYS:N    | 2.31                     | 0.64              |
| 1:A:689:SER:C     | 1:A:690:GLN:CD    | 2.66                     | 0.64              |
| 1:A:874:THR:O     | 1:A:878:LEU:HG    | 1.98                     | 0.64              |
| 1:B:874:THR:O     | 1:B:878:LEU:HG    | 1.98                     | 0.64              |
| 2:D:6:GLN:HG3     | 2:D:103:GLY:H     | 1.61                     | 0.64              |
| 1:A:461:LEU:HD12  | 1:A:461:LEU:O     | 1.98                     | 0.64              |
| 1:B:705:VAL:HG13  | 1:C:883:THR:HG21  | 1.78                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1129:VAL:CG2 | 1:B:917:TYR:CB   | 2.60                     | 0.64              |
| 2:D:6:GLN:OE1    | 2:D:104:GLY:N    | 2.30                     | 0.64              |
| 1:B:712:ILE:CB   | 1:B:1077:THR:CG2 | 2.75                     | 0.64              |
| 1:C:874:THR:O    | 1:C:878:LEU:HG   | 1.98                     | 0.64              |
| 1:A:102:ARG:H    | 1:A:242:LEU:HD23 | 1.63                     | 0.64              |
| 1:B:900:MET:HE2  | 1:B:904:TYR:CE2  | 2.33                     | 0.64              |
| 1:B:957:GLN:O    | 1:B:957:GLN:NE2  | 2.31                     | 0.64              |
| 1:C:461:LEU:HD12 | 1:C:461:LEU:O    | 1.98                     | 0.64              |
| 1:A:1006:THR:OG1 | 1:B:1005:GLN:NE2 | 2.30                     | 0.63              |
| 1:B:1097:SER:HB3 | 1:B:1102:TRP:CD2 | 2.34                     | 0.63              |
| 1:C:957:GLN:O    | 1:C:957:GLN:NE2  | 2.31                     | 0.63              |
| 1:B:102:ARG:H    | 1:B:242:LEU:HD23 | 1.63                     | 0.63              |
| 2:F:6:GLN:OE1    | 2:F:104:GLY:N    | 2.30                     | 0.63              |
| 1:A:472:ILE:HG22 | 1:A:472:ILE:O    | 1.98                     | 0.63              |
| 1:A:900:MET:HE2  | 1:A:904:TYR:CE2  | 2.33                     | 0.63              |
| 2:D:66:SER:HG    | 2:D:73:THR:HG1   | 1.45                     | 0.63              |
| 3:E:7:SER:OG     | 3:E:21:SER:OG    | 2.15                     | 0.63              |
| 1:C:900:MET:HE2  | 1:C:904:TYR:CE2  | 2.33                     | 0.63              |
| 1:A:1097:SER:HB3 | 1:A:1102:TRP:CD2 | 2.34                     | 0.63              |
| 1:B:775:ASP:O    | 1:B:779:GLN:CG   | 2.47                     | 0.63              |
| 1:C:689:SER:C    | 1:C:690:GLN:CD   | 2.66                     | 0.63              |
| 3:I:28:SER:OG    | 3:I:31:ASN:ND2   | 2.32                     | 0.63              |
| 1:A:108:THR:OG1  | 1:A:234:ASN:O    | 2.17                     | 0.63              |
| 1:A:712:ILE:CB   | 1:A:1077:THR:CG2 | 2.75                     | 0.63              |
| 3:E:90:ASP:OD1   | 3:E:90:ASP:O     | 2.17                     | 0.63              |
| 1:B:472:ILE:O    | 1:B:472:ILE:HG22 | 1.98                     | 0.63              |
| 1:A:1089:PHE:CE2 | 1:B:917:TYR:CD2  | 2.73                     | 0.63              |
| 1:A:957:GLN:O    | 1:A:957:GLN:NE2  | 2.31                     | 0.62              |
| 3:E:28:SER:OG    | 3:E:31:ASN:ND2   | 2.32                     | 0.62              |
| 1:B:689:SER:C    | 1:B:690:GLN:CD   | 2.66                     | 0.62              |
| 1:C:472:ILE:HG22 | 1:C:472:ILE:O    | 1.98                     | 0.62              |
| 1:A:597:VAL:HG13 | 1:A:609:ALA:O    | 1.99                     | 0.62              |
| 1:A:864:LEU:CD2  | 1:C:697:MET:HE1  | 2.29                     | 0.62              |
| 1:B:605:SER:OG   | 1:B:606:ASN:N    | 2.31                     | 0.62              |
| 3:I:93:MET:HE2   | 3:I:117:LYS:HG2  | 1.82                     | 0.62              |
| 1:A:772:VAL:HG12 | 1:A:772:VAL:O    | 2.00                     | 0.62              |
| 1:C:597:VAL:HG13 | 1:C:609:ALA:O    | 1.99                     | 0.62              |
| 2:H:34:VAL:HA    | 2:H:91:THR:OG1   | 1.98                     | 0.62              |
| 1:A:355:ARG:NH2  | 1:A:396:TYR:CE2  | 2.63                     | 0.62              |
| 1:A:697:MET:HE1  | 1:B:864:LEU:CD2  | 2.29                     | 0.62              |
| 3:G:28:SER:OG    | 3:G:31:ASN:ND2   | 2.32                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:102:ARG:H    | 1:C:242:LEU:HD23 | 1.63                     | 0.62              |
| 3:G:90:ASP:OD1   | 3:G:90:ASP:O     | 2.17                     | 0.62              |
| 1:B:1129:VAL:CB  | 1:C:917:TYR:HB3  | 2.30                     | 0.62              |
| 1:C:775:ASP:O    | 1:C:779:GLN:CG   | 2.47                     | 0.61              |
| 3:I:90:ASP:OD1   | 3:I:90:ASP:O     | 2.17                     | 0.61              |
| 1:B:597:VAL:HG13 | 1:B:609:ALA:O    | 1.99                     | 0.61              |
| 1:B:697:MET:HE1  | 1:C:864:LEU:CD2  | 2.29                     | 0.61              |
| 1:A:775:ASP:O    | 1:A:779:GLN:CG   | 2.47                     | 0.61              |
| 3:E:93:MET:HE2   | 3:E:117:LYS:HG2  | 1.82                     | 0.61              |
| 3:G:6:GLN:NE2    | 3:G:96:CYS:H     | 1.99                     | 0.61              |
| 1:A:1031:GLU:OE1 | 1:A:1042:PHE:HE2 | 1.82                     | 0.61              |
| 2:F:28:ASN:HB3   | 2:F:93:HIS:HA    | 1.83                     | 0.61              |
| 3:I:6:GLN:NE2    | 3:I:96:CYS:H     | 1.99                     | 0.61              |
| 3:E:87:LYS:HG2   | 3:E:90:ASP:HB2   | 1.82                     | 0.61              |
| 1:C:1097:SER:HB3 | 1:C:1102:TRP:CD2 | 2.34                     | 0.61              |
| 3:G:87:LYS:HG2   | 3:G:90:ASP:HB2   | 1.82                     | 0.61              |
| 1:B:1031:GLU:OE1 | 1:B:1042:PHE:HE2 | 1.82                     | 0.61              |
| 1:A:917:TYR:HB3  | 1:C:1129:VAL:CB  | 2.31                     | 0.61              |
| 3:E:6:GLN:NE2    | 3:E:96:CYS:H     | 1.99                     | 0.61              |
| 2:H:28:ASN:HB3   | 2:H:93:HIS:HA    | 1.83                     | 0.61              |
| 3:G:93:MET:HE2   | 3:G:117:LYS:HG2  | 1.82                     | 0.61              |
| 2:D:28:ASN:HB3   | 2:D:93:HIS:HA    | 1.82                     | 0.60              |
| 1:B:108:THR:OG1  | 1:B:234:ASN:O    | 2.17                     | 0.60              |
| 1:B:309:GLU:O    | 1:B:313:TYR:OH   | 2.18                     | 0.60              |
| 1:A:1129:VAL:CB  | 1:B:917:TYR:HB3  | 2.31                     | 0.60              |
| 1:B:973:ILE:HG13 | 1:B:980:ILE:HG12 | 1.83                     | 0.60              |
| 3:G:7:SER:OG     | 3:G:21:SER:OG    | 2.15                     | 0.60              |
| 1:C:973:ILE:HG13 | 1:C:980:ILE:HG12 | 1.83                     | 0.60              |
| 1:B:772:VAL:HG12 | 1:B:772:VAL:O    | 2.00                     | 0.60              |
| 1:C:472:ILE:HG12 | 1:C:490:PHE:HB3  | 1.83                     | 0.60              |
| 1:C:605:SER:OG   | 1:C:606:ASN:N    | 2.31                     | 0.60              |
| 1:C:880:GLY:O    | 1:C:884:SER:OG   | 2.14                     | 0.60              |
| 1:B:472:ILE:HG12 | 1:B:490:PHE:HB3  | 1.83                     | 0.60              |
| 3:I:87:LYS:HG2   | 3:I:90:ASP:HB2   | 1.82                     | 0.60              |
| 2:D:50:TYR:O     | 2:D:52:ASN:N     | 2.35                     | 0.60              |
| 3:E:104:ASN:HB2  | 3:E:108:PHE:CE2  | 2.37                     | 0.60              |
| 1:C:712:ILE:CB   | 1:C:1077:THR:CG2 | 2.75                     | 0.60              |
| 2:H:50:TYR:O     | 2:H:52:ASN:N     | 2.35                     | 0.60              |
| 2:D:9:SER:OG     | 2:D:106:LYS:O    | 2.14                     | 0.60              |
| 1:B:231:ILE:HG21 | 1:B:233:ILE:HD12 | 1.84                     | 0.60              |
| 1:A:320:VAL:HG13 | 1:A:590:CYS:SG   | 2.42                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:520:ALA:HB1  | 1:A:521:PRO:HD2   | 1.83                     | 0.60              |
| 1:A:880:GLY:O    | 1:A:884:SER:OG    | 2.14                     | 0.60              |
| 1:B:786:LYS:HE2  | 1:B:786:LYS:H     | 1.67                     | 0.60              |
| 1:C:538:CYS:HG   | 1:C:590:CYS:HG    | 0.89                     | 0.60              |
| 1:C:1031:GLU:OE1 | 1:C:1042:PHE:HE2  | 1.82                     | 0.60              |
| 3:G:104:ASN:CB   | 3:G:108:PHE:CE2   | 2.85                     | 0.60              |
| 1:B:102:ARG:H    | 1:B:242:LEU:CD2   | 2.15                     | 0.59              |
| 3:E:104:ASN:CB   | 3:E:108:PHE:CE2   | 2.85                     | 0.59              |
| 1:C:108:THR:OG1  | 1:C:234:ASN:O     | 2.17                     | 0.59              |
| 1:B:320:VAL:HG13 | 1:B:590:CYS:SG    | 2.42                     | 0.59              |
| 1:B:520:ALA:HB1  | 1:B:521:PRO:HD2   | 1.83                     | 0.59              |
| 1:C:772:VAL:HG12 | 1:C:772:VAL:O     | 2.00                     | 0.59              |
| 1:C:393:THR:HG21 | 1:C:519:HIS:H     | 1.67                     | 0.59              |
| 2:F:50:TYR:O     | 2:F:52:ASN:N      | 2.35                     | 0.59              |
| 1:A:231:ILE:HG21 | 1:A:233:ILE:HD12  | 1.84                     | 0.59              |
| 2:H:45:PRO:HG2   | 3:I:45:LEU:HD21   | 1.85                     | 0.59              |
| 2:H:66:SER:HG    | 2:H:73:THR:HG1    | 1.42                     | 0.59              |
| 1:A:452:LEU:HD13 | 1:A:492:LEU:CB    | 2.33                     | 0.59              |
| 1:A:472:ILE:HG12 | 1:A:490:PHE:HB3   | 1.83                     | 0.59              |
| 1:A:605:SER:OG   | 1:A:606:ASN:N     | 2.31                     | 0.59              |
| 1:A:619:GLU:OE1  | 1:A:619:GLU:N     | 2.35                     | 0.59              |
| 1:B:381:GLY:O    | 1:C:983:ARG:NH1   | 2.36                     | 0.59              |
| 1:C:786:LYS:HE2  | 1:C:786:LYS:H     | 1.67                     | 0.59              |
| 1:A:973:ILE:HG13 | 1:A:980:ILE:HG12  | 1.83                     | 0.59              |
| 1:C:452:LEU:HD13 | 1:C:492:LEU:CB    | 2.33                     | 0.59              |
| 1:A:381:GLY:O    | 1:B:983:ARG:NH1   | 2.35                     | 0.59              |
| 1:A:461:LEU:HD12 | 1:A:462:LYS:O     | 2.02                     | 0.59              |
| 2:D:45:PRO:HG2   | 3:E:45:LEU:HD21   | 1.85                     | 0.59              |
| 1:A:393:THR:HG21 | 1:A:519:HIS:H     | 1.67                     | 0.58              |
| 1:C:102:ARG:H    | 1:C:242:LEU:CD2   | 2.15                     | 0.58              |
| 3:G:104:ASN:HB2  | 3:G:108:PHE:CE2   | 2.37                     | 0.58              |
| 1:A:439:ASN:O    | 1:A:443:SER:OG    | 2.15                     | 0.58              |
| 1:A:786:LYS:H    | 1:A:786:LYS:HE2   | 1.67                     | 0.58              |
| 3:E:104:ASN:CB   | 3:E:108:PHE:HE2   | 2.16                     | 0.58              |
| 1:B:393:THR:HG21 | 1:B:519:HIS:H     | 1.67                     | 0.58              |
| 1:B:619:GLU:N    | 1:B:619:GLU:OE1   | 2.36                     | 0.58              |
| 3:G:100:GLN:N    | 3:G:100:GLN:OE1   | 2.35                     | 0.58              |
| 1:A:102:ARG:H    | 1:A:242:LEU:CD2   | 2.15                     | 0.58              |
| 1:A:726:ILE:HG13 | 1:A:1061:VAL:HG22 | 1.86                     | 0.58              |
| 1:B:461:LEU:HD13 | 1:B:462:LYS:O     | 2.04                     | 0.58              |
| 1:C:231:ILE:HG21 | 1:C:233:ILE:HD12  | 1.84                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:461:LEU:HD13 | 1:C:462:LYS:O     | 2.04                     | 0.58              |
| 1:C:520:ALA:HB1  | 1:C:521:PRO:HD2   | 1.84                     | 0.58              |
| 1:C:726:ILE:HG13 | 1:C:1061:VAL:HG22 | 1.86                     | 0.58              |
| 1:A:461:LEU:HD13 | 1:A:462:LYS:O     | 2.04                     | 0.58              |
| 1:C:619:GLU:N    | 1:C:619:GLU:OE1   | 2.36                     | 0.58              |
| 1:B:231:ILE:CG2  | 1:B:233:ILE:HG13  | 2.32                     | 0.58              |
| 1:B:452:LEU:HD13 | 1:B:492:LEU:CB    | 2.33                     | 0.58              |
| 1:C:461:LEU:HD12 | 1:C:462:LYS:O     | 2.02                     | 0.58              |
| 1:B:461:LEU:HD12 | 1:B:462:LYS:O     | 2.02                     | 0.58              |
| 1:C:53:ASP:HB2   | 1:C:55:PHE:CE1    | 2.39                     | 0.58              |
| 1:C:385:THR:O    | 1:C:385:THR:HG22  | 2.04                     | 0.58              |
| 3:G:104:ASN:CB   | 3:G:108:PHE:HE2   | 2.16                     | 0.58              |
| 2:D:29:ILE:O     | 2:D:67:LYS:NZ     | 2.26                     | 0.58              |
| 2:F:45:PRO:HG2   | 3:G:45:LEU:HD21   | 1.85                     | 0.58              |
| 3:I:100:GLN:N    | 3:I:100:GLN:OE1   | 2.35                     | 0.58              |
| 1:A:385:THR:HG22 | 1:A:385:THR:O     | 2.04                     | 0.57              |
| 2:D:10:VAL:HG11  | 2:D:20:ILE:HG22   | 1.86                     | 0.57              |
| 1:C:101:ILE:CD1  | 1:C:242:LEU:HD11  | 2.34                     | 0.57              |
| 1:B:53:ASP:HB2   | 1:B:55:PHE:CE1    | 2.39                     | 0.57              |
| 1:A:983:ARG:NH1  | 1:C:381:GLY:O     | 2.38                     | 0.57              |
| 1:B:562:PHE:CE2  | 1:C:225:PRO:CD    | 2.85                     | 0.57              |
| 1:A:900:MET:HE2  | 1:A:904:TYR:HE2   | 1.69                     | 0.57              |
| 1:B:866:THR:HG22 | 1:B:867:ASP:N     | 2.19                     | 0.57              |
| 1:B:900:MET:HE2  | 1:B:904:TYR:HE2   | 1.69                     | 0.57              |
| 1:C:900:MET:HE2  | 1:C:904:TYR:HE2   | 1.69                     | 0.57              |
| 3:G:36:TRP:CH2   | 3:G:96:CYS:HB3    | 2.40                     | 0.57              |
| 1:A:53:ASP:HB2   | 1:A:55:PHE:CE1    | 2.39                     | 0.57              |
| 1:A:101:ILE:CD1  | 1:A:242:LEU:HD11  | 2.34                     | 0.57              |
| 1:A:1107:ARG:NH1 | 1:B:904:TYR:HD1   | 1.72                     | 0.57              |
| 1:A:978:ASN:O    | 1:A:982:SER:N     | 2.38                     | 0.57              |
| 2:D:93:HIS:HE1   | 2:D:96:LEU:HG     | 1.69                     | 0.57              |
| 1:C:866:THR:HG22 | 1:C:867:ASP:N     | 2.19                     | 0.57              |
| 2:H:10:VAL:HG11  | 2:H:20:ILE:HG22   | 1.86                     | 0.57              |
| 3:I:36:TRP:CH2   | 3:I:96:CYS:HB3    | 2.40                     | 0.57              |
| 2:D:34:VAL:HA    | 2:D:91:THR:OG1    | 2.04                     | 0.57              |
| 1:B:106:PHE:HD1  | 1:B:238:PHE:HB2   | 1.70                     | 0.57              |
| 1:B:373:SER:OG   | 3:G:105:TYR:O     | 2.22                     | 0.57              |
| 1:C:101:ILE:HA   | 1:C:242:LEU:CD2   | 2.35                     | 0.57              |
| 2:F:10:VAL:HG11  | 2:F:20:ILE:HG22   | 1.86                     | 0.57              |
| 1:B:101:ILE:HA   | 1:B:242:LEU:CD2   | 2.35                     | 0.57              |
| 1:A:101:ILE:HA   | 1:A:242:LEU:CD2   | 2.35                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:373:SER:OG   | 3:E:105:TYR:O     | 2.22                     | 0.57              |
| 1:A:866:THR:HG22 | 1:A:867:ASP:N     | 2.19                     | 0.57              |
| 1:B:726:ILE:HG13 | 1:B:1061:VAL:HG22 | 1.86                     | 0.57              |
| 1:C:106:PHE:HD1  | 1:C:238:PHE:HB2   | 1.70                     | 0.57              |
| 3:E:36:TRP:CH2   | 3:E:96:CYS:HB3    | 2.40                     | 0.56              |
| 1:C:978:ASN:O    | 1:C:982:SER:N     | 2.38                     | 0.56              |
| 1:B:101:ILE:CD1  | 1:B:242:LEU:HD11  | 2.34                     | 0.56              |
| 1:B:320:VAL:CG1  | 1:B:590:CYS:SG    | 2.93                     | 0.56              |
| 1:C:42:VAL:HG23  | 1:C:42:VAL:O      | 2.03                     | 0.56              |
| 1:C:299:THR:HG22 | 1:C:315:THR:CG2   | 2.36                     | 0.56              |
| 2:F:34:VAL:HA    | 2:F:91:THR:OG1    | 2.04                     | 0.56              |
| 2:H:92:TRP:CG    | 3:I:107:TYR:HH    | 2.23                     | 0.56              |
| 1:A:106:PHE:HD1  | 1:A:238:PHE:HB2   | 1.70                     | 0.56              |
| 1:A:566:GLY:HA2  | 1:B:43:PHE:O      | 2.06                     | 0.56              |
| 1:A:1096:VAL:O   | 1:A:1103:PHE:N    | 2.37                     | 0.56              |
| 1:B:392:PHE:CD1  | 1:B:517:LEU:HD11  | 2.41                     | 0.56              |
| 1:A:225:PRO:CD   | 1:C:562:PHE:CE2   | 2.85                     | 0.56              |
| 1:A:231:ILE:CG2  | 1:A:233:ILE:HG13  | 2.32                     | 0.56              |
| 1:A:320:VAL:CG1  | 1:A:590:CYS:SG    | 2.93                     | 0.56              |
| 1:A:392:PHE:CD1  | 1:A:517:LEU:HD11  | 2.41                     | 0.56              |
| 1:B:566:GLY:HA2  | 1:C:43:PHE:O      | 2.05                     | 0.56              |
| 1:C:53:ASP:HB2   | 1:C:55:PHE:HE1    | 1.71                     | 0.56              |
| 2:F:93:HIS:HE1   | 2:F:96:LEU:HG     | 1.69                     | 0.56              |
| 1:A:53:ASP:HB2   | 1:A:55:PHE:HE1    | 1.71                     | 0.56              |
| 1:B:385:THR:HG22 | 1:B:385:THR:O     | 2.04                     | 0.56              |
| 2:H:93:HIS:HE1   | 2:H:96:LEU:HG     | 1.69                     | 0.56              |
| 3:E:100:GLN:N    | 3:E:100:GLN:OE1   | 2.35                     | 0.56              |
| 1:B:597:VAL:HG22 | 1:B:610:VAL:CG2   | 2.36                     | 0.56              |
| 1:A:299:THR:HG22 | 1:A:315:THR:CG2   | 2.36                     | 0.55              |
| 1:A:454:ARG:NH1  | 1:A:467:ASP:O     | 2.39                     | 0.55              |
| 1:B:140:PHE:HA   | 1:B:243:ALA:HA    | 1.88                     | 0.55              |
| 1:C:37:TYR:OH    | 1:C:54:LEU:O      | 2.20                     | 0.55              |
| 1:C:454:ARG:NH1  | 1:C:467:ASP:O     | 2.39                     | 0.55              |
| 1:A:374:PHE:CD1  | 1:A:434:ILE:CG2   | 2.89                     | 0.55              |
| 1:A:444:LYS:HB3  | 1:A:446:GLY:O     | 2.06                     | 0.55              |
| 1:B:901:GLN:O    | 1:B:904:TYR:N     | 2.39                     | 0.55              |
| 1:A:140:PHE:HA   | 1:A:243:ALA:HA    | 1.88                     | 0.55              |
| 1:A:562:PHE:CE2  | 1:B:225:PRO:CD    | 2.87                     | 0.55              |
| 1:C:374:PHE:CD1  | 1:C:434:ILE:CG2   | 2.89                     | 0.55              |
| 2:F:9:SER:OG     | 2:F:106:LYS:O     | 2.14                     | 0.55              |
| 2:H:9:SER:OG     | 2:H:106:LYS:O     | 2.14                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:898:PHE:O    | 1:A:901:GLN:N     | 2.39                     | 0.55              |
| 1:A:1126:CYS:HB2 | 1:A:1132:ILE:HD12 | 1.89                     | 0.55              |
| 1:B:444:LYS:HB3  | 1:B:446:GLY:O     | 2.06                     | 0.55              |
| 1:C:140:PHE:HA   | 1:C:243:ALA:HA    | 1.88                     | 0.55              |
| 1:C:392:PHE:CD1  | 1:C:517:LEU:HD11  | 2.41                     | 0.55              |
| 1:C:826:VAL:HG21 | 1:C:1057:PRO:HG3  | 1.88                     | 0.55              |
| 1:A:43:PHE:O     | 1:C:566:GLY:HA2   | 2.07                     | 0.55              |
| 1:B:578:ASP:OD1  | 1:B:583:GLU:N     | 2.40                     | 0.55              |
| 1:C:898:PHE:O    | 1:C:901:GLN:N     | 2.39                     | 0.55              |
| 1:A:597:VAL:HG22 | 1:A:610:VAL:CG2   | 2.36                     | 0.55              |
| 1:B:816:SER:OG   | 1:B:817:PHE:N     | 2.40                     | 0.55              |
| 1:C:444:LYS:HB3  | 1:C:446:GLY:O     | 2.06                     | 0.55              |
| 1:B:299:THR:HG22 | 1:B:315:THR:CG2   | 2.36                     | 0.55              |
| 1:B:1056:ALA:HB1 | 1:B:1057:PRO:HD2  | 1.89                     | 0.55              |
| 1:C:441:LEU:HD13 | 3:I:103:TYR:HD2   | 1.71                     | 0.55              |
| 3:G:83:TRP:HZ2   | 3:G:94:TYR:HE2    | 1.55                     | 0.55              |
| 1:A:565:PHE:CE1  | 1:B:42:VAL:HG12   | 2.41                     | 0.55              |
| 1:A:816:SER:OG   | 1:A:817:PHE:N     | 2.40                     | 0.55              |
| 1:A:1056:ALA:HB1 | 1:A:1057:PRO:HD2  | 1.89                     | 0.55              |
| 1:B:898:PHE:O    | 1:B:901:GLN:N     | 2.39                     | 0.55              |
| 1:B:374:PHE:CD1  | 1:B:434:ILE:CG2   | 2.89                     | 0.55              |
| 1:B:449:TYR:HA   | 1:B:494:SER:OG    | 2.07                     | 0.55              |
| 2:F:22:CYS:CB    | 2:F:89:CYS:HG     | 2.18                     | 0.55              |
| 3:I:83:TRP:HZ2   | 3:I:94:TYR:HE2    | 1.55                     | 0.55              |
| 1:B:978:ASN:O    | 1:B:982:SER:N     | 2.38                     | 0.54              |
| 1:C:449:TYR:HA   | 1:C:494:SER:OG    | 2.07                     | 0.54              |
| 1:C:1096:VAL:O   | 1:C:1103:PHE:N    | 2.37                     | 0.54              |
| 3:G:6:GLN:NE2    | 3:G:116:GLY:HA3   | 2.22                     | 0.54              |
| 1:B:1126:CYS:HB2 | 1:B:1132:ILE:HD12 | 1.89                     | 0.54              |
| 1:A:578:ASP:OD1  | 1:A:583:GLU:N     | 2.40                     | 0.54              |
| 1:A:826:VAL:HG21 | 1:A:1057:PRO:HG3  | 1.88                     | 0.54              |
| 3:E:83:TRP:HZ2   | 3:E:94:TYR:HE2    | 1.55                     | 0.54              |
| 1:B:826:VAL:HG21 | 1:B:1057:PRO:HG3  | 1.88                     | 0.54              |
| 1:C:453:TYR:HE2  | 1:C:495:TYR:HB2   | 1.73                     | 0.54              |
| 1:C:777:ASN:O    | 1:C:781:VAL:HG23  | 2.08                     | 0.54              |
| 3:G:93:MET:HA    | 3:G:118:GLY:O     | 2.08                     | 0.54              |
| 1:A:770:ILE:O    | 1:A:774:GLN:HG2   | 2.07                     | 0.54              |
| 1:B:454:ARG:NH1  | 1:B:467:ASP:O     | 2.40                     | 0.54              |
| 1:C:770:ILE:O    | 1:C:774:GLN:HG2   | 2.07                     | 0.54              |
| 1:A:37:TYR:OH    | 1:A:54:LEU:O      | 2.20                     | 0.54              |
| 1:A:309:GLU:O    | 1:A:313:TYR:OH    | 2.18                     | 0.54              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:231:ILE:CG2  | 1:C:233:ILE:HG13  | 2.32                     | 0.54              |
| 3:G:51:ILE:HD12  | 3:G:58:THR:HG22   | 1.90                     | 0.54              |
| 3:I:6:GLN:NE2    | 3:I:116:GLY:HA3   | 2.22                     | 0.54              |
| 1:A:453:TYR:HE2  | 1:A:495:TYR:HB2   | 1.73                     | 0.54              |
| 1:B:192:PHE:HA   | 1:B:204:TYR:O     | 2.08                     | 0.54              |
| 1:B:770:ILE:O    | 1:B:774:GLN:HG2   | 2.07                     | 0.54              |
| 1:B:777:ASN:O    | 1:B:781:VAL:HG23  | 2.08                     | 0.54              |
| 1:B:1040:VAL:HB  | 1:C:1030:SER:O    | 2.08                     | 0.54              |
| 1:A:192:PHE:HA   | 1:A:204:TYR:O     | 2.08                     | 0.54              |
| 1:A:449:TYR:HA   | 1:A:494:SER:OG    | 2.07                     | 0.54              |
| 3:E:93:MET:HA    | 3:E:118:GLY:O     | 2.08                     | 0.54              |
| 2:H:92:TRP:HH2   | 3:I:59:ARG:HD2    | 1.73                     | 0.54              |
| 1:A:130:VAL:HG13 | 1:A:233:ILE:HD13  | 1.90                     | 0.54              |
| 1:A:901:GLN:O    | 1:A:904:TYR:N     | 2.39                     | 0.54              |
| 1:A:1030:SER:O   | 1:C:1040:VAL:HB   | 2.06                     | 0.54              |
| 3:E:6:GLN:NE2    | 3:E:116:GLY:HA3   | 2.22                     | 0.53              |
| 1:A:101:ILE:HA   | 1:A:242:LEU:HD21  | 1.91                     | 0.53              |
| 1:A:777:ASN:O    | 1:A:781:VAL:HG23  | 2.08                     | 0.53              |
| 1:C:101:ILE:HA   | 1:C:242:LEU:HD21  | 1.91                     | 0.53              |
| 1:C:192:PHE:HA   | 1:C:204:TYR:O     | 2.08                     | 0.53              |
| 2:H:84:GLU:HG2   | 2:H:108:THR:HA    | 1.91                     | 0.53              |
| 1:C:1056:ALA:HB1 | 1:C:1057:PRO:HD2  | 1.89                     | 0.53              |
| 1:C:1126:CYS:HB2 | 1:C:1132:ILE:HD12 | 1.89                     | 0.53              |
| 1:A:42:VAL:HG12  | 1:C:565:PHE:CE1   | 2.42                     | 0.53              |
| 1:B:53:ASP:HB2   | 1:B:55:PHE:HE1    | 1.71                     | 0.53              |
| 1:B:858:LEU:HD22 | 1:B:959:LEU:HD11  | 1.91                     | 0.53              |
| 1:C:816:SER:OG   | 1:C:817:PHE:N     | 2.40                     | 0.53              |
| 1:A:225:PRO:HG2  | 1:C:562:PHE:CD2   | 2.43                     | 0.53              |
| 1:B:112:SER:HA   | 1:B:132:GLU:HB3   | 1.91                     | 0.53              |
| 1:B:453:TYR:HE2  | 1:B:495:TYR:HB2   | 1.73                     | 0.53              |
| 1:C:112:SER:HA   | 1:C:132:GLU:HB3   | 1.91                     | 0.53              |
| 1:C:343:ASN:HA   | 3:I:104:ASN:HA    | 1.90                     | 0.53              |
| 1:C:858:LEU:HD22 | 1:C:959:LEU:HD11  | 1.91                     | 0.53              |
| 1:A:665:PRO:HA   | 1:A:671:CYS:SG    | 2.49                     | 0.53              |
| 2:D:84:GLU:HB2   | 2:D:109:VAL:HG23  | 1.91                     | 0.53              |
| 2:D:92:TRP:HH2   | 3:E:59:ARG:HD2    | 1.73                     | 0.53              |
| 1:A:1040:VAL:HB  | 1:B:1030:SER:O    | 2.09                     | 0.53              |
| 2:D:79:LEU:HD21  | 2:D:109:VAL:HG22  | 1.91                     | 0.53              |
| 1:B:101:ILE:HA   | 1:B:242:LEU:HD21  | 1.91                     | 0.53              |
| 1:C:974:SER:O    | 1:C:980:ILE:CD1   | 2.57                     | 0.53              |
| 1:A:858:LEU:HD22 | 1:A:959:LEU:HD11  | 1.91                     | 0.53              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:84:GLU:HG2   | 2:D:108:THR:HA   | 1.91                     | 0.53              |
| 1:B:355:ARG:NH2  | 1:B:396:TYR:CD1  | 2.76                     | 0.53              |
| 1:B:901:GLN:HE21 | 1:B:905:ARG:HE   | 1.57                     | 0.53              |
| 2:F:79:LEU:HD21  | 2:F:109:VAL:HG22 | 1.91                     | 0.53              |
| 3:I:93:MET:HA    | 3:I:118:GLY:O    | 2.08                     | 0.53              |
| 1:A:112:SER:HA   | 1:A:132:GLU:HB3  | 1.91                     | 0.53              |
| 1:A:901:GLN:HE21 | 1:A:905:ARG:HE   | 1.57                     | 0.53              |
| 3:E:51:ILE:HD12  | 3:E:58:THR:HG22  | 1.90                     | 0.53              |
| 1:B:974:SER:O    | 1:B:980:ILE:CD1  | 2.57                     | 0.53              |
| 1:C:901:GLN:O    | 1:C:904:TYR:N    | 2.39                     | 0.53              |
| 1:A:974:SER:O    | 1:A:980:ILE:CD1  | 2.57                     | 0.53              |
| 1:B:780:GLU:O    | 1:B:784:GLN:NE2  | 2.36                     | 0.53              |
| 1:C:29:THR:OG1   | 1:C:62:VAL:HG22  | 2.10                     | 0.52              |
| 2:F:92:TRP:HH2   | 3:G:59:ARG:HD2   | 1.73                     | 0.52              |
| 1:B:562:PHE:CD2  | 1:C:225:PRO:HG2  | 2.44                     | 0.52              |
| 1:B:580:GLN:HB3  | 4:B:1306:NAG:H82 | 1.91                     | 0.52              |
| 2:F:22:CYS:SG    | 2:F:36:TRP:HH2   | 2.21                     | 0.52              |
| 1:C:101:ILE:HD12 | 1:C:242:LEU:CG   | 2.39                     | 0.52              |
| 1:C:136:CYS:SG   | 1:C:161:SER:HB3  | 2.50                     | 0.52              |
| 1:C:277:LEU:HD23 | 1:C:285:ILE:HD13 | 1.91                     | 0.52              |
| 3:I:51:ILE:HD12  | 3:I:58:THR:HG22  | 1.90                     | 0.52              |
| 3:E:113:ASP:OD1  | 3:E:113:ASP:N    | 2.42                     | 0.52              |
| 1:C:597:VAL:HG22 | 1:C:610:VAL:CG2  | 2.36                     | 0.52              |
| 2:F:29:ILE:O     | 2:F:67:LYS:NZ    | 2.26                     | 0.52              |
| 1:B:29:THR:OG1   | 1:B:62:VAL:HG22  | 2.10                     | 0.52              |
| 2:H:79:LEU:HD21  | 2:H:109:VAL:HG22 | 1.91                     | 0.52              |
| 1:A:310:LYS:HG3  | 1:A:600:PRO:HA   | 1.91                     | 0.52              |
| 1:B:665:PRO:HA   | 1:B:671:CYS:SG   | 2.49                     | 0.52              |
| 1:C:578:ASP:OD1  | 1:C:583:GLU:N    | 2.40                     | 0.52              |
| 2:H:84:GLU:HB2   | 2:H:109:VAL:HG23 | 1.91                     | 0.52              |
| 1:A:136:CYS:SG   | 1:A:161:SER:HB3  | 2.50                     | 0.52              |
| 1:A:355:ARG:NH2  | 1:A:396:TYR:CD1  | 2.76                     | 0.52              |
| 1:B:130:VAL:HG13 | 1:B:233:ILE:HD13 | 1.90                     | 0.52              |
| 1:C:665:PRO:HA   | 1:C:671:CYS:SG   | 2.49                     | 0.52              |
| 3:I:113:ASP:OD1  | 3:I:113:ASP:N    | 2.42                     | 0.52              |
| 1:A:580:GLN:HB3  | 4:A:1306:NAG:H82 | 1.91                     | 0.52              |
| 1:B:310:LYS:HG3  | 1:B:600:PRO:HA   | 1.91                     | 0.52              |
| 1:B:948:LEU:HD21 | 1:B:1059:GLY:HA3 | 1.92                     | 0.52              |
| 3:G:97:THR:HG21  | 3:G:111:TYR:CE1  | 2.45                     | 0.52              |
| 1:B:241:LEU:O    | 1:B:242:LEU:HG   | 2.10                     | 0.52              |
| 2:F:84:GLU:HB2   | 2:F:109:VAL:HG23 | 1.91                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:29:THR:OG1   | 1:A:62:VAL:HG22  | 2.10                     | 0.52              |
| 1:A:241:LEU:O    | 1:A:242:LEU:HG   | 2.10                     | 0.52              |
| 1:A:796:ASP:O    | 1:A:798:GLY:N    | 2.43                     | 0.52              |
| 1:B:101:ILE:HD12 | 1:B:242:LEU:CG   | 2.39                     | 0.52              |
| 2:F:55:ARG:NH2   | 2:F:63:PHE:O     | 2.38                     | 0.51              |
| 1:B:136:CYS:SG   | 1:B:161:SER:HB3  | 2.50                     | 0.51              |
