



## Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 09:49 PM UTC

PDB ID : 7P5V / pdb\_00007p5v  
EMDB ID : EMD-13202  
Title : Structure of homomeric LRRC8A Volume-Regulated Anion Channel in complex with synthetic nanobody Sb1  
Authors : Deneka, D.; Rutz, S.; Sawicka, M.  
Deposited on : 2021-07-15  
Resolution : 3.06 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

---

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

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

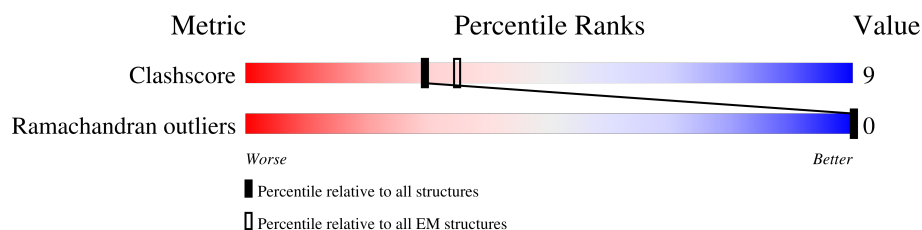
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.06 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 229148                      | 23984                       |
| Ramachandran outliers | 224038                      | 23583                       |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain                                                                                 |
|-----|-------|--------|--------------------------------------------------------------------------------------------------|
| 1   | A     | 810    |  65% 23% 11% |
| 1   | B     | 810    |  69% 22% 10% |
| 1   | C     | 810    |  67% 21% 11% |
| 1   | D     | 810    |  71% 20% 10% |
| 1   | E     | 810    |  66% 22% 11% |
| 1   | F     | 810    |  69% 21% 10% |
| 2   | G     | 144    |  61% 18% 21% |
| 2   | H     | 144    |  58% 22% 21% |
| 2   | I     | 144    |  61% 18% 21% |
| 2   | J     | 144    |  62% 17% 21% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain                                                                                  |
|-----|-------|--------|---------------------------------------------------------------------------------------------------|
| 2   | K     | 144    | <br>56% 23% 21% |
| 2   | L     | 144    | <br>62% 17% 21% |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41274 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 Volume-regulated anion channel subunit LRRC8A.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 718      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 5922  | 3853 | 997  | 1047 | 25 |         |       |
| 1   | B     | 732      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6030  | 3916 | 1018 | 1071 | 25 |         |       |
| 1   | C     | 718      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 5922  | 3853 | 997  | 1047 | 25 |         |       |
| 1   | D     | 732      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6030  | 3916 | 1018 | 1071 | 25 |         |       |
| 1   | E     | 718      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 5922  | 3853 | 997  | 1047 | 25 |         |       |
| 1   | F     | 732      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6030  | 3916 | 1018 | 1071 | 25 |         |       |