| 1:B:277:LEU:HD23 | 1:B:285:ILE:HD13 | 1.91                     | 0.51              |
| 2:F:92:TRP:CG    | 3:G:107:TYR:OH   | 2.63                     | 0.51              |
| 1:A:439:ASN:HB3  | 1:A:507:PRO:HD2  | 1.92                     | 0.51              |
| 1:C:901:GLN:HE21 | 1:C:905:ARG:HE   | 1.57                     | 0.51              |
| 1:A:277:LEU:HD23 | 1:A:285:ILE:HD13 | 1.91                     | 0.51              |
| 2:F:84:GLU:HG2   | 2:F:108:THR:HA   | 1.91                     | 0.51              |
| 3:E:4:LEU:HA     | 3:E:23:LYS:O     | 2.11                     | 0.51              |
| 1:B:51:THR:OG1   | 1:B:53:ASP:OD1   | 2.29                     | 0.51              |
| 1:B:91:TYR:OH    | 1:B:191:GLU:OE2  | 2.29                     | 0.51              |
| 1:C:241:LEU:O    | 1:C:242:LEU:HG   | 2.10                     | 0.51              |
| 1:C:580:GLN:HB3  | 4:C:1306:NAG:H82 | 1.91                     | 0.51              |
| 2:H:29:ILE:O     | 2:H:67:LYS:NZ    | 2.26                     | 0.51              |
| 1:A:51:THR:OG1   | 1:A:53:ASP:OD1   | 2.29                     | 0.51              |
| 1:B:603:ASN:OD1  | 1:B:603:ASN:N    | 2.43                     | 0.51              |
| 2:D:92:TRP:CG    | 3:E:107:TYR:OH   | 2.63                     | 0.51              |
| 1:B:353:TRP:O    | 1:B:466:ARG:NH1  | 2.44                     | 0.51              |
| 1:C:51:THR:OG1   | 1:C:53:ASP:OD1   | 2.29                     | 0.51              |
| 1:C:603:ASN:N    | 1:C:603:ASN:OD1  | 2.43                     | 0.51              |
| 1:A:353:TRP:O    | 1:A:466:ARG:NH1  | 2.44                     | 0.51              |
| 1:A:562:PHE:CD2  | 1:B:225:PRO:HG2  | 2.46                     | 0.51              |
| 1:B:320:VAL:HG13 | 1:B:538:CYS:HG   | 1.76                     | 0.51              |
| 1:B:1096:VAL:O   | 1:B:1103:PHE:N   | 2.37                     | 0.51              |
| 3:I:97:THR:HG21  | 3:I:111:TYR:CE1  | 2.45                     | 0.51              |
| 1:A:91:TYR:OH    | 1:A:191:GLU:OE2  | 2.29                     | 0.51              |
| 1:A:796:ASP:OD2  | 1:C:709:ASN:HB3  | 2.11                     | 0.51              |
| 1:C:343:ASN:HD21 | 4:C:1307:NAG:C7  | 2.24                     | 0.51              |
| 2:H:51:ASP:OD1   | 2:H:52:ASN:N     | 2.43                     | 0.51              |
| 1:B:900:MET:HE1  | 1:B:904:TYR:OH   | 2.10                     | 0.51              |
| 1:C:948:LEU:HD21 | 1:C:1059:GLY:HA3 | 1.92                     | 0.51              |
| 1:B:439:ASN:HB3  | 1:B:507:PRO:HD2  | 1.92                     | 0.50              |
| 1:A:689:SER:CA   | 1:A:690:GLN:OE1  | 2.60                     | 0.50              |
| 1:A:883:THR:HG21 | 1:C:705:VAL:HG11 | 1.92                     | 0.50              |
| 1:C:310:LYS:HG3  | 1:C:600:PRO:HA   | 1.91                     | 0.50              |
| 1:C:355:ARG:NH2  | 1:C:396:TYR:CD1  | 2.76                     | 0.50              |
| 3:G:5:VAL:HG23   | 3:G:23:LYS:HB2   | 1.93                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:472:ILE:CG2   | 1:B:488:CYS:O     | 2.49                     | 0.50              |
| 3:G:4:LEU:HA      | 3:G:23:LYS:O      | 2.11                     | 0.50              |
| 1:B:973:ILE:CG1   | 1:B:980:ILE:HG12  | 2.41                     | 0.50              |
| 1:C:91:TYR:OH     | 1:C:191:GLU:OE2   | 2.29                     | 0.50              |
| 1:C:439:ASN:HB3   | 1:C:507:PRO:HD2   | 1.92                     | 0.50              |
| 1:C:973:ILE:CG1   | 1:C:980:ILE:HG12  | 2.41                     | 0.50              |
| 3:G:10:GLU:O      | 3:G:119:THR:HG23  | 2.12                     | 0.50              |
| 1:A:101:ILE:HD12  | 1:A:242:LEU:CG    | 2.39                     | 0.50              |
| 1:A:1035:GLY:HA3  | 1:C:1040:VAL:HG21 | 1.93                     | 0.50              |
| 3:I:4:LEU:HA      | 3:I:23:LYS:O      | 2.11                     | 0.50              |
| 3:I:10:GLU:O      | 3:I:119:THR:HG23  | 2.12                     | 0.50              |
| 1:A:796:ASP:OD1   | 1:A:796:ASP:N     | 2.45                     | 0.50              |
| 1:A:973:ILE:CG1   | 1:A:980:ILE:HG12  | 2.41                     | 0.50              |
| 1:B:343:ASN:HD21  | 4:B:1307:NAG:C7   | 2.24                     | 0.50              |
| 1:B:689:SER:CA    | 1:B:690:GLN:OE1   | 2.60                     | 0.50              |
| 1:B:897:PRO:HG2   | 1:B:900:MET:HB2   | 1.94                     | 0.50              |
| 1:C:651:ILE:HG13  | 1:C:651:ILE:O     | 2.12                     | 0.50              |
| 1:A:570:ALA:CB    | 1:B:963:VAL:HG12  | 2.42                     | 0.50              |
| 1:A:900:MET:HE1   | 1:A:904:TYR:OH    | 2.10                     | 0.50              |
| 1:B:34:ARG:NH1    | 1:B:221:SER:OG    | 2.45                     | 0.50              |
| 1:C:134:GLN:HB2   | 1:C:161:SER:HB2   | 1.94                     | 0.50              |
| 1:A:461:LEU:C     | 1:A:461:LEU:CD1   | 2.84                     | 0.49              |
| 1:A:651:ILE:O     | 1:A:651:ILE:HG13  | 2.12                     | 0.49              |
| 1:C:353:TRP:O     | 1:C:466:ARG:NH1   | 2.44                     | 0.49              |
| 2:F:51:ASP:OD1    | 2:F:52:ASN:N      | 2.43                     | 0.49              |
| 1:A:948:LEU:HD21  | 1:A:1059:GLY:HA3  | 1.92                     | 0.49              |
| 3:E:5:VAL:HG23    | 3:E:23:LYS:HB2    | 1.93                     | 0.49              |
| 1:A:134:GLN:HB2   | 1:A:161:SER:HB2   | 1.94                     | 0.49              |
| 1:A:716:THR:O     | 1:A:717:ASN:CG    | 2.56                     | 0.49              |
| 1:A:472:ILE:CG2   | 1:A:488:CYS:O     | 2.49                     | 0.49              |
| 1:A:1040:VAL:HG21 | 1:B:1035:GLY:HA3  | 1.94                     | 0.49              |
| 1:B:134:GLN:HB2   | 1:B:161:SER:HB2   | 1.94                     | 0.49              |
| 1:B:782:PHE:CZ    | 1:B:1060:VAL:HG22 | 2.47                     | 0.49              |
| 1:C:101:ILE:CG1   | 1:C:242:LEU:HD21  | 2.41                     | 0.49              |
| 1:C:472:ILE:CG2   | 1:C:488:CYS:O     | 2.48                     | 0.49              |
| 3:I:5:VAL:HG23    | 3:I:23:LYS:HB2    | 1.93                     | 0.49              |
| 1:B:1040:VAL:HG21 | 1:C:1035:GLY:HA3  | 1.95                     | 0.49              |
| 1:C:689:SER:CA    | 1:C:690:GLN:OE1   | 2.60                     | 0.49              |
| 1:C:782:PHE:CZ    | 1:C:1060:VAL:HG22 | 2.47                     | 0.49              |
| 3:G:104:ASN:N     | 3:G:108:PHE:CE2   | 2.67                     | 0.49              |
| 1:A:320:VAL:HG13  | 1:A:538:CYS:HG    | 1.76                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:130:VAL:HG13 | 1:C:233:ILE:HD13  | 1.90                     | 0.49              |
| 1:A:343:ASN:HD21 | 4:A:1307:NAG:C7   | 2.24                     | 0.49              |
| 1:A:736:VAL:HG22 | 1:A:858:LEU:HD23  | 1.95                     | 0.49              |
| 1:A:816:SER:HB3  | 1:A:819:GLU:HG3   | 1.95                     | 0.49              |
| 1:B:645:THR:OG1  | 1:B:647:ALA:N     | 2.46                     | 0.49              |
| 1:A:191:GLU:O    | 1:A:205:SER:HA    | 2.12                     | 0.49              |
| 1:A:782:PHE:CZ   | 1:A:1060:VAL:HG22 | 2.48                     | 0.49              |
| 1:B:716:THR:O    | 1:B:717:ASN:CG    | 2.56                     | 0.49              |
| 1:C:816:SER:HB3  | 1:C:819:GLU:HG3   | 1.95                     | 0.49              |
| 3:G:113:ASP:OD1  | 3:G:113:ASP:N     | 2.42                     | 0.49              |
| 3:E:10:GLU:O     | 3:E:119:THR:HG23  | 2.12                     | 0.49              |
| 1:B:651:ILE:O    | 1:B:651:ILE:HG13  | 2.12                     | 0.49              |
| 1:C:431:GLY:H    | 1:C:514:SER:HA    | 1.78                     | 0.49              |
| 1:A:41:LYS:O     | 1:A:42:VAL:C      | 2.56                     | 0.49              |
| 1:A:645:THR:OG1  | 1:A:647:ALA:N     | 2.46                     | 0.49              |
| 1:A:780:GLU:O    | 1:A:784:GLN:NE2   | 2.37                     | 0.49              |
| 1:A:963:VAL:HG12 | 1:C:570:ALA:CB    | 2.43                     | 0.49              |
| 1:C:748:GLU:H    | 1:C:748:GLU:CD    | 2.20                     | 0.49              |
| 3:I:99:HIS:HD2   | 3:I:111:TYR:CE1   | 2.31                     | 0.49              |
| 2:D:89:CYS:O     | 2:D:102:GLY:N     | 2.43                     | 0.48              |
| 1:B:298:GLU:O    | 1:B:302:THR:HG23  | 2.12                     | 0.48              |
| 1:C:897:PRO:HG2  | 1:C:900:MET:HB2   | 1.94                     | 0.48              |
| 2:H:17:LYS:NZ    | 2:H:78:GLY:H      | 2.11                     | 0.48              |
| 1:A:1031:GLU:OE2 | 1:A:1039:ARG:CG   | 2.58                     | 0.48              |
| 3:G:97:THR:OG1   | 3:G:113:ASP:O     | 2.25                     | 0.48              |
| 1:B:191:GLU:O    | 1:B:205:SER:HA    | 2.12                     | 0.48              |
| 1:B:736:VAL:HG22 | 1:B:858:LEU:HD23  | 1.95                     | 0.48              |
| 1:B:748:GLU:H    | 1:B:748:GLU:CD    | 2.20                     | 0.48              |
| 1:B:816:SER:HB3  | 1:B:819:GLU:HG3   | 1.95                     | 0.48              |
| 1:C:191:GLU:O    | 1:C:205:SER:HA    | 2.12                     | 0.48              |
| 1:C:298:GLU:O    | 1:C:302:THR:HG23  | 2.12                     | 0.48              |
| 1:C:716:THR:O    | 1:C:717:ASN:CG    | 2.56                     | 0.48              |
| 1:C:780:GLU:O    | 1:C:784:GLN:NE2   | 2.37                     | 0.48              |
| 1:C:900:MET:CE   | 1:C:904:TYR:CZ    | 2.97                     | 0.48              |
| 1:A:431:GLY:H    | 1:A:514:SER:HA    | 1.78                     | 0.48              |
| 1:B:538:CYS:SG   | 1:B:590:CYS:HB3   | 2.54                     | 0.48              |
| 1:C:900:MET:HE1  | 1:C:904:TYR:OH    | 2.11                     | 0.48              |
| 1:A:298:GLU:O    | 1:A:302:THR:HG23  | 2.13                     | 0.48              |
| 1:A:705:VAL:HG11 | 1:B:883:THR:HG21  | 1.92                     | 0.48              |
| 2:D:17:LYS:NZ    | 2:D:78:GLY:H      | 2.11                     | 0.48              |
| 1:B:709:ASN:HB3  | 1:C:796:ASP:OD2   | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:343:ASN:OD1  | 1:C:343:ASN:C    | 2.56                     | 0.48              |
| 3:I:97:THR:CG2   | 3:I:111:TYR:CE1  | 2.97                     | 0.48              |
| 3:E:104:ASN:N    | 3:E:108:PHE:CE2  | 2.67                     | 0.48              |
| 1:B:431:GLY:H    | 1:B:514:SER:HA   | 1.78                     | 0.48              |
| 1:C:1031:GLU:OE2 | 1:C:1039:ARG:CG  | 2.58                     | 0.48              |
| 1:A:343:ASN:OD1  | 1:A:343:ASN:C    | 2.56                     | 0.48              |
| 1:A:538:CYS:SG   | 1:A:590:CYS:HB3  | 2.54                     | 0.48              |
| 1:A:897:PRO:HG2  | 1:A:900:MET:HB2  | 1.94                     | 0.48              |
| 1:A:900:MET:CE   | 1:A:904:TYR:CZ   | 2.97                     | 0.48              |
| 2:D:51:ASP:OD1   | 2:D:52:ASN:N     | 2.43                     | 0.48              |
| 1:C:402:ILE:HD11 | 1:C:418:ILE:HG12 | 1.96                     | 0.48              |
| 1:C:796:ASP:O    | 1:C:798:GLY:N    | 2.43                     | 0.48              |
| 1:C:796:ASP:OD1  | 1:C:796:ASP:N    | 2.45                     | 0.48              |
| 2:F:17:LYS:NZ    | 2:F:78:GLY:H     | 2.11                     | 0.48              |
| 2:F:79:LEU:HD23  | 2:F:80:GLN:N     | 2.29                     | 0.48              |
| 2:H:55:ARG:NH2   | 2:H:63:PHE:O     | 2.38                     | 0.48              |
| 1:A:748:GLU:H    | 1:A:748:GLU:CD   | 2.20                     | 0.48              |
| 1:A:772:VAL:O    | 1:A:772:VAL:CG1  | 2.62                     | 0.48              |
| 2:H:79:LEU:HD23  | 2:H:80:GLN:N     | 2.29                     | 0.48              |
| 3:I:47:TRP:CZ3   | 3:I:49:GLY:HA2   | 2.49                     | 0.48              |
| 2:D:79:LEU:HD23  | 2:D:80:GLN:N     | 2.29                     | 0.48              |
| 1:B:1083:HIS:CE1 | 1:B:1136:THR:HA  | 2.49                     | 0.48              |
| 1:C:538:CYS:CB   | 1:C:590:CYS:CB   | 2.90                     | 0.48              |
| 1:C:708:SER:OG   | 1:C:711:SER:N    | 2.46                     | 0.48              |
| 1:C:772:VAL:O    | 1:C:772:VAL:CG1  | 2.62                     | 0.48              |
| 1:C:1083:HIS:CE1 | 1:C:1136:THR:HA  | 2.49                     | 0.48              |
| 3:G:47:TRP:CZ3   | 3:G:49:GLY:HA2   | 2.49                     | 0.48              |
| 1:B:402:ILE:HD11 | 1:B:418:ILE:HG12 | 1.96                     | 0.47              |
| 1:B:494:SER:OG   | 1:B:495:TYR:N    | 2.46                     | 0.47              |
| 1:B:566:GLY:CA   | 1:C:43:PHE:O     | 2.62                     | 0.47              |
| 3:G:99:HIS:HD2   | 3:G:111:TYR:CE1  | 2.31                     | 0.47              |
| 1:A:708:SER:OG   | 1:A:711:SER:N    | 2.46                     | 0.47              |
| 1:B:538:CYS:CB   | 1:B:590:CYS:CB   | 2.90                     | 0.47              |
| 1:B:570:ALA:CB   | 1:C:963:VAL:HG12 | 2.43                     | 0.47              |
| 1:B:703:ASN:OD1  | 1:C:787:GLN:CB   | 2.62                     | 0.47              |
| 1:C:645:THR:OG1  | 1:C:647:ALA:N    | 2.46                     | 0.47              |
| 1:C:736:VAL:HG22 | 1:C:858:LEU:HD23 | 1.95                     | 0.47              |
| 2:H:47:LEU:HD23  | 2:H:56:PRO:HG3   | 1.96                     | 0.47              |
| 1:A:740:MET:HE1  | 1:C:592:PHE:CZ   | 2.50                     | 0.47              |
| 1:A:1083:HIS:CE1 | 1:A:1136:THR:HA  | 2.49                     | 0.47              |
| 1:B:461:LEU:C    | 1:B:461:LEU:CD1  | 2.84                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:89:CYS:O     | 2:H:102:GLY:N    | 2.43                     | 0.47              |
| 3:I:83:TRP:CZ2   | 3:I:94:TYR:HE2   | 2.32                     | 0.47              |
| 1:A:494:SER:OG   | 1:A:495:TYR:N    | 2.46                     | 0.47              |
| 1:B:418:ILE:HA   | 1:B:422:ASN:ND2  | 2.30                     | 0.47              |
| 1:B:641:ASN:OD1  | 1:B:642:VAL:N    | 2.44                     | 0.47              |
| 1:B:900:MET:CE   | 1:B:904:TYR:CZ   | 2.97                     | 0.47              |
| 2:H:86:ASP:HB3   | 2:H:88:TYR:CE1   | 2.49                     | 0.47              |
| 2:D:5:THR:N      | 2:D:23:SER:O     | 2.29                     | 0.47              |
| 3:E:36:TRP:CZ3   | 3:E:96:CYS:HB3   | 2.49                     | 0.47              |
| 1:C:494:SER:OG   | 1:C:495:TYR:N    | 2.46                     | 0.47              |
| 3:I:23:LYS:HE3   | 3:I:23:LYS:HB3   | 1.74                     | 0.47              |
| 1:A:43:PHE:O     | 1:C:566:GLY:CA   | 2.63                     | 0.47              |
| 1:A:782:PHE:O    | 1:A:784:GLN:N    | 2.46                     | 0.47              |
| 1:A:787:GLN:CB   | 1:C:703:ASN:OD1  | 2.63                     | 0.47              |
| 2:D:13:ALA:O     | 2:D:16:GLN:HG3   | 2.15                     | 0.47              |
| 2:D:86:ASP:HB3   | 2:D:88:TYR:CE1   | 2.49                     | 0.47              |
| 3:E:47:TRP:CZ3   | 3:E:49:GLY:HA2   | 2.49                     | 0.47              |
| 1:B:697:MET:HE1  | 1:C:864:LEU:HD21 | 1.97                     | 0.47              |
| 1:B:854:LYS:HE3  | 1:B:854:LYS:HB3  | 1.80                     | 0.47              |
| 4:C:1307:NAG:O6  | 3:I:104:ASN:HB2  | 2.14                     | 0.47              |
| 3:I:36:TRP:CZ3   | 3:I:96:CYS:HB3   | 2.49                     | 0.47              |
| 1:A:1031:GLU:HG2 | 1:A:1037:SER:HB2 | 1.97                     | 0.47              |
| 2:D:48:LEU:HG    | 2:D:49:ILE:HG12  | 1.97                     | 0.47              |
| 1:B:708:SER:OG   | 1:B:711:SER:N    | 2.46                     | 0.47              |
| 1:A:34:ARG:NH1   | 1:A:221:SER:OG   | 2.45                     | 0.47              |
| 1:A:443:SER:O    | 1:A:448:ASN:HB2  | 2.15                     | 0.47              |
| 1:A:566:GLY:CA   | 1:B:43:PHE:O     | 2.62                     | 0.47              |
| 1:B:772:VAL:O    | 1:B:772:VAL:CG1  | 2.62                     | 0.47              |
| 2:H:48:LEU:HG    | 2:H:49:ILE:HG12  | 1.97                     | 0.47              |
| 3:G:99:HIS:CD2   | 3:G:111:TYR:CE1  | 3.03                     | 0.47              |
| 3:I:99:HIS:CD2   | 3:I:111:TYR:CE1  | 3.03                     | 0.47              |
| 1:A:658:ASN:ND2  | 1:A:660:TYR:OH   | 2.46                     | 0.47              |
| 1:A:709:ASN:HB3  | 1:B:796:ASP:OD2  | 2.15                     | 0.47              |
| 2:D:47:LEU:HD23  | 2:D:56:PRO:HG3   | 1.96                     | 0.47              |
| 1:B:402:ILE:HD11 | 1:B:418:ILE:HG21 | 1.97                     | 0.47              |
| 1:B:605:SER:HG   | 1:B:607:GLN:H    | 1.62                     | 0.47              |
| 2:F:13:ALA:O     | 2:F:16:GLN:HG3   | 2.15                     | 0.47              |
| 2:F:86:ASP:HB3   | 2:F:88:TYR:CE1   | 2.49                     | 0.47              |
| 3:G:97:THR:CG2   | 3:G:111:TYR:CE1  | 2.97                     | 0.47              |
| 1:B:343:ASN:C    | 1:B:343:ASN:OD1  | 2.56                     | 0.46              |
| 1:B:347:PHE:CE1  | 1:B:399:SER:HB2  | 2.50                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:796:ASP:O    | 1:B:798:GLY:N     | 2.43                     | 0.46              |
| 1:C:418:ILE:HA   | 1:C:422:ASN:ND2   | 2.30                     | 0.46              |
| 1:C:1029:MET:HE3 | 1:C:1029:MET:HB2  | 1.86                     | 0.46              |
| 2:F:47:LEU:HD23  | 2:F:56:PRO:HG3    | 1.96                     | 0.46              |
| 2:H:92:TRP:HA    | 2:H:99:GLY:CA     | 2.43                     | 0.46              |
| 1:A:347:PHE:CE1  | 1:A:399:SER:HB2   | 2.50                     | 0.46              |
| 1:B:231:ILE:HG21 | 1:B:233:ILE:CD1   | 2.45                     | 0.46              |
| 1:B:418:ILE:HA   | 1:B:422:ASN:HD22  | 1.79                     | 0.46              |
| 1:C:206:LYS:HD2  | 1:C:206:LYS:HA    | 1.71                     | 0.46              |
| 1:C:900:MET:CE   | 1:C:904:TYR:CE2   | 2.98                     | 0.46              |
| 2:H:5:THR:N      | 2:H:23:SER:O      | 2.29                     | 0.46              |
| 2:H:106:LYS:HB3  | 2:H:106:LYS:HE3   | 1.63                     | 0.46              |
| 1:A:538:CYS:CB   | 1:A:590:CYS:CB    | 2.90                     | 0.46              |
| 1:B:443:SER:O    | 1:B:448:ASN:HB2   | 2.15                     | 0.46              |
| 2:F:92:TRP:HA    | 2:F:99:GLY:CA     | 2.43                     | 0.46              |
| 1:A:231:ILE:CG2  | 1:A:233:ILE:CD1   | 2.94                     | 0.46              |
| 1:A:402:ILE:HD11 | 1:A:418:ILE:HG12  | 1.96                     | 0.46              |
| 1:A:418:ILE:HA   | 1:A:422:ASN:ND2   | 2.30                     | 0.46              |
| 1:A:1087:ALA:O   | 1:A:1122:VAL:HG23 | 2.16                     | 0.46              |
| 2:D:55:ARG:NH2   | 2:D:63:PHE:O      | 2.38                     | 0.46              |
| 1:C:355:ARG:CZ   | 1:C:396:TYR:CD1   | 2.99                     | 0.46              |
| 1:C:1031:GLU:HG2 | 1:C:1037:SER:HB2  | 1.97                     | 0.46              |
| 1:C:1049:LEU:HB2 | 1:C:1065:VAL:O    | 2.15                     | 0.46              |
| 3:G:36:TRP:CZ3   | 3:G:96:CYS:HB3    | 2.49                     | 0.46              |
| 1:A:641:ASN:OD1  | 1:A:642:VAL:N     | 2.44                     | 0.46              |
| 1:A:873:TYR:CE2  | 1:C:699:LEU:HD22  | 2.51                     | 0.46              |
| 1:A:1030:SER:HB3 | 1:C:1041:ASP:HB3  | 1.97                     | 0.46              |
| 1:C:231:ILE:CG2  | 1:C:233:ILE:CD1   | 2.94                     | 0.46              |
| 2:F:5:THR:N      | 2:F:23:SER:O      | 2.29                     | 0.46              |
| 3:G:83:TRP:CZ2   | 3:G:94:TYR:HE2    | 2.32                     | 0.46              |
| 1:A:101:ILE:CG1  | 1:A:242:LEU:HD21  | 2.41                     | 0.46              |
| 1:B:139:PRO:HB3  | 1:B:241:LEU:HD22  | 1.97                     | 0.46              |
| 1:B:280:ASN:OD1  | 1:B:281:GLU:N     | 2.46                     | 0.46              |
| 1:B:1041:ASP:O   | 1:B:1041:ASP:CG   | 2.59                     | 0.46              |
| 1:B:1087:ALA:O   | 1:B:1122:VAL:HG23 | 2.16                     | 0.46              |
| 1:C:234:ASN:ND2  | 4:C:1305:NAG:O7   | 2.49                     | 0.46              |
| 1:C:339:GLY:O    | 1:C:343:ASN:N     | 2.36                     | 0.46              |
| 3:G:99:HIS:HB3   | 3:G:111:TYR:CD1   | 2.51                     | 0.46              |
| 1:A:231:ILE:HG21 | 1:A:233:ILE:CD1   | 2.45                     | 0.46              |
| 1:A:391:CYS:HB3  | 1:A:522:ALA:HB1   | 1.98                     | 0.46              |
| 1:A:703:ASN:OD1  | 1:B:787:GLN:CB    | 2.64                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:981:LEU:HD13 | 1:A:993:ILE:HD11  | 1.98                     | 0.46              |
| 2:D:22:CYS:CB    | 2:D:89:CYS:SG     | 3.04                     | 0.46              |
| 2:D:106:LYS:HE3  | 2:D:106:LYS:HB3   | 1.63                     | 0.46              |
| 1:B:355:ARG:CZ   | 1:B:396:TYR:CD1   | 2.99                     | 0.46              |
| 1:B:900:MET:CE   | 1:B:904:TYR:CE2   | 2.98                     | 0.46              |
| 1:C:139:PRO:HB3  | 1:C:241:LEU:HD22  | 1.97                     | 0.46              |
| 1:C:443:SER:O    | 1:C:448:ASN:HB2   | 2.15                     | 0.46              |
| 2:F:106:LYS:HE3  | 2:F:106:LYS:HB3   | 1.63                     | 0.46              |
| 2:H:13:ALA:O     | 2:H:16:GLN:HG3    | 2.15                     | 0.46              |
| 1:A:234:ASN:ND2  | 4:A:1305:NAG:O7   | 2.49                     | 0.46              |
| 1:A:355:ARG:CZ   | 1:A:396:TYR:CD1   | 2.99                     | 0.46              |
| 1:A:418:ILE:HA   | 1:A:422:ASN:HD22  | 1.80                     | 0.46              |
| 1:B:234:ASN:ND2  | 4:B:1305:NAG:O7   | 2.49                     | 0.46              |
| 1:C:1087:ALA:O   | 1:C:1122:VAL:HG23 | 2.16                     | 0.46              |
| 2:H:32:ASN:HA    | 2:H:33:PRO:HD3    | 1.86                     | 0.46              |
| 1:A:402:ILE:HD11 | 1:A:418:ILE:HG21  | 1.97                     | 0.46              |
| 1:A:749:CYS:SG   | 1:A:997:ILE:HD11  | 2.56                     | 0.46              |
| 1:B:231:ILE:CG2  | 1:B:233:ILE:CD1   | 2.94                     | 0.46              |
| 1:B:289:VAL:HG23 | 1:B:306:PHE:CZ    | 2.51                     | 0.46              |
| 1:B:1028:LYS:NZ  | 1:B:1042:PHE:O    | 2.49                     | 0.46              |
| 1:B:1031:GLU:HG2 | 1:B:1037:SER:HB2  | 1.97                     | 0.46              |
| 1:C:347:PHE:CE1  | 1:C:399:SER:HB2   | 2.50                     | 0.46              |
| 1:C:418:ILE:HA   | 1:C:422:ASN:HD22  | 1.80                     | 0.46              |
| 3:E:12:LYS:HB3   | 3:E:16:GLU:OE1    | 2.16                     | 0.46              |
| 1:B:749:CYS:SG   | 1:B:997:ILE:HD11  | 2.56                     | 0.46              |
| 1:C:964:LYS:HB3  | 1:C:964:LYS:HE3   | 1.59                     | 0.46              |
| 2:H:4:LEU:HB2    | 2:H:102:GLY:HA2   | 1.99                     | 0.46              |
| 3:I:51:ILE:HD11  | 3:I:56:SER:HA     | 1.97                     | 0.46              |
| 3:I:99:HIS:HB3   | 3:I:111:TYR:CD1   | 2.51                     | 0.46              |
| 1:A:699:LEU:HD22 | 1:B:873:TYR:CE2   | 2.51                     | 0.45              |
| 1:A:866:THR:CG2  | 1:A:867:ASP:N     | 2.80                     | 0.45              |
| 1:A:914:ASN:OD1  | 1:A:915:VAL:N     | 2.49                     | 0.45              |
| 2:D:49:ILE:HD13  | 2:D:49:ILE:HA     | 1.82                     | 0.45              |
| 3:E:36:TRP:CZ2   | 3:E:81:LEU:HD11   | 2.51                     | 0.45              |
| 1:B:391:CYS:HB3  | 1:B:522:ALA:HB1   | 1.98                     | 0.45              |
| 1:B:914:ASN:OD1  | 1:B:915:VAL:N     | 2.49                     | 0.45              |
| 1:A:603:ASN:OD1  | 1:A:603:ASN:N     | 2.43                     | 0.45              |
| 1:A:1041:ASP:HB3 | 1:B:1030:SER:HB3  | 1.98                     | 0.45              |
| 1:B:658:ASN:ND2  | 1:B:660:TYR:OH    | 2.46                     | 0.45              |
| 1:B:1041:ASP:HB3 | 1:C:1030:SER:HB3  | 1.98                     | 0.45              |
| 1:C:41:LYS:O     | 1:C:42:VAL:C      | 2.59                     | 0.45              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:402:ILE:HD11 | 1:C:418:ILE:HG21  | 1.97                     | 0.45              |
| 2:F:22:CYS:CB    | 2:F:89:CYS:SG     | 3.04                     | 0.45              |
| 3:G:36:TRP:CZ2   | 3:G:81:LEU:HD11   | 2.51                     | 0.45              |
| 3:I:36:TRP:CZ2   | 3:I:81:LEU:HD11   | 2.51                     | 0.45              |
| 1:A:289:VAL:HG23 | 1:A:306:PHE:CZ    | 2.51                     | 0.45              |
| 1:A:339:GLY:O    | 1:A:343:ASN:N     | 2.36                     | 0.45              |
| 1:A:1041:ASP:O   | 1:A:1041:ASP:CG   | 2.59                     | 0.45              |
| 1:A:1049:LEU:HB2 | 1:A:1065:VAL:O    | 2.16                     | 0.45              |
| 2:D:22:CYS:SG    | 2:D:36:TRP:HH2    | 2.21                     | 0.45              |
| 3:E:6:GLN:NE2    | 3:E:96:CYS:SG     | 2.84                     | 0.45              |
| 3:E:51:ILE:HD11  | 3:E:56:SER:HA     | 1.97                     | 0.45              |
| 3:E:83:TRP:CZ2   | 3:E:94:TYR:HE2    | 2.32                     | 0.45              |
| 1:C:122:ASN:C    | 1:C:124:THR:H     | 2.25                     | 0.45              |
| 1:C:391:CYS:HB3  | 1:C:522:ALA:HB1   | 1.98                     | 0.45              |
| 1:A:122:ASN:C    | 1:A:124:THR:H     | 2.25                     | 0.45              |
| 1:A:902:MET:HE3  | 1:A:1049:LEU:HD13 | 1.98                     | 0.45              |
| 1:B:112:SER:N    | 1:B:133:PHE:O     | 2.50                     | 0.45              |
| 1:B:592:PHE:CZ   | 1:C:740:MET:HE1   | 2.50                     | 0.45              |
| 1:B:916:LEU:O    | 1:B:920:GLN:N     | 2.50                     | 0.45              |
| 2:D:4:LEU:HB2    | 2:D:102:GLY:HA2   | 1.99                     | 0.45              |
| 1:C:1041:ASP:O   | 1:C:1041:ASP:CG   | 2.59                     | 0.45              |
| 2:F:48:LEU:HG    | 2:F:49:ILE:HG12   | 1.97                     | 0.45              |
| 2:H:92:TRP:CH2   | 3:I:59:ARG:HD2    | 2.52                     | 0.45              |
| 3:G:12:LYS:HB3   | 3:G:16:GLU:OE1    | 2.16                     | 0.45              |
| 1:A:134:GLN:N    | 1:A:161:SER:OG    | 2.48                     | 0.45              |
| 1:A:139:PRO:HB3  | 1:A:241:LEU:HD22  | 1.97                     | 0.45              |
| 1:A:347:PHE:CD1  | 1:A:399:SER:HB2   | 2.52                     | 0.45              |
| 3:E:95:TYR:HB3   | 3:E:114:VAL:HG11  | 1.99                     | 0.45              |
| 1:B:40:ASP:HB3   | 1:B:42:VAL:HG22   | 1.98                     | 0.45              |
| 1:C:280:ASN:OD1  | 1:C:281:GLU:N     | 2.46                     | 0.45              |
| 2:F:4:LEU:HB2    | 2:F:102:GLY:HA2   | 1.99                     | 0.45              |
| 3:I:6:GLN:NE2    | 3:I:96:CYS:SG     | 2.84                     | 0.45              |
| 3:I:100:GLN:HE22 | 3:I:112:ILE:HD11  | 1.82                     | 0.45              |
| 1:A:374:PHE:CD1  | 1:A:434:ILE:HG21  | 2.52                     | 0.45              |
| 2:D:92:TRP:HA    | 2:D:99:GLY:CA     | 2.43                     | 0.45              |
| 3:E:6:GLN:HE22   | 3:E:96:CYS:H      | 1.65                     | 0.45              |
| 1:B:101:ILE:CG1  | 1:B:242:LEU:HD21  | 2.41                     | 0.45              |
| 1:B:1049:LEU:HB2 | 1:B:1065:VAL:O    | 2.16                     | 0.45              |
| 1:B:1095:PHE:CE1 | 1:B:1104:VAL:HG12 | 2.52                     | 0.45              |
| 1:C:134:GLN:N    | 1:C:161:SER:OG    | 2.48                     | 0.45              |
| 1:C:289:VAL:HG23 | 1:C:306:PHE:CZ    | 2.51                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:749:CYS:SG    | 1:C:997:ILE:HD11  | 2.56                     | 0.45              |
| 1:C:981:LEU:HD12  | 1:C:981:LEU:HA    | 1.77                     | 0.45              |
| 1:C:981:LEU:HD13  | 1:C:993:ILE:HD11  | 1.97                     | 0.45              |
| 3:I:12:LYS:HB3    | 3:I:16:GLU:OE1    | 2.16                     | 0.45              |
| 1:A:112:SER:N     | 1:A:133:PHE:O     | 2.50                     | 0.45              |
| 1:A:900:MET:CE    | 1:A:904:TYR:CE2   | 2.98                     | 0.45              |
| 3:E:97:THR:OG1    | 3:E:113:ASP:O     | 2.25                     | 0.45              |
| 3:E:100:GLN:HE22  | 3:E:112:ILE:HD11  | 1.82                     | 0.45              |
| 1:B:339:GLY:O     | 1:B:343:ASN:N     | 2.36                     | 0.45              |
| 1:B:439:ASN:O     | 1:B:443:SER:OG    | 2.15                     | 0.45              |
| 1:B:981:LEU:HD13  | 1:B:993:ILE:HD11  | 1.98                     | 0.45              |
| 1:C:309:GLU:O     | 1:C:313:TYR:OH    | 2.18                     | 0.45              |
| 1:C:854:LYS:HE3   | 1:C:854:LYS:HB3   | 1.80                     | 0.45              |
| 1:C:1095:PHE:CE1  | 1:C:1104:VAL:HG12 | 2.52                     | 0.45              |
| 1:A:443:SER:O     | 1:A:444:LYS:HB2   | 2.17                     | 0.45              |
| 1:A:916:LEU:O     | 1:A:920:GLN:N     | 2.50                     | 0.45              |
| 1:A:1095:PHE:CE1  | 1:A:1104:VAL:HG12 | 2.52                     | 0.45              |
| 1:C:231:ILE:HG21  | 1:C:233:ILE:CD1   | 2.45                     | 0.45              |
| 1:C:538:CYS:CB    | 1:C:590:CYS:SG    | 3.05                     | 0.45              |
| 1:C:870:ILE:O     | 1:C:874:THR:HG23  | 2.17                     | 0.45              |
| 1:C:914:ASN:OD1   | 1:C:915:VAL:N     | 2.49                     | 0.45              |
| 1:C:916:LEU:O     | 1:C:920:GLN:N     | 2.50                     | 0.45              |
| 3:G:51:ILE:HD11   | 3:G:56:SER:HA     | 1.97                     | 0.45              |
| 1:A:592:PHE:CZ    | 1:B:740:MET:HE1   | 2.52                     | 0.45              |
| 1:A:1082:CYS:HB2  | 1:A:1126:CYS:HB2  | 1.91                     | 0.45              |
| 1:A:1129:VAL:HG23 | 1:B:917:TYR:CB    | 2.38                     | 0.45              |
| 1:B:443:SER:O     | 1:B:444:LYS:HB2   | 2.17                     | 0.45              |
| 1:B:1031:GLU:OE2  | 1:B:1039:ARG:CG   | 2.58                     | 0.45              |
| 1:C:443:SER:O     | 1:C:444:LYS:HB2   | 2.17                     | 0.45              |
| 1:C:641:ASN:OD1   | 1:C:642:VAL:N     | 2.44                     | 0.45              |
| 1:C:658:ASN:ND2   | 1:C:660:TYR:OH    | 2.46                     | 0.45              |
| 2:F:93:HIS:H      | 2:F:99:GLY:HA2    | 1.82                     | 0.45              |
| 2:H:22:CYS:CB     | 2:H:89:CYS:SG     | 3.04                     | 0.45              |
| 3:I:6:GLN:CD      | 3:I:116:GLY:HA3   | 2.42                     | 0.45              |
| 1:A:538:CYS:CB    | 1:A:590:CYS:SG    | 3.05                     | 0.44              |
| 1:A:656:VAL:HG22  | 1:A:695:TYR:HB3   | 1.99                     | 0.44              |
| 1:A:697:MET:HE1   | 1:B:864:LEU:HD21  | 1.97                     | 0.44              |
| 1:B:866:THR:CG2   | 1:B:867:ASP:N     | 2.79                     | 0.44              |
| 2:F:92:TRP:CH2    | 3:G:59:ARG:HD2    | 2.52                     | 0.44              |
| 3:G:99:HIS:HD2    | 3:G:111:TYR:HE1   | 1.63                     | 0.44              |
| 1:A:280:ASN:OD1   | 1:A:281:GLU:N     | 2.46                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1028:LYS:NZ  | 1:A:1042:PHE:O    | 2.49                     | 0.44              |
| 1:B:134:GLN:N    | 1:B:161:SER:OG    | 2.48                     | 0.44              |
| 1:B:347:PHE:CD1  | 1:B:399:SER:HB2   | 2.52                     | 0.44              |
| 1:B:782:PHE:O    | 1:B:784:GLN:N     | 2.46                     | 0.44              |
| 1:B:870:ILE:O    | 1:B:874:THR:HG23  | 2.17                     | 0.44              |
| 1:C:866:THR:CG2  | 1:C:867:ASP:N     | 2.80                     | 0.44              |
| 1:C:1028:LYS:NZ  | 1:C:1042:PHE:O    | 2.49                     | 0.44              |
| 3:I:99:HIS:HD2   | 3:I:111:TYR:HE1   | 1.63                     | 0.44              |
| 1:A:201:PHE:O    | 1:A:228:ASP:HA    | 2.17                     | 0.44              |
| 1:A:303:LEU:HD21 | 1:A:313:TYR:CE2   | 2.53                     | 0.44              |
| 1:A:870:ILE:O    | 1:A:874:THR:HG23  | 2.17                     | 0.44              |
| 1:A:974:SER:H    | 1:A:980:ILE:HD11  | 1.82                     | 0.44              |
| 1:B:902:MET:HE3  | 1:B:1049:LEU:HD13 | 1.98                     | 0.44              |
| 3:G:100:GLN:HE22 | 3:G:112:ILE:HD11  | 1.82                     | 0.44              |
| 1:B:206:LYS:HD2  | 1:B:206:LYS:HA    | 1.71                     | 0.44              |
| 1:B:320:VAL:HG13 | 1:B:320:VAL:O     | 2.18                     | 0.44              |
| 1:B:374:PHE:CD1  | 1:B:434:ILE:HG21  | 2.52                     | 0.44              |
| 1:B:538:CYS:CB   | 1:B:590:CYS:SG    | 3.05                     | 0.44              |
| 1:B:656:VAL:HG22 | 1:B:695:TYR:HB3   | 2.00                     | 0.44              |
| 1:B:802:PHE:HZ   | 1:B:898:PHE:CZ    | 2.35                     | 0.44              |
| 1:C:656:VAL:HG22 | 1:C:695:TYR:HB3   | 2.00                     | 0.44              |
| 1:C:767:LEU:HD23 | 1:C:767:LEU:HA    | 1.84                     | 0.44              |
| 1:B:66:HIS:HD2   | 1:B:264:ALA:HB2   | 1.83                     | 0.44              |
| 1:B:1055:SER:OG  | 1:B:1056:ALA:N    | 2.51                     | 0.44              |
| 1:C:347:PHE:CD1  | 1:C:399:SER:HB2   | 2.52                     | 0.44              |
| 3:I:6:GLN:HE22   | 3:I:96:CYS:H      | 1.65                     | 0.44              |
| 1:A:802:PHE:HZ   | 1:A:898:PHE:CZ    | 2.35                     | 0.44              |
| 3:E:6:GLN:CD     | 3:E:116:GLY:HA3   | 2.42                     | 0.44              |
| 3:E:23:LYS:HE3   | 3:E:23:LYS:HB3    | 1.74                     | 0.44              |
| 1:B:592:PHE:CE2  | 1:C:740:MET:HE1   | 2.53                     | 0.44              |
| 1:C:66:HIS:HD2   | 1:C:264:ALA:HB2   | 1.83                     | 0.44              |
| 2:H:93:HIS:H     | 2:H:99:GLY:HA2    | 1.82                     | 0.44              |
| 3:G:6:GLN:CD     | 3:G:116:GLY:HA3   | 2.42                     | 0.44              |
| 1:A:320:VAL:HG13 | 1:A:538:CYS:SG    | 2.58                     | 0.44              |
| 1:A:1055:SER:OG  | 1:A:1056:ALA:N    | 2.51                     | 0.44              |
| 2:D:13:ALA:N     | 2:D:110:LEU:HD12  | 2.33                     | 0.44              |
| 1:B:303:LEU:HD21 | 1:B:313:TYR:CE2   | 2.53                     | 0.44              |
| 1:B:320:VAL:HG13 | 1:B:538:CYS:SG    | 2.58                     | 0.44              |
| 1:B:974:SER:H    | 1:B:980:ILE:HD11  | 1.82                     | 0.44              |
| 1:B:981:LEU:HD12 | 1:B:981:LEU:HA    | 1.77                     | 0.44              |
| 1:C:112:SER:N    | 1:C:133:PHE:O     | 2.50                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:303:LEU:HD21 | 1:C:313:TYR:CE2   | 2.53                     | 0.44              |
| 1:C:886:TRP:N    | 1:C:886:TRP:CD1   | 2.84                     | 0.44              |
| 1:C:902:MET:HE3  | 1:C:1049:LEU:HD13 | 1.98                     | 0.44              |
| 2:F:6:GLN:HG2    | 2:F:22:CYS:HB2    | 2.00                     | 0.44              |
| 1:A:320:VAL:HG13 | 1:A:320:VAL:O     | 2.18                     | 0.44              |
| 1:A:900:MET:HE2  | 1:A:900:MET:HB3   | 1.68                     | 0.44              |
| 1:B:195:LYS:CB   | 1:B:202:LYS:HE2   | 2.48                     | 0.44              |
| 3:G:95:TYR:HB3   | 3:G:114:VAL:HG11  | 1.99                     | 0.44              |
| 1:A:195:LYS:CB   | 1:A:202:LYS:HE2   | 2.48                     | 0.44              |
| 1:A:904:TYR:CZ   | 1:C:1094:VAL:HG12 | 2.53                     | 0.44              |
| 1:A:864:LEU:HD21 | 1:C:697:MET:HE1   | 1.98                     | 0.43              |
| 2:D:93:HIS:H     | 2:D:99:GLY:HA2    | 1.82                     | 0.43              |
| 1:B:392:PHE:HD1  | 1:B:517:LEU:HD11  | 1.83                     | 0.43              |
| 1:B:900:MET:HE2  | 1:B:900:MET:HB3   | 1.67                     | 0.43              |
| 1:C:201:PHE:O    | 1:C:228:ASP:HA    | 2.17                     | 0.43              |
| 1:C:802:PHE:HZ   | 1:C:898:PHE:CZ    | 2.35                     | 0.43              |
| 1:C:1055:SER:OG  | 1:C:1056:ALA:N    | 2.51                     | 0.43              |
| 1:C:1067:TYR:CD1 | 1:C:1067:TYR:C    | 2.96                     | 0.43              |
| 3:G:6:GLN:HE22   | 3:G:96:CYS:H      | 1.65                     | 0.43              |
| 1:A:48:LEU:HD13  | 1:A:305:SER:HA    | 2.00                     | 0.43              |
| 1:A:392:PHE:HD1  | 1:A:517:LEU:CD1   | 2.31                     | 0.43              |
| 2:D:11:SER:OG    | 2:D:108:THR:O     | 2.27                     | 0.43              |
| 1:C:95:THR:O     | 1:C:95:THR:OG1    | 2.36                     | 0.43              |
| 1:B:699:LEU:HD22 | 1:C:873:TYR:CE2   | 2.51                     | 0.43              |
| 1:B:1082:CYS:HB2 | 1:B:1126:CYS:HB2  | 1.91                     | 0.43              |
| 1:C:782:PHE:O    | 1:C:784:GLN:N     | 2.46                     | 0.43              |
| 1:C:974:SER:H    | 1:C:980:ILE:HD11  | 1.82                     | 0.43              |
| 2:F:13:ALA:N     | 2:F:110:LEU:HD12  | 2.33                     | 0.43              |
| 1:A:353:TRP:CD1  | 1:A:353:TRP:H     | 2.37                     | 0.43              |
| 1:A:666:ILE:HD11 | 1:A:672:ALA:HB2   | 2.00                     | 0.43              |
| 1:A:1067:TYR:CD1 | 1:A:1067:TYR:C    | 2.96                     | 0.43              |
| 1:B:48:LEU:HD13  | 1:B:305:SER:HA    | 2.00                     | 0.43              |
| 1:B:201:PHE:O    | 1:B:228:ASP:HA    | 2.17                     | 0.43              |
| 1:B:392:PHE:HD1  | 1:B:517:LEU:CD1   | 2.31                     | 0.43              |
| 1:B:715:PRO:CD   | 1:C:894:LEU:HD11  | 2.40                     | 0.43              |
| 1:C:101:ILE:HD12 | 1:C:242:LEU:HD11  | 2.01                     | 0.43              |
| 2:H:6:GLN:HG2    | 2:H:22:CYS:HB2    | 2.00                     | 0.43              |
| 3:G:29:PHE:CG    | 3:G:77:SER:HB3    | 2.53                     | 0.43              |
| 3:I:29:PHE:CG    | 3:I:77:SER:HB3    | 2.53                     | 0.43              |
| 1:A:740:MET:HE1  | 1:C:592:PHE:CE2   | 2.52                     | 0.43              |
| 1:A:886:TRP:CD1  | 1:A:886:TRP:N     | 2.84                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:705:VAL:HG11 | 1:C:883:THR:HG21  | 1.94                     | 0.43              |
| 1:C:374:PHE:CD1  | 1:C:434:ILE:HG21  | 2.52                     | 0.43              |
| 1:C:452:LEU:HD12 | 1:C:452:LEU:C     | 2.44                     | 0.43              |
| 1:C:538:CYS:SG   | 1:C:590:CYS:HB3   | 2.54                     | 0.43              |
| 3:I:95:TYR:HB3   | 3:I:114:VAL:HG11  | 1.99                     | 0.43              |
| 3:I:100:GLN:HB2  | 3:I:110:TYR:CD2   | 2.54                     | 0.43              |
| 1:A:40:ASP:HB3   | 1:A:42:VAL:HG22   | 2.00                     | 0.43              |
| 1:A:942:ALA:O    | 1:A:943:SER:OG    | 2.26                     | 0.43              |
| 3:E:104:ASN:CA   | 3:E:108:PHE:HE2   | 2.32                     | 0.43              |
| 1:B:574:ASP:OD1  | 1:B:575:ALA:N     | 2.52                     | 0.43              |
| 1:B:1019:ARG:O   | 1:B:1023:ASN:ND2  | 2.52                     | 0.43              |
| 1:B:1059:GLY:O   | 1:B:1060:VAL:HG23 | 2.19                     | 0.43              |
| 1:B:1102:TRP:HB2 | 1:B:1135:ASN:HD21 | 1.84                     | 0.43              |
| 2:H:13:ALA:N     | 2:H:110:LEU:HD12  | 2.33                     | 0.43              |
| 1:A:452:LEU:HD12 | 1:A:452:LEU:C     | 2.44                     | 0.43              |
| 2:D:6:GLN:HG2    | 2:D:22:CYS:HB2    | 2.00                     | 0.43              |
| 3:E:29:PHE:CG    | 3:E:77:SER:HB3    | 2.53                     | 0.43              |
| 1:B:122:ASN:C    | 1:B:124:THR:H     | 2.25                     | 0.43              |
| 1:B:779:GLN:CD   | 1:B:865:LEU:CD1   | 2.81                     | 0.43              |
| 1:B:797:PHE:O    | 1:B:800:PHE:N     | 2.49                     | 0.43              |
| 1:A:392:PHE:HD1  | 1:A:517:LEU:HD11  | 1.83                     | 0.43              |
| 1:B:666:ILE:HD11 | 1:B:672:ALA:HB2   | 2.00                     | 0.43              |
| 1:C:195:LYS:CB   | 1:C:202:LYS:HE2   | 2.48                     | 0.43              |
| 1:C:353:TRP:CD1  | 1:C:353:TRP:H     | 2.37                     | 0.43              |
| 1:C:392:PHE:HD1  | 1:C:517:LEU:CD1   | 2.31                     | 0.43              |
| 1:C:395:VAL:HG22 | 1:C:515:PHE:HD1   | 1.84                     | 0.43              |
| 2:H:92:TRP:CD1   | 3:I:107:TYR:HH    | 2.37                     | 0.43              |
| 1:A:574:ASP:OD1  | 1:A:575:ALA:N     | 2.52                     | 0.43              |
| 1:A:977:LEU:O    | 1:A:981:LEU:HB2   | 2.19                     | 0.43              |
| 1:A:1059:GLY:O   | 1:A:1060:VAL:HG23 | 2.19                     | 0.43              |
| 2:D:32:ASN:HA    | 2:D:33:PRO:HD3    | 1.84                     | 0.43              |
| 1:B:122:ASN:HB3  | 1:B:125:ASN:H     | 1.84                     | 0.43              |
| 1:B:965:GLN:HE22 | 1:C:758:SER:N     | 2.00                     | 0.43              |
| 1:A:66:HIS:HD2   | 1:A:264:ALA:HB2   | 1.83                     | 0.43              |
| 1:A:1107:ARG:NH1 | 1:B:904:TYR:CB    | 2.75                     | 0.43              |
| 1:A:1144:GLU:N   | 1:A:1144:GLU:OE2  | 2.52                     | 0.43              |
| 1:B:355:ARG:CZ   | 1:B:396:TYR:CG    | 3.02                     | 0.43              |
| 1:C:355:ARG:CZ   | 1:C:396:TYR:CG    | 3.02                     | 0.43              |
| 3:G:13:LYS:HA    | 3:G:13:LYS:HD2    | 1.91                     | 0.43              |
| 3:G:21:SER:HA    | 3:G:80:TYR:HD1    | 1.84                     | 0.43              |
| 1:A:101:ILE:HD12 | 1:A:242:LEU:HD11  | 2.01                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:570:ALA:HB2   | 1:B:963:VAL:HG12  | 2.01                     | 0.42              |
| 1:B:1029:MET:HE3  | 1:B:1029:MET:HB2  | 1.86                     | 0.42              |
| 1:C:122:ASN:HB3   | 1:C:125:ASN:H     | 1.84                     | 0.42              |
| 3:I:21:SER:HA     | 3:I:80:TYR:HD1    | 1.84                     | 0.42              |
| 3:I:38:ARG:HG3    | 3:I:94:TYR:CE1    | 2.54                     | 0.42              |
| 1:A:395:VAL:HG22  | 1:A:515:PHE:HD1   | 1.84                     | 0.42              |
| 1:A:712:ILE:H     | 1:A:1077:THR:HG23 | 1.84                     | 0.42              |
| 1:A:856:ASN:OD1   | 1:A:856:ASN:N     | 2.53                     | 0.42              |
| 1:A:894:LEU:HD11  | 1:C:715:PRO:CD    | 2.39                     | 0.42              |
| 3:E:39:HIS:HB2    | 3:E:45:LEU:HG     | 2.01                     | 0.42              |
| 1:B:317:ASN:ND2   | 1:C:737:ASP:OD2   | 2.52                     | 0.42              |
| 3:G:38:ARG:HG3    | 3:G:94:TYR:CE1    | 2.54                     | 0.42              |
| 3:I:6:GLN:OE1     | 3:I:117:LYS:N     | 2.42                     | 0.42              |
| 1:A:122:ASN:HB3   | 1:A:125:ASN:H     | 1.84                     | 0.42              |
| 1:A:206:LYS:HA    | 1:A:206:LYS:HD2   | 1.71                     | 0.42              |
| 1:A:317:ASN:ND2   | 1:B:737:ASP:OD2   | 2.53                     | 0.42              |
| 1:B:101:ILE:HD12  | 1:B:242:LEU:HD11  | 2.01                     | 0.42              |
| 1:C:977:LEU:O     | 1:C:981:LEU:HB2   | 2.19                     | 0.42              |
| 1:A:1019:ARG:O    | 1:A:1023:ASN:ND2  | 2.52                     | 0.42              |
| 3:E:37:VAL:HG13   | 3:E:46:GLU:O      | 2.19                     | 0.42              |
| 1:B:964:LYS:HE3   | 1:B:964:LYS:HB3   | 1.59                     | 0.42              |
| 1:C:48:LEU:HD13   | 1:C:305:SER:HA    | 2.00                     | 0.42              |
| 1:C:856:ASN:OD1   | 1:C:856:ASN:N     | 2.53                     | 0.42              |
| 1:C:1059:GLY:O    | 1:C:1060:VAL:HG23 | 2.19                     | 0.42              |
| 1:C:1102:TRP:HB2  | 1:C:1135:ASN:HD21 | 1.84                     | 0.42              |
| 1:A:54:LEU:HA     | 1:A:271:GLN:O     | 2.20                     | 0.42              |
| 1:A:1029:MET:HE3  | 1:A:1029:MET:HB2  | 1.86                     | 0.42              |
| 1:B:353:TRP:CD1   | 1:B:353:TRP:H     | 2.37                     | 0.42              |
| 1:B:1067:TYR:CD1  | 1:B:1067:TYR:C    | 2.96                     | 0.42              |
| 1:B:1080:ALA:HB3  | 1:B:1132:ILE:HG22 | 2.02                     | 0.42              |
| 1:B:1107:ARG:HH12 | 1:C:904:TYR:CB    | 2.16                     | 0.42              |
| 1:C:574:ASP:OD1   | 1:C:575:ALA:N     | 2.52                     | 0.42              |
| 1:C:712:ILE:H     | 1:C:1077:THR:HG23 | 1.84                     | 0.42              |
| 3:I:97:THR:CG2    | 3:I:111:TYR:HE1   | 2.33                     | 0.42              |
| 1:A:598:ILE:HG23  | 1:A:664:ILE:HG21  | 2.01                     | 0.42              |
| 2:D:50:TYR:N      | 2:D:54:LYS:O      | 2.36                     | 0.42              |
| 2:D:92:TRP:CH2    | 3:E:59:ARG:HD2    | 2.52                     | 0.42              |
| 1:B:452:LEU:C     | 1:B:452:LEU:HD12  | 2.44                     | 0.42              |
| 1:B:537:LYS:O     | 1:B:539:VAL:HG13  | 2.19                     | 0.42              |
| 1:B:942:ALA:O     | 1:B:943:SER:OG    | 2.26                     | 0.42              |
| 1:C:1144:GLU:N    | 1:C:1144:GLU:OE2  | 2.52                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:13:ALA:HA     | 2:H:110:LEU:HB2   | 2.02                     | 0.42              |
| 3:G:100:GLN:HB2   | 3:G:110:TYR:CD2   | 2.54                     | 0.42              |
| 3:E:21:SER:HA     | 3:E:80:TYR:HD1    | 1.84                     | 0.42              |
| 1:B:662:CYS:HB2   | 1:B:671:CYS:HB2   | 1.42                     | 0.42              |
| 1:B:886:TRP:N     | 1:B:886:TRP:CD1   | 2.84                     | 0.42              |
| 1:B:977:LEU:O     | 1:B:981:LEU:HB2   | 2.19                     | 0.42              |
| 1:C:1019:ARG:O    | 1:C:1023:ASN:ND2  | 2.52                     | 0.42              |
| 1:C:1080:ALA:HB3  | 1:C:1132:ILE:HG22 | 2.02                     | 0.42              |
| 3:I:37:VAL:HG13   | 3:I:46:GLU:O      | 2.19                     | 0.42              |
| 3:I:60:TYR:OH     | 3:I:70:ILE:N      | 2.33                     | 0.42              |
| 1:A:537:LYS:O     | 1:A:539:VAL:HG13  | 2.19                     | 0.42              |
| 1:A:592:PHE:CE2   | 1:B:740:MET:HE1   | 2.54                     | 0.42              |
| 1:A:758:SER:N     | 1:C:965:GLN:HE22  | 2.00                     | 0.42              |
| 1:A:1102:TRP:HB2  | 1:A:1135:ASN:HD21 | 1.84                     | 0.42              |
| 1:B:395:VAL:HG22  | 1:B:515:PHE:HD1   | 1.84                     | 0.42              |
| 1:B:712:ILE:H     | 1:B:1077:THR:HG23 | 1.84                     | 0.42              |
| 1:B:796:ASP:OD1   | 1:B:796:ASP:N     | 2.45                     | 0.42              |
| 2:H:49:ILE:HD13   | 2:H:49:ILE:HA     | 1.82                     | 0.42              |
| 3:G:104:ASN:CA    | 3:G:108:PHE:HE2   | 2.32                     | 0.42              |
| 1:B:54:LEU:HA     | 1:B:271:GLN:O     | 2.20                     | 0.42              |
| 1:C:54:LEU:HA     | 1:C:271:GLN:O     | 2.20                     | 0.42              |
| 1:C:537:LYS:O     | 1:C:539:VAL:HG13  | 2.19                     | 0.42              |
| 2:F:36:TRP:CH2    | 2:F:89:CYS:HB3    | 2.55                     | 0.42              |
| 1:A:34:ARG:O      | 1:A:56:LEU:HD23   | 2.20                     | 0.42              |
| 2:D:36:TRP:CH2    | 2:D:89:CYS:HB3    | 2.55                     | 0.42              |
| 2:D:62:ARG:NH1    | 2:D:80:GLN:NE2    | 2.68                     | 0.42              |
| 1:B:34:ARG:O      | 1:B:56:LEU:HD23   | 2.20                     | 0.42              |
| 1:C:461:LEU:C     | 1:C:461:LEU:CD1   | 2.84                     | 0.42              |
| 2:H:62:ARG:NH1    | 2:H:80:GLN:NE2    | 2.68                     | 0.42              |
| 1:A:1080:ALA:HB3  | 1:A:1132:ILE:HG22 | 2.02                     | 0.41              |
| 1:B:1144:GLU:OE2  | 1:B:1144:GLU:N    | 2.52                     | 0.41              |
| 2:H:84:GLU:HG2    | 2:H:107:LEU:O     | 2.20                     | 0.41              |
| 3:G:23:LYS:HE3    | 3:G:23:LYS:HB3    | 1.74                     | 0.41              |
| 3:G:37:VAL:HG13   | 3:G:46:GLU:O      | 2.19                     | 0.41              |
| 1:A:662:CYS:HB2   | 1:A:671:CYS:HB2   | 1.42                     | 0.41              |
| 1:A:1094:VAL:HG12 | 1:B:904:TYR:CZ    | 2.54                     | 0.41              |
| 1:B:385:THR:O     | 1:B:385:THR:CG2   | 2.68                     | 0.41              |
| 1:B:437:ASN:HB2   | 1:B:508:TYR:CZ    | 2.55                     | 0.41              |
| 1:C:568:ASP:OD1   | 1:C:572:THR:OG1   | 2.29                     | 0.41              |
| 1:C:598:ILE:HG23  | 1:C:664:ILE:HG21  | 2.01                     | 0.41              |
| 1:C:666:ILE:HD11  | 1:C:672:ALA:HB2   | 2.00                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:797:PHE:O    | 1:C:800:PHE:N     | 2.49                     | 0.41              |
| 3:G:97:THR:CG2   | 3:G:111:TYR:HE1   | 2.33                     | 0.41              |
| 1:A:1082:CYS:HB2 | 1:A:1132:ILE:HD12 | 2.03                     | 0.41              |
| 3:E:103:TYR:CZ   | 3:E:107:TYR:HB2   | 2.55                     | 0.41              |
| 1:B:570:ALA:HB2  | 1:C:963:VAL:HG12  | 2.02                     | 0.41              |
| 1:C:41:LYS:O     | 1:C:43:PHE:N      | 2.53                     | 0.41              |
| 1:A:737:ASP:OD2  | 1:C:317:ASN:ND2   | 2.52                     | 0.41              |
| 2:D:84:GLU:HG2   | 2:D:107:LEU:O     | 2.20                     | 0.41              |
| 1:C:437:ASN:HB2  | 1:C:508:TYR:CZ    | 2.55                     | 0.41              |
| 1:C:900:MET:HE2  | 1:C:900:MET:HB3   | 1.68                     | 0.41              |
| 2:H:71:SER:OG    | 2:H:72:ALA:N      | 2.53                     | 0.41              |
| 3:G:115:TRP:CE3  | 3:G:115:TRP:HA    | 2.56                     | 0.41              |
| 1:A:904:TYR:CB   | 1:C:1107:ARG:HH12 | 2.14                     | 0.41              |
| 2:D:13:ALA:HA    | 2:D:110:LEU:HB2   | 2.02                     | 0.41              |
| 1:C:1082:CYS:HB2 | 1:C:1132:ILE:HD12 | 2.03                     | 0.41              |
| 1:A:317:ASN:HA   | 1:A:594:GLY:HA2   | 2.03                     | 0.41              |
| 1:A:437:ASN:HB2  | 1:A:508:TYR:CZ    | 2.55                     | 0.41              |
| 2:D:22:CYS:SG    | 2:D:89:CYS:HB3    | 2.60                     | 0.41              |
| 1:B:29:THR:OG1   | 1:B:62:VAL:CG2    | 2.68                     | 0.41              |
| 1:B:562:PHE:HE2  | 1:C:225:PRO:HD2   | 1.77                     | 0.41              |
| 1:C:317:ASN:HA   | 1:C:594:GLY:HA2   | 2.03                     | 0.41              |
| 1:C:662:CYS:HB2  | 1:C:671:CYS:HB2   | 1.42                     | 0.41              |
| 1:C:754:LEU:HD23 | 1:C:754:LEU:HA    | 1.79                     | 0.41              |
| 2:F:71:SER:OG    | 2:F:72:ALA:N      | 2.53                     | 0.41              |
| 2:F:89:CYS:O     | 2:F:102:GLY:N     | 2.43                     | 0.41              |
| 2:H:36:TRP:HB2   | 2:H:49:ILE:HB     | 2.01                     | 0.41              |
| 2:D:7:PRO:HD3    | 2:D:21:SER:O      | 2.21                     | 0.41              |
| 3:E:38:ARG:HG3   | 3:E:94:TYR:CE1    | 2.56                     | 0.41              |
| 2:F:36:TRP:HA    | 2:F:88:TYR:O      | 2.21                     | 0.41              |
| 2:F:62:ARG:NH1   | 2:F:80:GLN:NE2    | 2.68                     | 0.41              |
| 1:A:102:ARG:N    | 1:A:242:LEU:HD23  | 2.34                     | 0.41              |
| 1:A:385:THR:O    | 1:A:385:THR:CG2   | 2.68                     | 0.41              |
| 1:A:1059:GLY:C   | 1:A:1060:VAL:HG23 | 2.46                     | 0.41              |
| 1:B:1037:SER:OG  | 1:B:1039:ARG:HG3  | 2.20                     | 0.41              |
| 1:B:1059:GLY:C   | 1:B:1060:VAL:HG23 | 2.46                     | 0.41              |
| 1:C:29:THR:OG1   | 1:C:62:VAL:CG2    | 2.68                     | 0.41              |
| 1:C:439:ASN:O    | 1:C:443:SER:OG    | 2.15                     | 0.41              |
| 1:C:441:LEU:HD13 | 3:I:103:TYR:CD2   | 2.54                     | 0.41              |
| 1:C:1102:TRP:HB2 | 1:C:1135:ASN:ND2  | 2.36                     | 0.41              |
| 1:A:29:THR:OG1   | 1:A:62:VAL:CG2    | 2.68                     | 0.41              |
| 1:A:105:ILE:HG22 | 1:A:239:GLN:O     | 2.21                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:355:ARG:CZ    | 1:A:396:TYR:CG    | 3.02                     | 0.41              |
| 1:A:1037:SER:OG   | 1:A:1039:ARG:HG3  | 2.20                     | 0.41              |
| 2:D:71:SER:OG     | 2:D:72:ALA:N      | 2.53                     | 0.41              |
| 3:E:60:TYR:OH     | 3:E:70:ILE:N      | 2.33                     | 0.41              |
| 1:B:106:PHE:HB2   | 1:B:235:ILE:HD13  | 2.03                     | 0.41              |
| 1:C:29:THR:O      | 1:C:61:ASN:HA     | 2.21                     | 0.41              |
| 1:C:597:VAL:HG12  | 1:C:598:ILE:N     | 2.36                     | 0.41              |
| 1:C:1145:LEU:HD23 | 1:C:1145:LEU:HA   | 1.87                     | 0.41              |
| 2:F:7:PRO:HD3     | 2:F:21:SER:O      | 2.21                     | 0.41              |
| 2:F:13:ALA:HA     | 2:F:110:LEU:HB2   | 2.02                     | 0.41              |
| 3:G:39:HIS:HB2    | 3:G:45:LEU:HG     | 2.02                     | 0.41              |
| 3:I:115:TRP:HA    | 3:I:115:TRP:CE3   | 2.56                     | 0.41              |
| 1:A:41:LYS:O      | 1:A:43:PHE:N      | 2.54                     | 0.41              |
| 1:A:917:TYR:HB3   | 1:C:1129:VAL:HB   | 2.02                     | 0.41              |
| 1:A:1129:VAL:HB   | 1:B:917:TYR:HB3   | 2.03                     | 0.41              |
| 3:E:100:GLN:HB2   | 3:E:110:TYR:CB    | 2.49                     | 0.41              |
| 1:B:826:VAL:HG11  | 1:B:1057:PRO:HG3  | 2.03                     | 0.41              |
| 1:C:294:ASP:OD1   | 1:C:296:LEU:N     | 2.46                     | 0.41              |
| 1:C:392:PHE:HD1   | 1:C:517:LEU:HD11  | 1.83                     | 0.41              |
| 1:C:1059:GLY:C    | 1:C:1060:VAL:HG23 | 2.46                     | 0.41              |
| 3:E:6:GLN:OE1     | 3:E:117:LYS:N     | 2.42                     | 0.40              |
| 1:B:1082:CYS:HB2  | 1:B:1132:ILE:HD12 | 2.03                     | 0.40              |
| 1:B:1107:ARG:NH1  | 1:C:904:TYR:CB    | 2.75                     | 0.40              |
| 1:C:106:PHE:HB2   | 1:C:235:ILE:HD13  | 2.03                     | 0.40              |
| 2:F:84:GLU:HG2    | 2:F:107:LEU:O     | 2.20                     | 0.40              |
| 2:H:7:PRO:HD3     | 2:H:21:SER:O      | 2.21                     | 0.40              |
| 3:G:7:SER:HG      | 3:G:21:SER:HG     | 1.50                     | 0.40              |
| 3:E:115:TRP:CE3   | 3:E:115:TRP:HA    | 2.55                     | 0.40              |
| 1:B:767:LEU:HD23  | 1:B:767:LEU:HA    | 1.84                     | 0.40              |
| 1:C:42:VAL:HG23   | 1:C:44:ARG:NH1    | 2.36                     | 0.40              |
| 1:C:105:ILE:HG22  | 1:C:239:GLN:O     | 2.21                     | 0.40              |
| 2:F:28:ASN:OD1    | 2:F:29:ILE:HG12   | 2.21                     | 0.40              |
| 2:H:22:CYS:SG     | 2:H:89:CYS:HB3    | 2.60                     | 0.40              |
| 3:G:19:LYS:HG3    | 3:G:81:LEU:O      | 2.21                     | 0.40              |
| 3:I:13:LYS:HA     | 3:I:13:LYS:HD2    | 1.91                     | 0.40              |
| 1:A:417:LYS:O     | 1:A:422:ASN:ND2   | 2.55                     | 0.40              |
| 1:A:457:ARG:HG3   | 1:A:458:LYS:N     | 2.36                     | 0.40              |
| 1:A:568:ASP:N     | 1:A:574:ASP:OD2   | 2.55                     | 0.40              |
| 1:A:699:LEU:HB2   | 1:B:788:ILE:HG13  | 2.03                     | 0.40              |
| 3:E:19:LYS:HG3    | 3:E:81:LEU:O      | 2.21                     | 0.40              |
| 1:B:597:VAL:HG12  | 1:B:598:ILE:N     | 2.36                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:856:ASN:N    | 1:B:856:ASN:OD1  | 2.53                     | 0.40              |
| 1:C:417:LYS:O    | 1:C:422:ASN:ND2  | 2.55                     | 0.40              |
| 1:C:1082:CYS:HB2 | 1:C:1126:CYS:HB2 | 1.91                     | 0.40              |
| 1:B:317:ASN:HA   | 1:B:594:GLY:HA2  | 2.03                     | 0.40              |
| 1:B:598:ILE:HG23 | 1:B:664:ILE:HG21 | 2.01                     | 0.40              |
| 1:C:439:ASN:HA   | 1:C:507:PRO:HG2  | 2.03                     | 0.40              |
| 1:C:1037:SER:OG  | 1:C:1039:ARG:HG3 | 2.20                     | 0.40              |
| 3:I:97:THR:OG1   | 3:I:113:ASP:O    | 2.25                     | 0.40              |
| 1:A:904:TYR:CB   | 1:C:1107:ARG:NH1 | 2.72                     | 0.40              |
| 1:C:355:ARG:NE   | 1:C:396:TYR:CG   | 2.85                     | 0.40              |
| 1:C:385:THR:O    | 1:C:385:THR:CG2  | 2.68                     | 0.40              |
| 1:C:560:LEU:O    | 1:C:562:PHE:N    | 2.55                     | 0.40              |
| 1:C:806:LEU:HD23 | 1:C:806:LEU:HA   | 1.68                     | 0.40              |
| 1:C:826:VAL:HG11 | 1:C:1057:PRO:HG3 | 2.03                     | 0.40              |
| 3:G:6:GLN:NE2    | 3:G:96:CYS:SG    | 2.85                     | 0.40              |
| 3:I:19:LYS:HG3   | 3:I:81:LEU:O     | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 1   | A     | 964/1208 (80%) | 872 (90%) | 90 (9%)  | 2 (0%)   | 43          | 71  |
| 1   | B     | 964/1208 (80%) | 872 (90%) | 90 (9%)  | 2 (0%)   | 43          | 71  |
| 1   | C     | 964/1208 (80%) | 871 (90%) | 91 (9%)  | 2 (0%)   | 43          | 71  |
| 2   | D     | 109/216 (50%)  | 96 (88%)  | 12 (11%) | 1 (1%)   | 14          | 42  |
| 2   | F     | 109/216 (50%)  | 96 (88%)  | 12 (11%) | 1 (1%)   | 14          | 42  |
| 2   | H     | 109/216 (50%)  | 96 (88%)  | 12 (11%) | 1 (1%)   | 14          | 42  |
| 3   | E     | 118/237 (50%)  | 107 (91%) | 11 (9%)  | 0        | 100         | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 3   | G     | 118/237 (50%)   | 106 (90%)  | 12 (10%)  | 0        | 100         | 100 |
| 3   | I     | 118/237 (50%)   | 107 (91%)  | 11 (9%)   | 0        | 100         | 100 |
| All | All   | 3573/4983 (72%) | 3223 (90%) | 341 (10%) | 9 (0%)   | 37          | 65  |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 42  | VAL  |
| 1   | B     | 42  | VAL  |
| 1   | C     | 42  | VAL  |
| 1   | A     | 444 | LYS  |
| 2   | D     | 51  | ASP  |
| 1   | B     | 444 | LYS  |
| 1   | C     | 444 | LYS  |
| 2   | F     | 51  | ASP  |
| 2   | H     | 51  | ASP  |