There are 96 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 1       | MET      | -      | initiating methionine | UNP Q80WG5 |
| A     | 2       | ILE      | -      | expression tag        | UNP Q80WG5 |
| A     | 3       | PRO      | -      | expression tag        | UNP Q80WG5 |
| A     | 4       | VAL      | -      | expression tag        | UNP Q80WG5 |
| A     | 5       | THR      | -      | expression tag        | UNP Q80WG5 |
| A     | 6       | GLU      | -      | expression tag        | UNP Q80WG5 |
| A     | 7       | LEU      | -      | expression tag        | UNP Q80WG5 |
| A     | 8       | ARG      | -      | expression tag        | UNP Q80WG5 |
| A     | 9       | TYR      | -      | expression tag        | UNP Q80WG5 |
| A     | 10      | PHE      | -      | expression tag        | UNP Q80WG5 |
| A     | 11      | ALA      | -      | expression tag        | UNP Q80WG5 |
| A     | 12      | ASP      | -      | expression tag        | UNP Q80WG5 |
| A     | 13      | THR      | -      | expression tag        | UNP Q80WG5 |
| A     | 14      | GLN      | -      | expression tag        | UNP Q80WG5 |
| A     | 809     | GLN      | -      | expression tag        | UNP Q80WG5 |
| A     | 810     | ALA      | -      | expression tag        | UNP Q80WG5 |
| B     | 1       | MET      | -      | initiating methionine | UNP Q80WG5 |
| B     | 2       | ILE      | -      | expression tag        | UNP Q80WG5 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| B     | 3       | PRO      | -      | expression tag        | UNP Q80WG5 |
| B     | 4       | VAL      | -      | expression tag        | UNP Q80WG5 |
| B     | 5       | THR      | -      | expression tag        | UNP Q80WG5 |
| B     | 6       | GLU      | -      | expression tag        | UNP Q80WG5 |
| B     | 7       | LEU      | -      | expression tag        | UNP Q80WG5 |
| B     | 8       | ARG      | -      | expression tag        | UNP Q80WG5 |
| B     | 9       | TYR      | -      | expression tag        | UNP Q80WG5 |
| B     | 10      | PHE      | -      | expression tag        | UNP Q80WG5 |
| B     | 11      | ALA      | -      | expression tag        | UNP Q80WG5 |
| B     | 12      | ASP      | -      | expression tag        | UNP Q80WG5 |
| B     | 13      | THR      | -      | expression tag        | UNP Q80WG5 |
| B     | 14      | GLN      | -      | expression tag        | UNP Q80WG5 |
| B     | 809     | GLN      | -      | expression tag        | UNP Q80WG5 |
| B     | 810     | ALA      | -      | expression tag        | UNP Q80WG5 |
| C     | 1       | MET      | -      | initiating methionine | UNP Q80WG5 |
| C     | 2       | ILE      | -      | expression tag        | UNP Q80WG5 |
| C     | 3       | PRO      | -      | expression tag        | UNP Q80WG5 |
| C     | 4       | VAL      | -      | expression tag        | UNP Q80WG5 |
| C     | 5       | THR      | -      | expression tag        | UNP Q80WG5 |
| C     | 6       | GLU      | -      | expression tag        | UNP Q80WG5 |
| C     | 7       | LEU      | -      | expression tag        | UNP Q80WG5 |
| C     | 8       | ARG      | -      | expression tag        | UNP Q80WG5 |
| C     | 9       | TYR      | -      | expression tag        | UNP Q80WG5 |
| C     | 10      | PHE      | -      | expression tag        | UNP Q80WG5 |
| C     | 11      | ALA      | -      | expression tag        | UNP Q80WG5 |
| C     | 12      | ASP      | -      | expression tag        | UNP Q80WG5 |
| C     | 13      | THR      | -      | expression tag        | UNP Q80WG5 |
| C     | 14      | GLN      | -      | expression tag        | UNP Q80WG5 |
| C     | 809     | GLN      | -      | expression tag        | UNP Q80WG5 |
| C     | 810     | ALA      | -      | expression tag        | UNP Q80WG5 |
| D     | 1       | MET      | -      | initiating methionine | UNP Q80WG5 |
| D     | 2       | ILE      | -      | expression tag        | UNP Q80WG5 |
| D     | 3       | PRO      | -      | expression tag        | UNP Q80WG5 |
| D     | 4       | VAL      | -      | expression tag        | UNP Q80WG5 |
| D     | 5       | THR      | -      | expression tag        | UNP Q80WG5 |
| D     | 6       | GLU      | -      | expression tag        | UNP Q80WG5 |
| D     | 7       | LEU      | -      | expression tag        | UNP Q80WG5 |
| D     | 8       | ARG      | -      | expression tag        | UNP Q80WG5 |
| D     | 9       | TYR      | -      | expression tag        | UNP Q80WG5 |
| D     | 10      | PHE      | -      | expression tag        | UNP Q80WG5 |
| D     | 11      | ALA      | -      | expression tag        | UNP Q80WG5 |
| D     | 12      | ASP      | -      | expression tag        | UNP Q80WG5 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| D     | 13      | THR      | -      | expression tag        | UNP Q80WG5 |
| D     | 14      | GLN      | -      | expression tag        | UNP Q80WG5 |
| D     | 809     | GLN      | -      | expression tag        | UNP Q80WG5 |
| D     | 810     | ALA      | -      | expression tag        | UNP Q80WG5 |
| E     | 1       | MET      | -      | initiating methionine | UNP Q80WG5 |
| E     | 2       | ILE      | -      | expression tag        | UNP Q80WG5 |
| E     | 3       | PRO      | -      | expression tag        | UNP Q80WG5 |
| E     | 4       | VAL      | -      | expression tag        | UNP Q80WG5 |
| E     | 5       | THR      | -      | expression tag        | UNP Q80WG5 |
| E     | 6       | GLU      | -      | expression tag        | UNP Q80WG5 |
| E     | 7       | LEU      | -      | expression tag        | UNP Q80WG5 |
| E     | 8       | ARG      | -      | expression tag        | UNP Q80WG5 |
| E     | 9       | TYR      | -      | expression tag        | UNP Q80WG5 |
| E     | 10      | PHE      | -      | expression tag        | UNP Q80WG5 |
| E     | 11      | ALA      | -      | expression tag        | UNP Q80WG5 |
| E     | 12      | ASP      | -      | expression tag        | UNP Q80WG5 |
| E     | 13      | THR      | -      | expression tag        | UNP Q80WG5 |
| E     | 14      | GLN      | -      | expression tag        | UNP Q80WG5 |
| E     | 809     | GLN      | -      | expression tag        | UNP Q80WG5 |
| E     | 810     | ALA      | -      | expression tag        | UNP Q80WG5 |
| F     | 1       | MET      | -      | initiating methionine | UNP Q80WG5 |
| F     | 2       | ILE      | -      | expression tag        | UNP Q80WG5 |
| F     | 3       | PRO      | -      | expression tag        | UNP Q80WG5 |
| F     | 4       | VAL      | -      | expression tag        | UNP Q80WG5 |
| F     | 5       | THR      | -      | expression tag        | UNP Q80WG5 |
| F     | 6       | GLU      | -      | expression tag        | UNP Q80WG5 |
| F     | 7       | LEU      | -      | expression tag        | UNP Q80WG5 |
| F     | 8       | ARG      | -      | expression tag        | UNP Q80WG5 |
| F     | 9       | TYR      | -      | expression tag        | UNP Q80WG5 |
| F     | 10      | PHE      | -      | expression tag        | UNP Q80WG5 |
| F     | 11      | ALA      | -      | expression tag        | UNP Q80WG5 |
| F     | 12      | ASP      | -      | expression tag        | UNP Q80WG5 |
| F     | 13      | THR      | -      | expression tag        | UNP Q80WG5 |
| F     | 14      | GLN      | -      | expression tag        | UNP Q80WG5 |
| F     | 809     | GLN      | -      | expression tag        | UNP Q80WG5 |
| F     | 810     | ALA      | -      | expression tag        | UNP Q80WG5 |

- Molecule 2 is a protein called Synthetic nanobody Sb1.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 2   | G     | 114      | Total | C   | N   | O   | S       |       |
|     |       |          | 903   | 575 | 152 | 172 | 4       | 0     |