### 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     | 796/1053 (76%)  | 774 (97%)  | 22 (3%)  | 38          | 60 |
| 1   | B     | 796/1053 (76%)  | 774 (97%)  | 22 (3%)  | 38          | 60 |
| 1   | C     | 796/1053 (76%)  | 775 (97%)  | 21 (3%)  | 40          | 61 |
| 2   | D     | 89/181 (49%)    | 88 (99%)   | 1 (1%)   | 65          | 74 |
| 2   | F     | 89/181 (49%)    | 88 (99%)   | 1 (1%)   | 65          | 74 |
| 2   | H     | 89/181 (49%)    | 88 (99%)   | 1 (1%)   | 65          | 74 |
| 3   | E     | 102/205 (50%)   | 100 (98%)  | 2 (2%)   | 48          | 65 |
| 3   | G     | 102/205 (50%)   | 100 (98%)  | 2 (2%)   | 48          | 65 |
| 3   | I     | 102/205 (50%)   | 100 (98%)  | 2 (2%)   | 48          | 65 |
| All | All   | 2961/4317 (69%) | 2887 (98%) | 74 (2%)  | 42          | 62 |

All (74) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 42   | VAL  |
| 1   | A     | 312  | ILE  |
| 1   | A     | 362  | VAL  |
| 1   | A     | 438  | SER  |
| 1   | A     | 511  | VAL  |
| 1   | A     | 584  | ILE  |
| 1   | A     | 610  | VAL  |
| 1   | A     | 615  | VAL  |
| 1   | A     | 620  | VAL  |
| 1   | A     | 645  | THR  |
| 1   | A     | 656  | VAL  |
| 1   | A     | 716  | THR  |
| 1   | A     | 729  | VAL  |
| 1   | A     | 786  | LYS  |
| 1   | A     | 818  | ILE  |
| 1   | A     | 909  | ILE  |
| 1   | A     | 922  | LEU  |
| 1   | A     | 976  | VAL  |
| 1   | A     | 981  | LEU  |
| 1   | A     | 997  | ILE  |
| 1   | A     | 1123 | SER  |
| 1   | A     | 1133 | VAL  |
| 2   | D     | 28   | ASN  |
| 3   | E     | 68   | VAL  |
| 3   | E     | 89   | SER  |
| 1   | B     | 42   | VAL  |
| 1   | B     | 312  | ILE  |
| 1   | B     | 362  | VAL  |
| 1   | B     | 438  | SER  |
| 1   | B     | 511  | VAL  |
| 1   | B     | 584  | ILE  |
| 1   | B     | 610  | VAL  |
| 1   | B     | 615  | VAL  |
| 1   | B     | 620  | VAL  |
| 1   | B     | 645  | THR  |
| 1   | B     | 656  | VAL  |
| 1   | B     | 716  | THR  |
| 1   | B     | 729  | VAL  |
| 1   | B     | 786  | LYS  |
| 1   | B     | 818  | ILE  |
| 1   | B     | 909  | ILE  |
| 1   | B     | 922  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 976  | VAL  |
| 1   | B     | 981  | LEU  |
| 1   | B     | 997  | ILE  |
| 1   | B     | 1123 | SER  |
| 1   | B     | 1133 | VAL  |
| 1   | C     | 312  | ILE  |
| 1   | C     | 362  | VAL  |
| 1   | C     | 438  | SER  |
| 1   | C     | 511  | VAL  |
| 1   | C     | 584  | ILE  |
| 1   | C     | 610  | VAL  |
| 1   | C     | 615  | VAL  |
| 1   | C     | 620  | VAL  |
| 1   | C     | 645  | THR  |
| 1   | C     | 656  | VAL  |
| 1   | C     | 716  | THR  |
| 1   | C     | 729  | VAL  |
| 1   | C     | 786  | LYS  |
| 1   | C     | 818  | ILE  |
| 1   | C     | 909  | ILE  |
| 1   | C     | 922  | LEU  |
| 1   | C     | 976  | VAL  |
| 1   | C     | 981  | LEU  |
| 1   | C     | 997  | ILE  |
| 1   | C     | 1123 | SER  |
| 1   | C     | 1133 | VAL  |
| 2   | F     | 28   | ASN  |
| 2   | H     | 28   | ASN  |
| 3   | G     | 68   | VAL  |
| 3   | G     | 89   | SER  |
| 3   | I     | 68   | VAL  |
| 3   | I     | 89   | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 61  | ASN  |
| 1   | A     | 99  | ASN  |
| 1   | A     | 121 | ASN  |
| 1   | A     | 422 | ASN  |
| 1   | A     | 437 | ASN  |
| 1   | A     | 448 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 487  | ASN  |
| 1   | A     | 536  | ASN  |
| 1   | A     | 564  | GLN  |
| 1   | A     | 644  | GLN  |
| 1   | A     | 655  | HIS  |
| 1   | A     | 717  | ASN  |
| 1   | A     | 751  | ASN  |
| 1   | A     | 755  | GLN  |
| 1   | A     | 901  | GLN  |
| 1   | A     | 960  | ASN  |
| 1   | A     | 965  | GLN  |
| 1   | A     | 1002 | GLN  |
| 1   | A     | 1005 | GLN  |
| 1   | A     | 1088 | HIS  |
| 1   | A     | 1101 | HIS  |
| 2   | D     | 31   | ASN  |
| 2   | D     | 39   | GLN  |
| 3   | E     | 31   | ASN  |
| 3   | E     | 39   | HIS  |
| 1   | B     | 61   | ASN  |
| 1   | B     | 99   | ASN  |
| 1   | B     | 121  | ASN  |
| 1   | B     | 422  | ASN  |
| 1   | B     | 437  | ASN  |
| 1   | B     | 448  | ASN  |
| 1   | B     | 487  | ASN  |
| 1   | B     | 536  | ASN  |
| 1   | B     | 564  | GLN  |
| 1   | B     | 644  | GLN  |
| 1   | B     | 655  | HIS  |
| 1   | B     | 717  | ASN  |
| 1   | B     | 751  | ASN  |
| 1   | B     | 755  | GLN  |
| 1   | B     | 901  | GLN  |
| 1   | B     | 960  | ASN  |
| 1   | B     | 965  | GLN  |
| 1   | B     | 1002 | GLN  |
| 1   | B     | 1005 | GLN  |
| 1   | B     | 1101 | HIS  |
| 1   | C     | 61   | ASN  |
| 1   | C     | 99   | ASN  |
| 1   | C     | 121  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 422  | ASN  |
| 1   | C     | 437  | ASN  |
| 1   | C     | 448  | ASN  |
| 1   | C     | 487  | ASN  |
| 1   | C     | 536  | ASN  |
| 1   | C     | 564  | GLN  |
| 1   | C     | 644  | GLN  |
| 1   | C     | 655  | HIS  |
| 1   | C     | 717  | ASN  |
| 1   | C     | 751  | ASN  |
| 1   | C     | 755  | GLN  |
| 1   | C     | 901  | GLN  |
| 1   | C     | 960  | ASN  |
| 1   | C     | 965  | GLN  |
| 1   | C     | 1002 | GLN  |
| 1   | C     | 1005 | GLN  |
| 1   | C     | 1101 | HIS  |
| 2   | F     | 31   | ASN  |
| 2   | F     | 39   | GLN  |
| 2   | H     | 39   | GLN  |
| 3   | G     | 31   | ASN  |
| 3   | G     | 39   | HIS  |
| 3   | I     | 31   | ASN  |
| 3   | I     | 39   | HIS  |
| 3   | I     | 104  | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