*Continued on next page...*

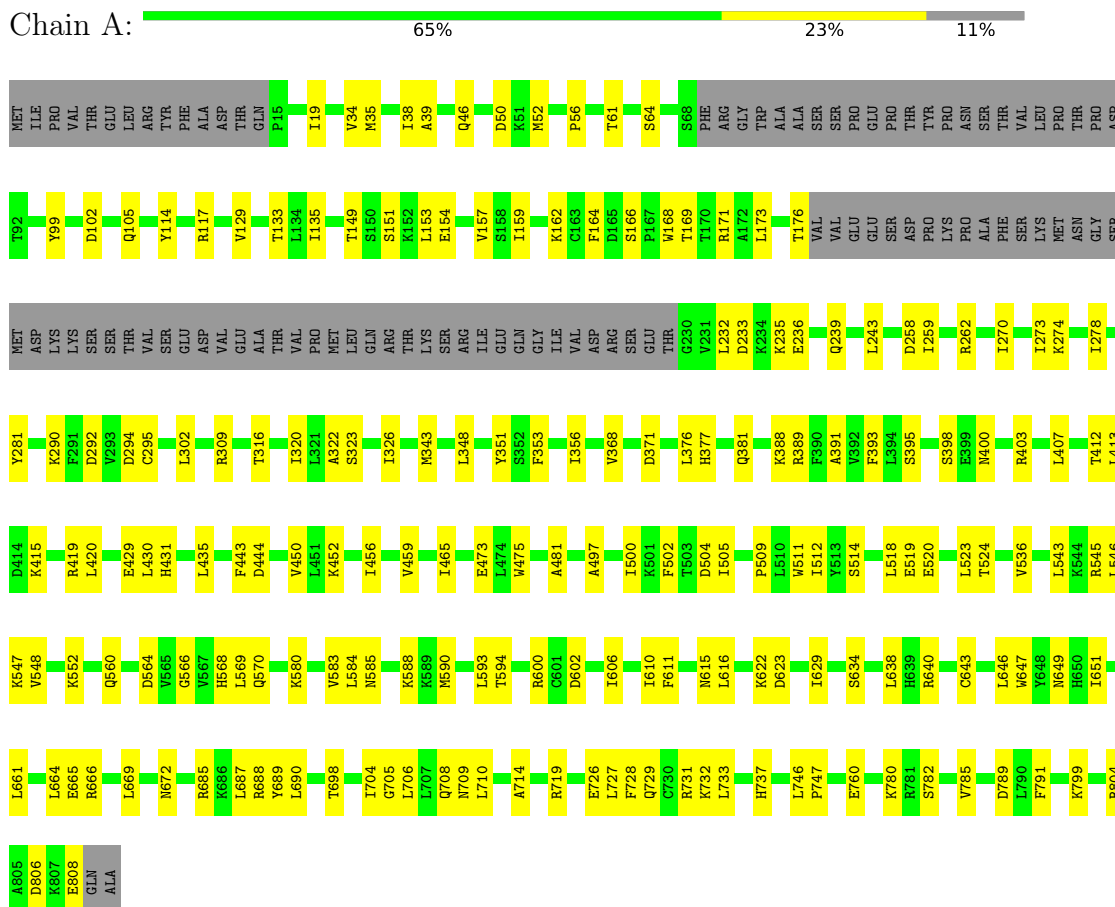
*Continued from previous page...*

| Mol | Chain | Residues | Atoms        |          |          |          |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 2   | H     | 114      | Total<br>903 | C<br>575 | N<br>152 | O<br>172 | S<br>4 | 0       | 0     |
| 2   | I     | 114      | Total<br>903 | C<br>575 | N<br>152 | O<br>172 | S<br>4 | 0       | 0     |
| 2   | J     | 114      | Total<br>903 | C<br>575 | N<br>152 | O<br>172 | S<br>4 | 0       | 0     |
| 2   | K     | 114      | Total<br>903 | C<br>575 | N<br>152 | O<br>172 | S<br>4 | 0       | 0     |
| 2   | L     | 114      | Total<br>903 | C<br>575 | N<br>152 | O<br>172 | S<br>4 | 0       | 0     |