24 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$ |
| 4   | NAG  | C     | 1305 | 1    | 14,14,15     | 0.43 | 0           | 17,19,21    | 0.65 | 1 (5%)      |
| 4   | NAG  | A     | 1303 | 1    | 14,14,15     | 0.31 | 0           | 17,19,21    | 0.59 | 0           |
| 4   | NAG  | B     | 1303 | 1    | 14,14,15     | 0.30 | 0           | 17,19,21    | 0.58 | 0           |
| 4   | NAG  | A     | 1304 | 1    | 14,14,15     | 0.22 | 0           | 17,19,21    | 0.50 | 0           |
| 4   | NAG  | B     | 1304 | 1    | 14,14,15     | 0.21 | 0           | 17,19,21    | 0.51 | 0           |
| 4   | NAG  | B     | 1307 | 1    | 14,14,15     | 0.35 | 0           | 17,19,21    | 0.37 | 0           |
| 4   | NAG  | A     | 1301 | 1    | 14,14,15     | 0.41 | 0           | 17,19,21    | 0.40 | 0           |
| 4   | NAG  | C     | 1303 | 1    | 14,14,15     | 0.31 | 0           | 17,19,21    | 0.58 | 0           |
| 4   | NAG  | B     | 1301 | 1    | 14,14,15     | 0.41 | 0           | 17,19,21    | 0.40 | 0           |
| 4   | NAG  | C     | 1304 | 1    | 14,14,15     | 0.22 | 0           | 17,19,21    | 0.50 | 0           |
| 4   | NAG  | B     | 1302 | 1    | 14,14,15     | 0.34 | 0           | 17,19,21    | 0.60 | 0           |
| 4   | NAG  | C     | 1308 | 1    | 14,14,15     | 0.40 | 0           | 17,19,21    | 1.87 | 4 (23%)     |
| 4   | NAG  | B     | 1308 | 1    | 14,14,15     | 0.37 | 0           | 17,19,21    | 1.56 | 1 (5%)      |
| 4   | NAG  | A     | 1302 | 1    | 14,14,15     | 0.34 | 0           | 17,19,21    | 0.60 | 0           |
| 4   | NAG  | A     | 1305 | 1    | 14,14,15     | 0.44 | 0           | 17,19,21    | 0.66 | 1 (5%)      |
| 4   | NAG  | B     | 1306 | 1    | 14,14,15     | 0.18 | 0           | 17,19,21    | 0.60 | 0           |
| 4   | NAG  | A     | 1306 | 1    | 14,14,15     | 0.19 | 0           | 17,19,21    | 0.59 | 0           |
| 4   | NAG  | C     | 1306 | 1    | 14,14,15     | 0.18 | 0           | 17,19,21    | 0.59 | 0           |
| 4   | NAG  | B     | 1305 | 1    | 14,14,15     | 0.44 | 0           | 17,19,21    | 0.65 | 1 (5%)      |
| 4   | NAG  | C     | 1301 | 1    | 14,14,15     | 0.39 | 0           | 17,19,21    | 0.41 | 0           |
| 4   | NAG  | A     | 1307 | 1    | 14,14,15     | 0.35 | 0           | 17,19,21    | 0.38 | 0           |
| 4   | NAG  | A     | 1308 | 1    | 14,14,15     | 0.37 | 0           | 17,19,21    | 1.59 | 1 (5%)      |
| 4   | NAG  | C     | 1302 | 1    | 14,14,15     | 0.33 | 0           | 17,19,21    | 0.60 | 0           |
| 4   | NAG  | C     | 1307 | 1    | 14,14,15     | 0.35 | 0           | 17,19,21    | 0.38 | 0           |