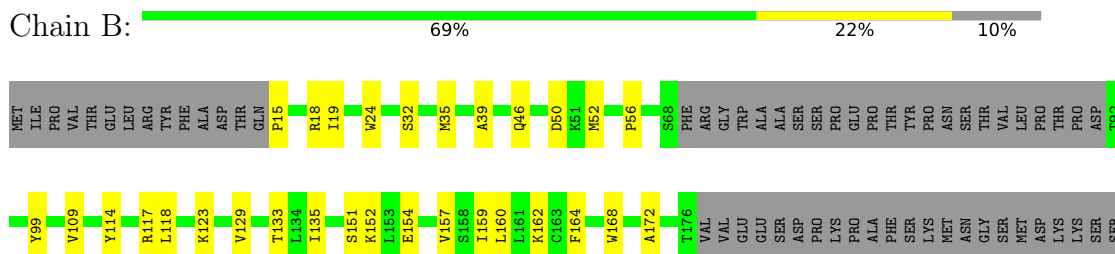
### 3 Residue-property plots

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

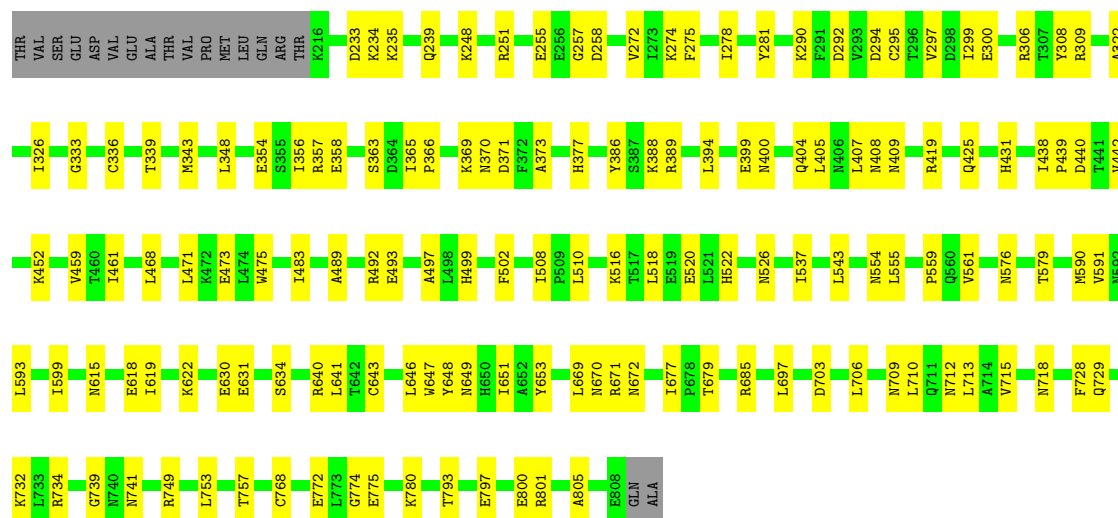
- Molecule 1: Volume-regulated anion channel subunit LRRC8A



- Molecule 1: Volume-regulated anion channel subunit LRRC8A

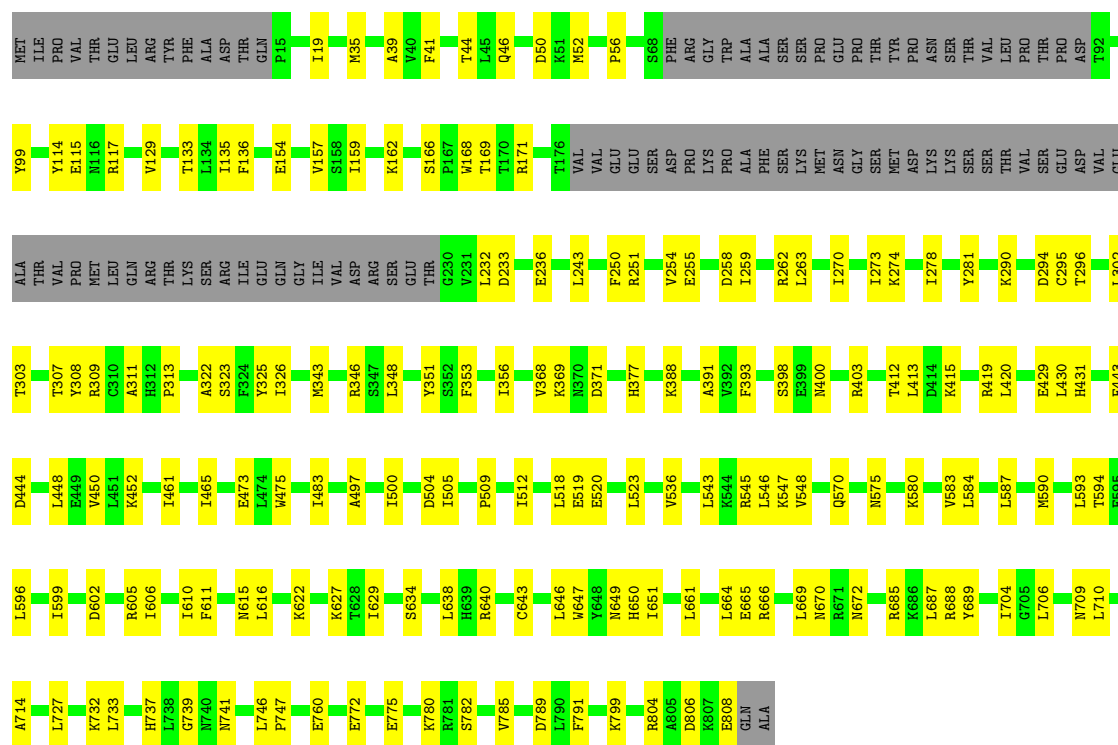






• Molecule 1: Volume-regulated anion channel subunit LRRC8A

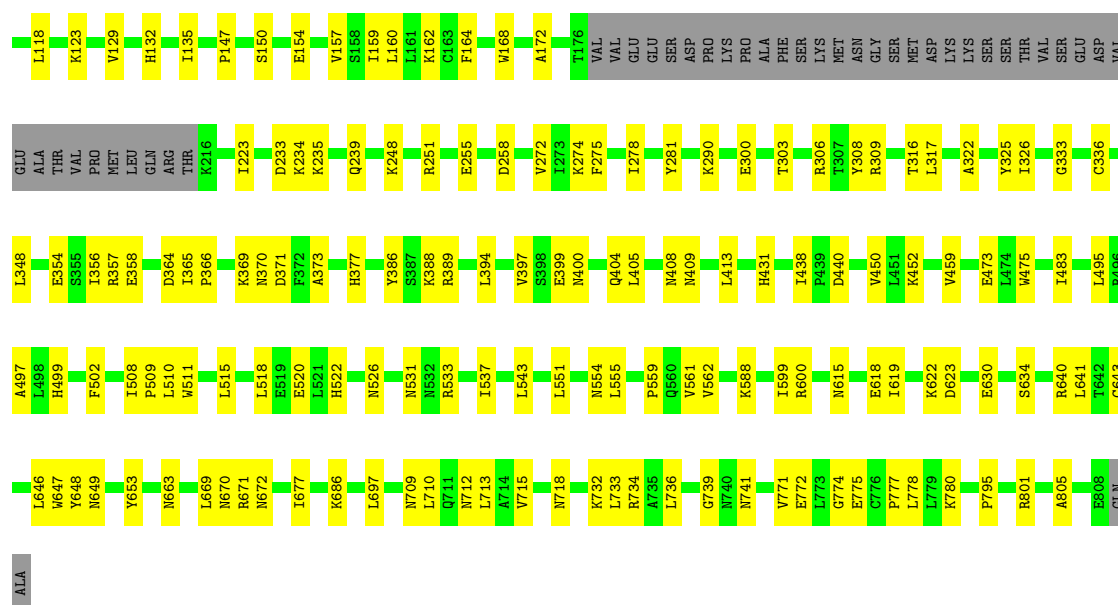
Chain C: 67% 21% 11%



• Molecule 1: Volume-regulated anion channel subunit LRRC8A

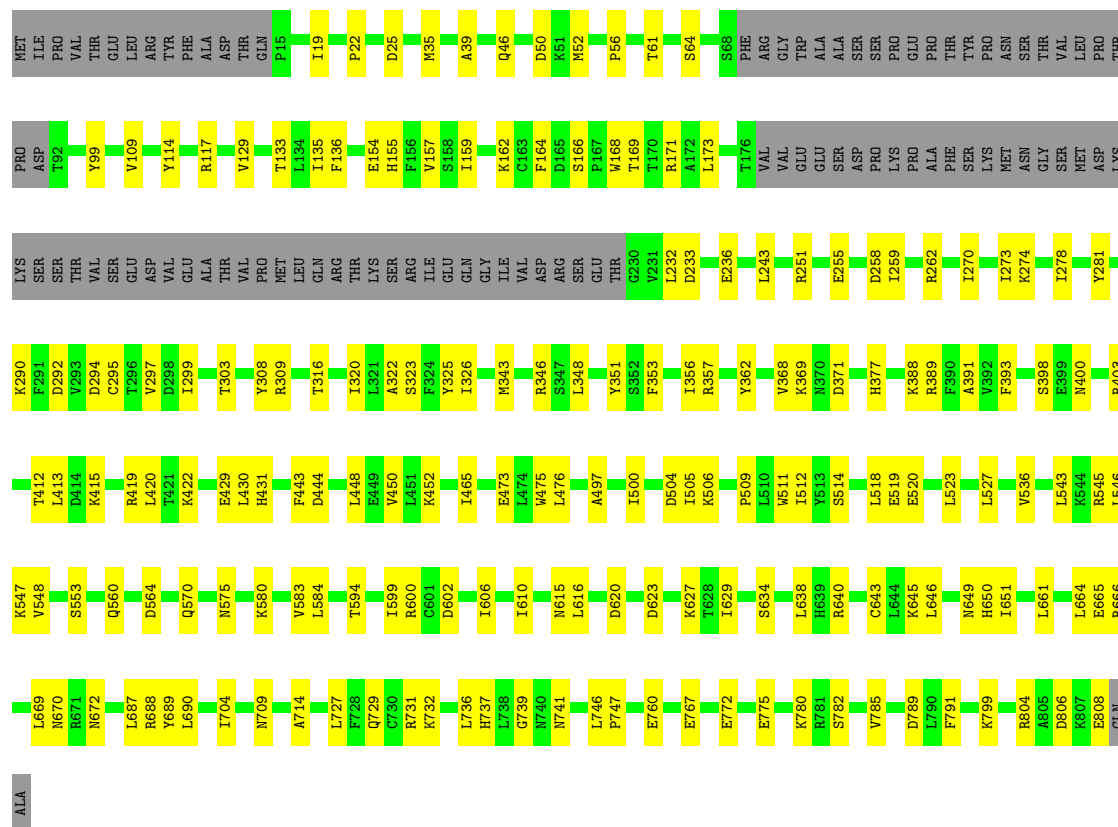
Chain D: 71% 20% 10%





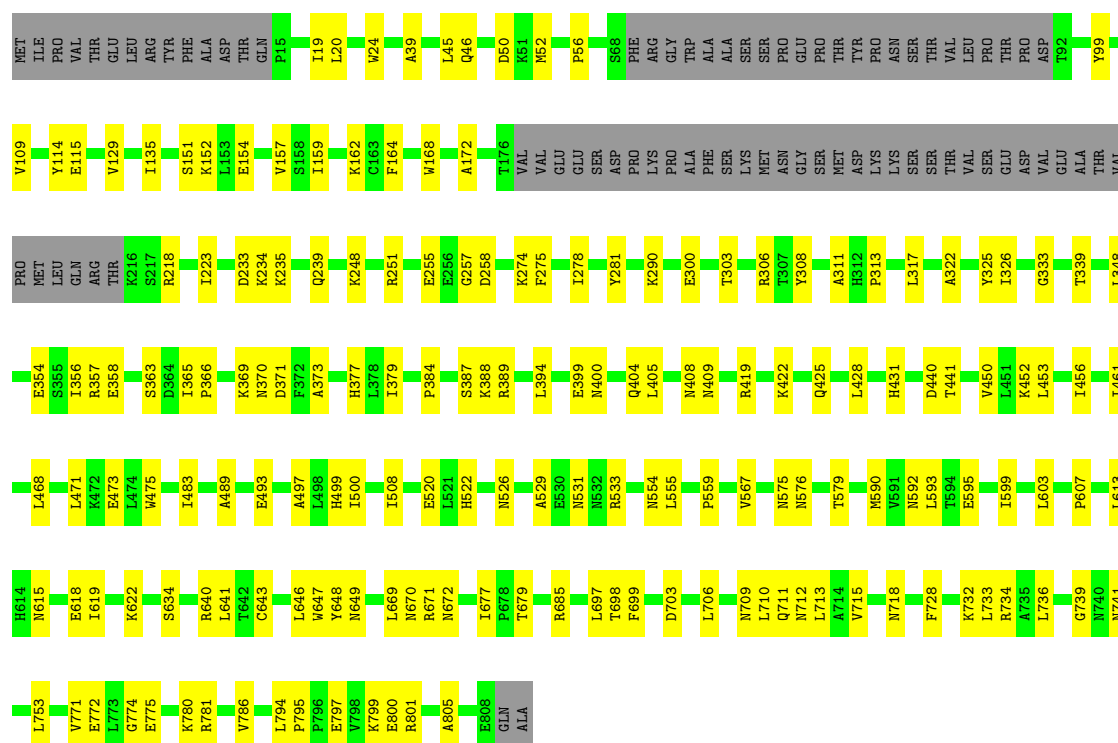
- Molecule 1: Volume-regulated anion channel subunit LRRC8A

Chain E: 66% 22% 11%



- Molecule 1: Volume-regulated anion channel subunit LRRC8A

Chain F: 69% 21% 10%



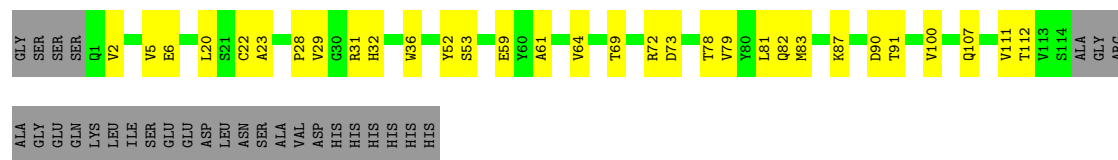
• Molecule 2: Synthetic nanobody Sb1