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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 4   | NAG  | C     | 1305 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1303 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1303 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1304 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1304 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1307 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1301 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1303 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1301 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1304 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1302 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1308 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1308 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1302 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1305 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1306 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1306 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1306 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1305 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1301 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1307 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1308 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1302 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1307 | 1    | -       | 0/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

All (9) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4   | A     | 1308 | NAG  | C1-O5-C5 | 5.10  | 119.02      | 112.19   |
| 4   | C     | 1308 | NAG  | C1-O5-C5 | 5.09  | 119.00      | 112.19   |
| 4   | B     | 1308 | NAG  | C1-O5-C5 | 5.05  | 118.96      | 112.19   |
| 4   | C     | 1308 | NAG  | C2-N2-C7 | -3.49 | 118.22      | 122.90   |
| 4   | C     | 1308 | NAG  | O5-C5-C6 | 2.65  | 112.82      | 107.66   |
| 4   | C     | 1308 | NAG  | C3-C4-C5 | 2.20  | 114.23      | 110.23   |
| 4   | A     | 1305 | NAG  | C1-O5-C5 | 2.13  | 115.04      | 112.19   |
| 4   | C     | 1305 | NAG  | C1-O5-C5 | 2.12  | 115.03      | 112.19   |
| 4   | B     | 1305 | NAG  | C1-O5-C5 | 2.08  | 114.98      | 112.19   |