Chain G: 61% 18% 21%



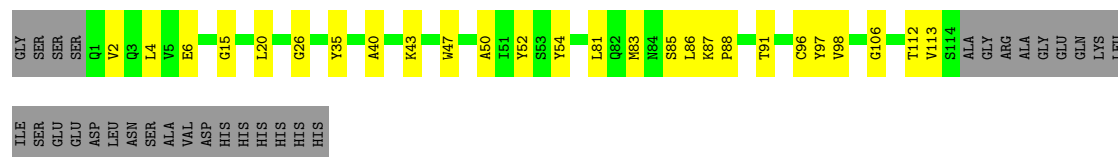
• Molecule 2: Synthetic nanobody Sb1

Chain H: 58% 22% 21%

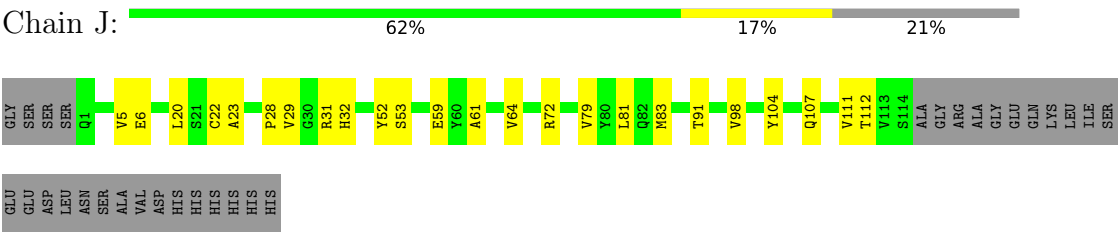


• Molecule 2: Synthetic nanobody Sb1

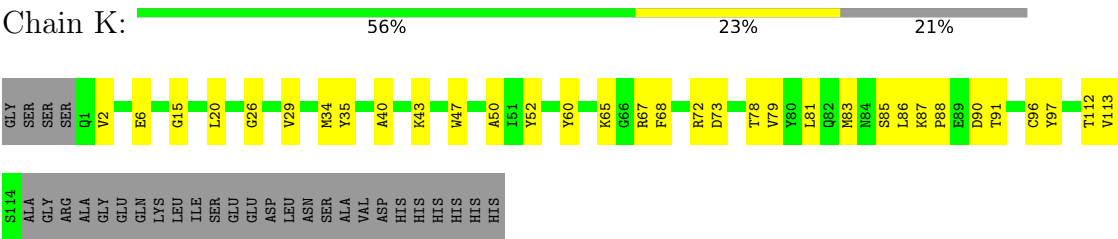
Chain I: 61% 18% 21%



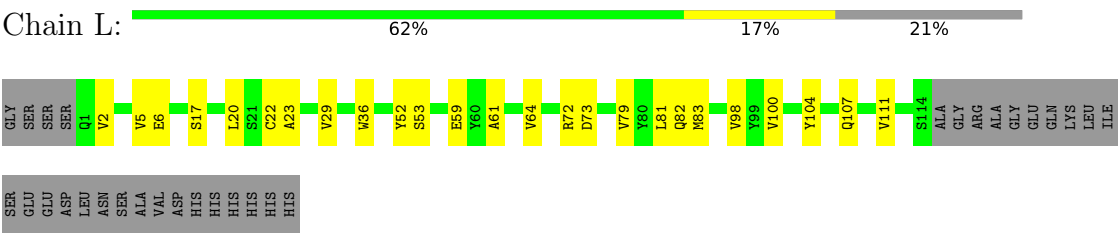
• Molecule 2: Synthetic nanobody Sb1



• Molecule 2: Synthetic nanobody Sb1



• Molecule 2: Synthetic nanobody Sb1



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 59962                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 67                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |

## 5 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | A     | 0.17         | 0/6055  | 0.31        | 0/8207  |
| 1   | B     | 0.17         | 0/6163  | 0.31        | 0/8352  |
| 1   | C     | 0.17         | 0/6055  | 0.30        | 0/8207  |
| 1   | D     | 0.17         | 0/6163  | 0.31        | 0/8352  |
| 1   | E     | 0.17         | 0/6055  | 0.30        | 0/8207  |
| 1   | F     | 0.17         | 0/6163  | 0.30        | 0/8352  |
| 2   | G     | 0.09         | 0/927   | 0.24        | 0/1258  |
| 2   | H     | 0.10         | 0/927   | 0.25        | 0/1258  |
| 2   | I     | 0.08         | 0/927   | 0.23        | 0/1258  |
| 2   | J     | 0.10         | 0/927   | 0.25        | 0/1258  |
| 2   | K     | 0.08         | 0/927   | 0.23        | 0/1258  |
| 2   | L     | 0.10         | 0/927   | 0.26        | 0/1258  |
| All | All   | 0.16         | 0/42216 | 0.30        | 0/57225 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5922  | 0        | 6081     | 121     | 0            |
| 1   | B     | 6030  | 0        | 6184     | 112     | 0            |
| 1   | C     | 5922  | 0        | 6081     | 113     | 0            |
| 1   | D     | 6030  | 0        | 6184     | 100     | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | E     | 5922  | 0        | 6081     | 115     | 0            |
| 1   | F     | 6030  | 0        | 6184     | 111     | 0            |
| 2   | G     | 903   | 0        | 852      | 16      | 0            |
| 2   | H     | 903   | 0        | 852      | 23      | 0            |
| 2   | I     | 903   | 0        | 852      | 16      | 0            |
| 2   | J     | 903   | 0        | 852      | 16      | 0            |
| 2   | K     | 903   | 0        | 852      | 22      | 0            |
| 2   | L     | 903   | 0        | 852      | 18      | 0            |
| All | All   | 41274 | 0        | 41907    | 766     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (766) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:83:MET:HB3   | 2:G:86:LEU:HD21  | 1.62                     | 0.81              |
| 1:E:634:SER:HG   | 2:K:52:TYR:HH    | 1.28                     | 0.81              |
| 2:K:83:MET:HB3   | 2:K:86:LEU:HD21  | 1.61                     | 0.80              |
| 1:C:35:MET:HE2   | 1:C:133:THR:HG22 | 1.70                     | 0.74              |
| 1:C:351:TYR:HB3  | 1:C:368:VAL:HG23 | 1.69                     | 0.73              |
| 1:E:135:ILE:HG12 | 1:E:274:LYS:HZ3  | 1.54                     | 0.73              |
| 1:C:643:CYS:SG   | 1:C:666:ARG:NH1  | 2.62                     | 0.73              |
| 1:E:643:CYS:SG   | 1:E:666:ARG:NH1  | 2.62                     | 0.73              |
| 1:E:429:GLU:HG3  | 1:E:452:LYS:HE3  | 1.71                     | 0.73              |
| 1:B:164:PHE:O    | 1:B:389:ARG:NH1  | 2.21                     | 0.72              |
| 1:B:405:LEU:O    | 1:B:409:ASN:ND2  | 2.23                     | 0.72              |
| 1:E:419:ARG:NH1  | 1:E:431:HIS:O    | 2.23                     | 0.72              |
| 1:E:473:GLU:HG2  | 1:E:497:ALA:HB3  | 1.72                     | 0.72              |
| 1:D:164:PHE:O    | 1:D:389:ARG:NH1  | 2.24                     | 0.71              |
| 1:A:35:MET:HE2   | 1:A:133:THR:HG22 | 1.72                     | 0.70              |
| 2:I:83:MET:HB3   | 2:I:86:LEU:HD21  | 1.71                     | 0.70              |
| 1:F:164:PHE:O    | 1:F:389:ARG:NH1  | 2.24                     | 0.69              |
| 1:D:258:ASP:H    | 1:D:371:ASP:HB2  | 1.57                     | 0.69              |
| 1:A:343:MET:HA   | 1:A:348:LEU:HD11 | 1.76                     | 0.68              |
| 1:A:643:CYS:SG   | 1:A:666:ARG:NH1  | 2.66                     | 0.68              |
| 1:D:618:GLU:HG3  | 1:D:643:CYS:HB3  | 1.74                     | 0.68              |
| 1:A:429:GLU:HG3  | 1:A:452:LYS:HE3  | 1.75                     | 0.68              |
| 1:C:294:ASP:OD1  | 1:C:309:ARG:NH1  | 2.27                     | 0.68              |
| 2:J:52:TYR:O     | 2:J:72:ARG:NH2   | 2.26                     | 0.68              |
| 1:E:351:TYR:HB3  | 1:E:368:VAL:HG23 | 1.75                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:2:VAL:HA     | 2:I:26:GLY:HA3   | 1.76                     | 0.67              |