There are no chirality outliers.

All (20) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 4   | A     | 1308 | NAG  | C3-C2-N2-C7 |
| 4   | A     | 1308 | NAG  | C8-C7-N2-C2 |
| 4   | A     | 1308 | NAG  | O7-C7-N2-C2 |
| 4   | B     | 1308 | NAG  | C3-C2-N2-C7 |
| 4   | B     | 1308 | NAG  | C8-C7-N2-C2 |
| 4   | B     | 1308 | NAG  | O7-C7-N2-C2 |
| 4   | C     | 1308 | NAG  | O5-C5-C6-O6 |
| 4   | C     | 1308 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 1302 | NAG  | C3-C2-N2-C7 |
| 4   | B     | 1302 | NAG  | C3-C2-N2-C7 |
| 4   | C     | 1302 | NAG  | C3-C2-N2-C7 |
| 4   | A     | 1301 | NAG  | C4-C5-C6-O6 |
| 4   | C     | 1301 | NAG  | C4-C5-C6-O6 |
| 4   | B     | 1301 | NAG  | C4-C5-C6-O6 |
| 4   | C     | 1301 | NAG  | O5-C5-C6-O6 |
| 4   | A     | 1301 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 1301 | NAG  | O5-C5-C6-O6 |
| 4   | A     | 1302 | NAG  | C1-C2-N2-C7 |
| 4   | B     | 1302 | NAG  | C1-C2-N2-C7 |
| 4   | C     | 1302 | NAG  | C1-C2-N2-C7 |

There are no ring outliers.

9 monomers are involved in 10 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | C     | 1305 | NAG  | 1       | 0            |
| 4   | B     | 1307 | NAG  | 1       | 0            |
| 4   | A     | 1305 | NAG  | 1       | 0            |
| 4   | B     | 1306 | NAG  | 1       | 0            |
| 4   | A     | 1306 | NAG  | 1       | 0            |
| 4   | C     | 1306 | NAG  | 1       | 0            |
| 4   | B     | 1305 | NAG  | 1       | 0            |
| 4   | A     | 1307 | NAG  | 1       | 0            |
| 4   | C     | 1307 | NAG  | 2       | 0            |

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

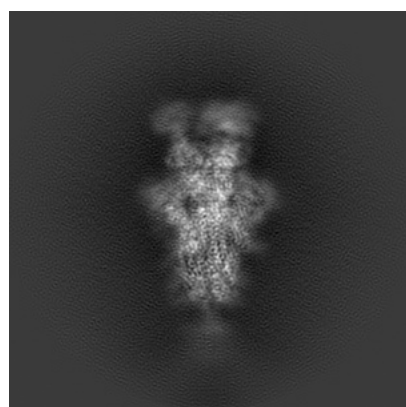
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31639. These allow visual inspection of the internal detail of the map and identification of artifacts.

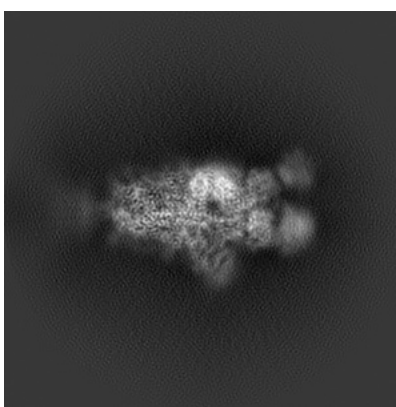
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

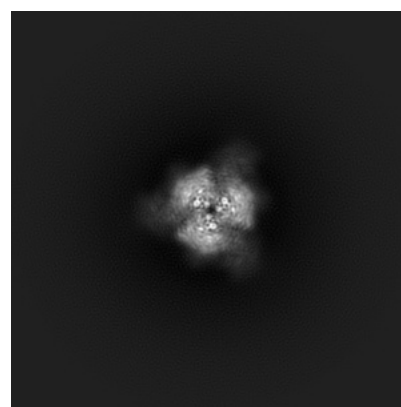
#### 6.1.1 Primary map



X



Y

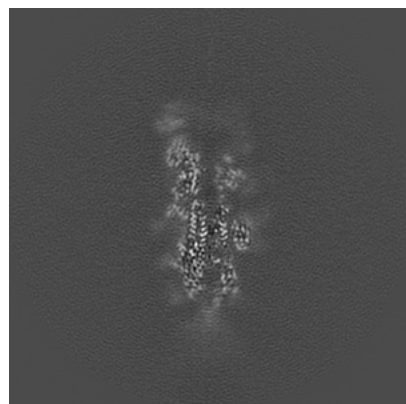


Z

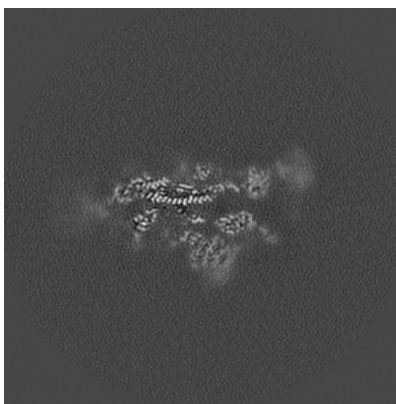
The images above show the map projected in three orthogonal directions.

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

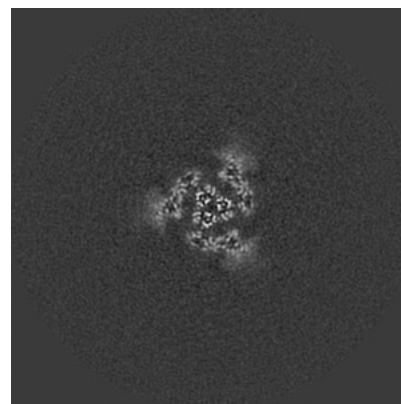
#### 6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

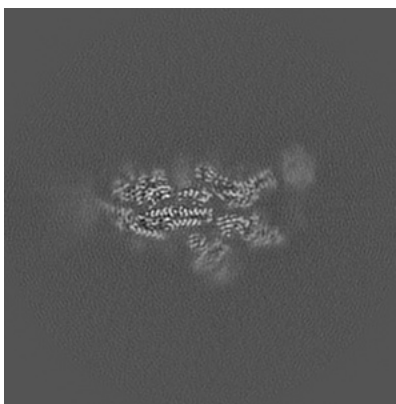
The images above show central slices of the map in three orthogonal directions.

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

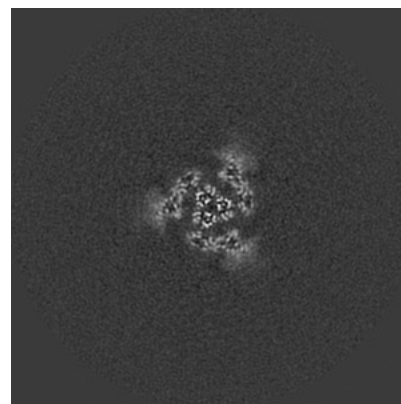
### 6.3.1 Primary map



X Index: 196



Y Index: 207

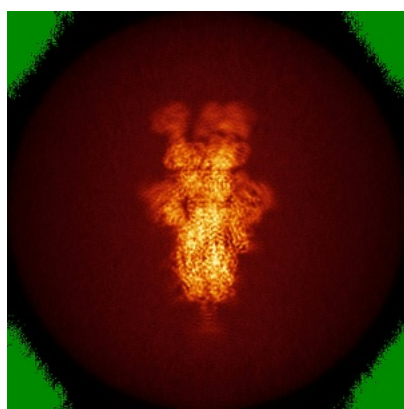


Z Index: 200

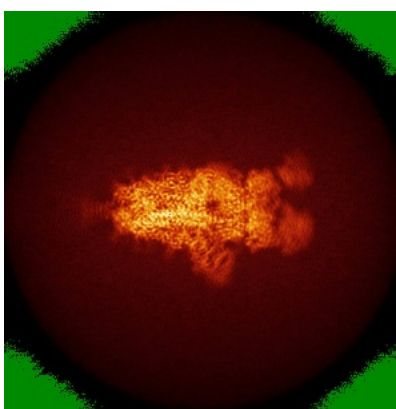
The images above show the largest variance slices of the map in three orthogonal directions.

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

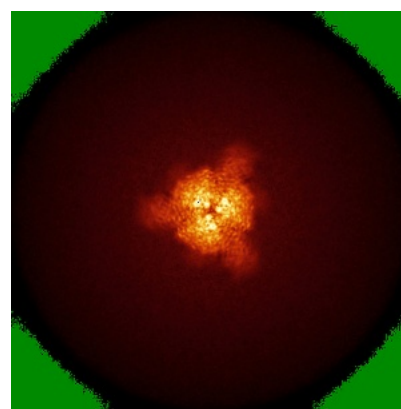
### 6.4.1 Primary map



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

This section was not generated.

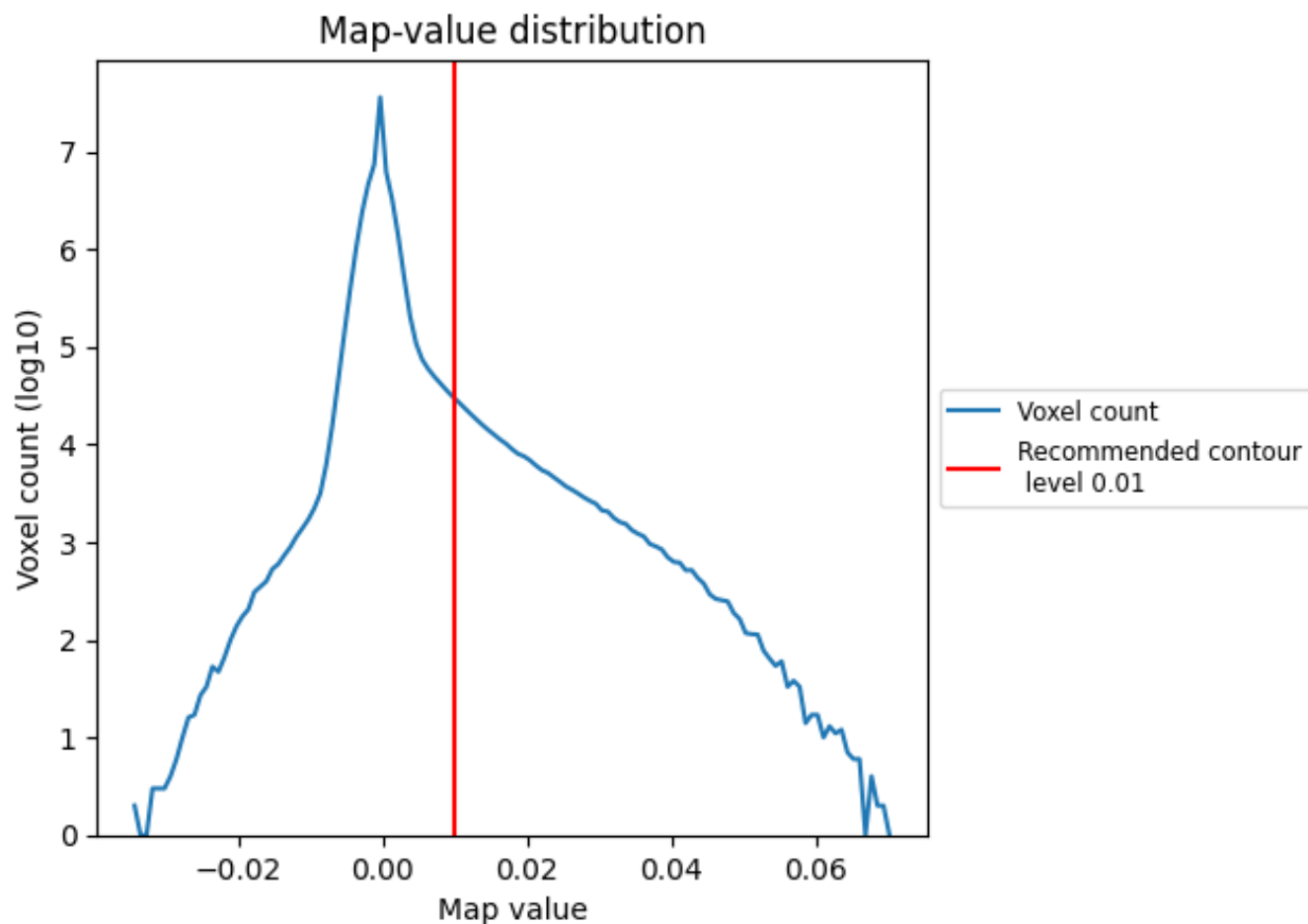
## 6.6 Mask visualisation

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

## 7 Map analysis [i](#)

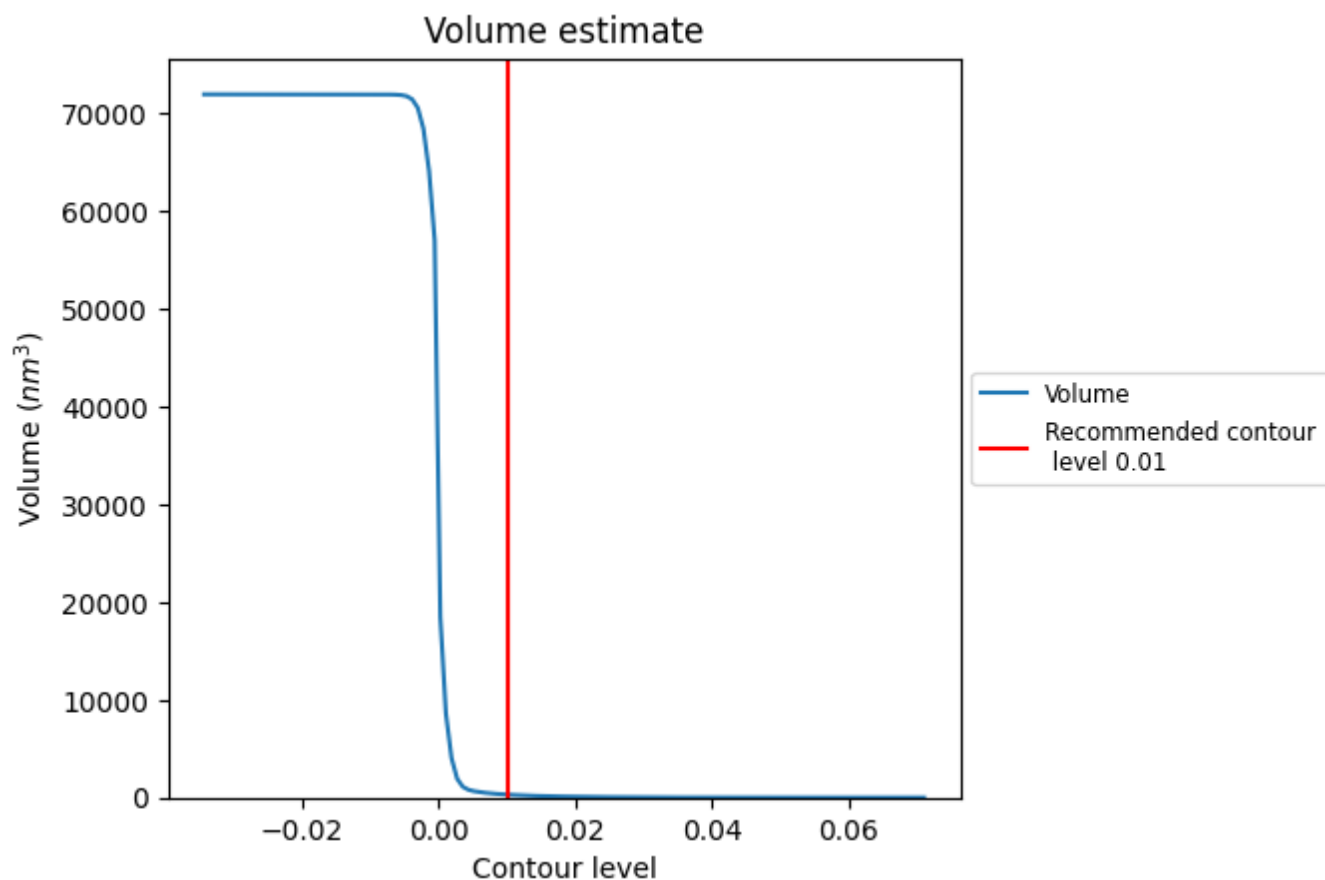
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)

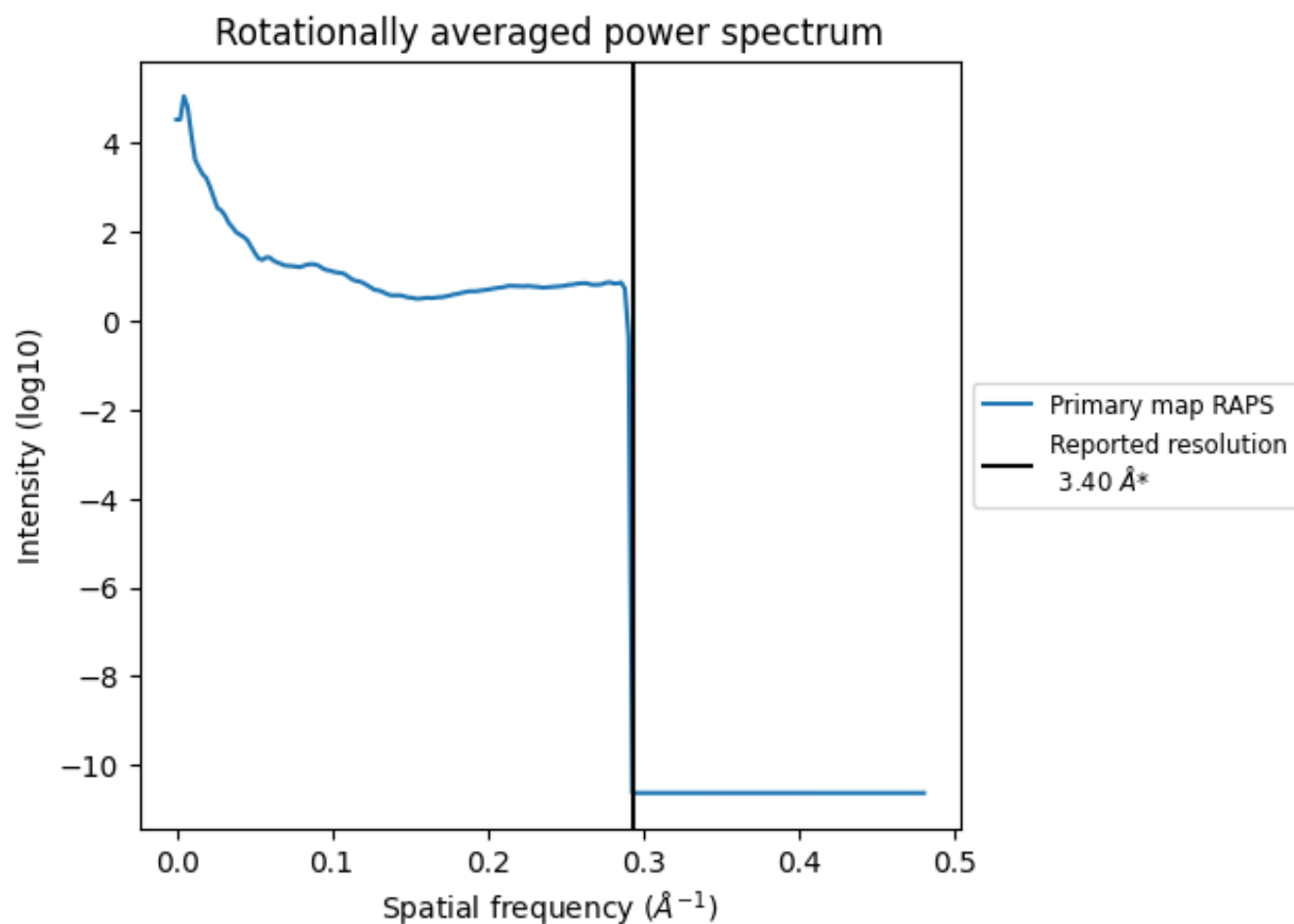


The volume at the recommended contour level is 300  $\text{nm}^3$ ; this corresponds to an approximate mass of 271 kDa.

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 0.294 Å<sup>-1</sup>

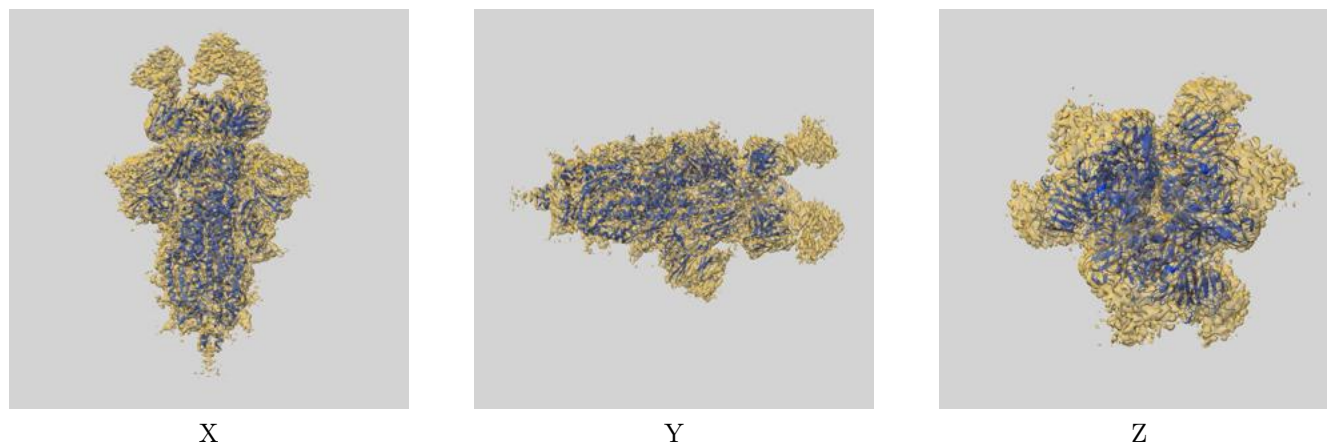
## 8 Fourier-Shell correlation ⓘ

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

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

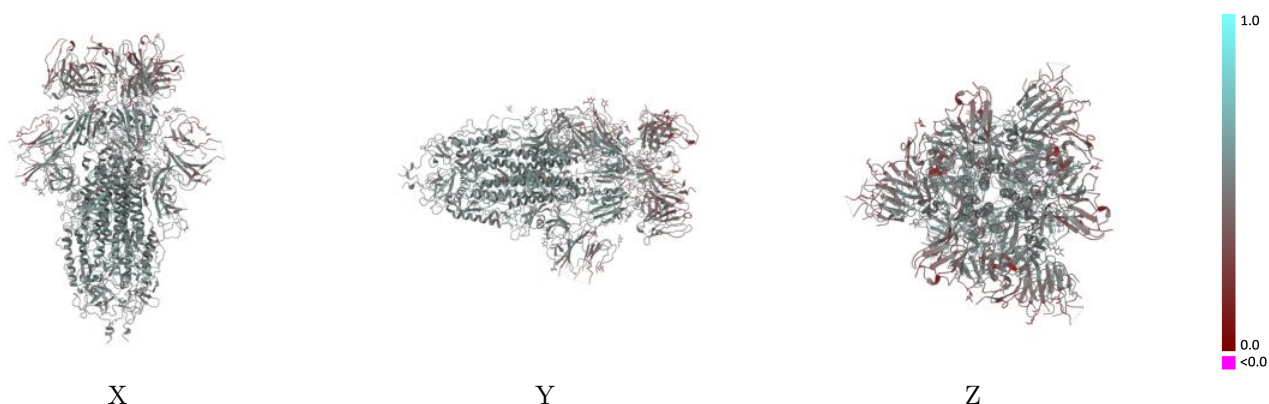
This section contains information regarding the fit between EMDB map EMD-31639 and PDB model 7V2A. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



The images above show the 3D surface view of the map at the recommended contour level 0.01 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](#)



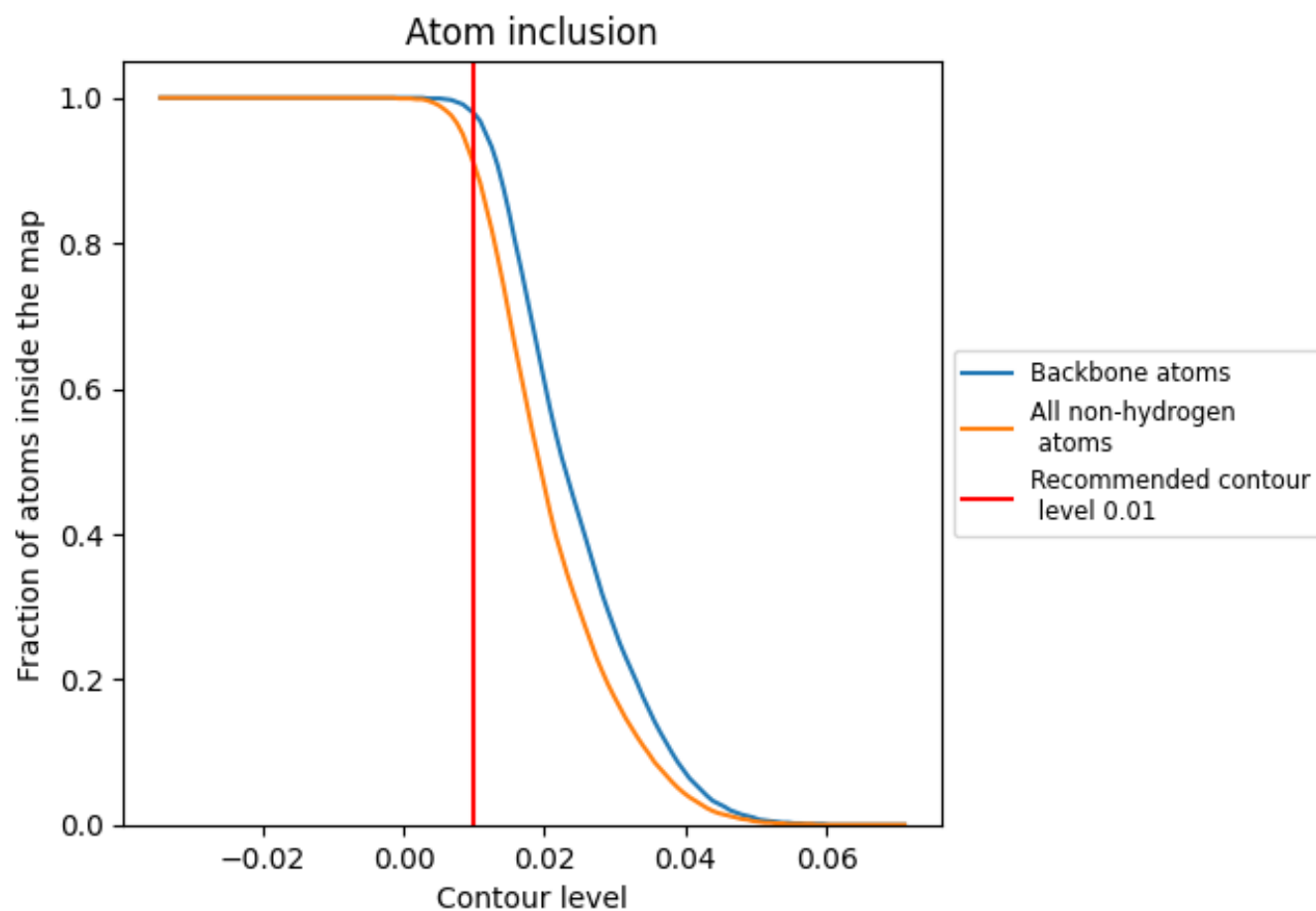
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.9100 | <div><div></div></div> 0.4820 |
| A     | <div><div></div></div> 0.9180 | <div><div></div></div> 0.5010 |
| B     | <div><div></div></div> 0.9170 | <div><div></div></div> 0.4990 |
| C     | <div><div></div></div> 0.9170 | <div><div></div></div> 0.4990 |
| D     | <div><div></div></div> 0.8770 | <div><div></div></div> 0.4070 |
| E     | <div><div></div></div> 0.8800 | <div><div></div></div> 0.4040 |
| F     | <div><div></div></div> 0.8730 | <div><div></div></div> 0.4050 |
| G     | <div><div></div></div> 0.8810 | <div><div></div></div> 0.4100 |
| H     | <div><div></div></div> 0.8740 | <div><div></div></div> 0.4070 |
| I     | <div><div></div></div> 0.8770 | <div><div></div></div> 0.4010 |

1.0

0.0

<0.0