| 1:A:294:ASP:OD1  | 1:A:309:ARG:NH1  | 2.28                     | 0.67              |
| 2:L:52:TYR:O     | 2:L:72:ARG:NH2   | 2.27                     | 0.67              |
| 1:C:473:GLU:HG2  | 1:C:497:ALA:HB3  | 1.77                     | 0.66              |
| 1:F:255:GLU:HG3  | 1:F:369:LYS:HB2  | 1.78                     | 0.66              |
| 2:G:2:VAL:HA     | 2:G:26:GLY:HA3   | 1.77                     | 0.66              |
| 1:C:429:GLU:HG3  | 1:C:452:LYS:HE3  | 1.77                     | 0.66              |
| 1:C:419:ARG:NH1  | 1:C:431:HIS:O    | 2.28                     | 0.66              |
| 2:H:20:LEU:HB2   | 2:H:81:LEU:HB3   | 1.79                     | 0.65              |
| 1:A:729:GLN:OE1  | 1:A:731:ARG:NH2  | 2.30                     | 0.65              |
| 1:E:615:ASN:HA   | 1:E:640:ARG:HE   | 1.61                     | 0.65              |
| 1:A:473:GLU:HG2  | 1:A:497:ALA:HB3  | 1.77                     | 0.65              |
| 1:B:300:GLU:OE2  | 1:B:306:ARG:NH1  | 2.29                     | 0.64              |
| 1:C:343:MET:HA   | 1:C:348:LEU:HD11 | 1.79                     | 0.64              |
| 1:F:300:GLU:OE2  | 1:F:306:ARG:NH1  | 2.30                     | 0.64              |
| 1:F:619:ILE:HG22 | 1:F:641:LEU:HD11 | 1.80                     | 0.64              |
| 1:D:118:LEU:HD23 | 1:D:123:LYS:HG3  | 1.80                     | 0.64              |
| 1:E:343:MET:HA   | 1:E:348:LEU:HD11 | 1.79                     | 0.64              |
| 2:H:52:TYR:O     | 2:H:72:ARG:NH2   | 2.30                     | 0.64              |
| 1:B:618:GLU:HG3  | 1:B:643:CYS:HB3  | 1.78                     | 0.64              |
| 1:B:438:ILE:HG13 | 1:B:459:VAL:HG21 | 1.79                     | 0.63              |
| 1:F:357:ARG:NH1  | 1:F:365:ILE:O    | 2.31                     | 0.63              |
| 1:B:619:ILE:HG22 | 1:B:641:LEU:HD11 | 1.80                     | 0.63              |
| 1:C:634:SER:HG   | 2:I:52:TYR:HH    | 1.37                     | 0.63              |
| 1:F:618:GLU:HG3  | 1:F:643:CYS:HB3  | 1.81                     | 0.63              |
| 1:B:373:ALA:O    | 1:B:377:HIS:ND1  | 2.32                     | 0.63              |
| 1:F:452:LYS:HA   | 1:F:475:TRP:HB2  | 1.81                     | 0.62              |
| 1:A:292:ASP:OD1  | 1:A:292:ASP:N    | 2.32                     | 0.62              |
| 1:B:255:GLU:HG3  | 1:B:369:LYS:HB2  | 1.80                     | 0.62              |
| 1:A:135:ILE:HG12 | 1:A:274:LYS:HZ2  | 1.65                     | 0.62              |
| 1:D:373:ALA:O    | 1:D:377:HIS:ND1  | 2.30                     | 0.62              |
| 1:F:405:LEU:O    | 1:F:409:ASN:ND2  | 2.27                     | 0.62              |
| 1:A:705:GLY:O    | 1:A:708:GLN:NE2  | 2.33                     | 0.62              |
| 1:B:258:ASP:H    | 1:B:371:ASP:HB2  | 1.65                     | 0.62              |
| 1:B:357:ARG:NH1  | 1:B:365:ILE:O    | 2.33                     | 0.62              |
| 1:E:429:GLU:HB2  | 1:E:450:VAL:HB   | 1.82                     | 0.61              |
| 1:B:292:ASP:OD1  | 1:B:292:ASP:N    | 2.33                     | 0.61              |
| 1:C:259:ILE:N    | 1:C:371:ASP:OD2  | 2.30                     | 0.61              |
| 1:A:669:LEU:O    | 1:A:672:ASN:ND2  | 2.33                     | 0.61              |
| 1:F:774:GLY:O    | 1:F:801:ARG:NH2  | 2.32                     | 0.61              |
| 1:B:712:ASN:OD1  | 1:B:734:ARG:NH2  | 2.32                     | 0.61              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:5:VAL:HG13   | 2:J:23:ALA:HB3   | 1.82                     | 0.61              |
| 2:J:29:VAL:O     | 2:J:72:ARG:NH1   | 2.34                     | 0.61              |
| 1:B:408:ASN:ND2  | 1:B:440:ASP:OD2  | 2.30                     | 0.61              |
| 1:D:438:ILE:HG13 | 1:D:459:VAL:HG21 | 1.83                     | 0.61              |
| 1:A:102:ASP:OD1  | 1:A:105:GLN:NE2  | 2.20                     | 0.61              |
| 1:E:412:THR:HG23 | 1:E:415:LYS:H    | 1.66                     | 0.61              |
| 2:H:20:LEU:HD22  | 2:H:81:LEU:HD23  | 1.81                     | 0.61              |
| 1:A:258:ASP:O    | 1:A:262:ARG:NH1  | 2.34                     | 0.60              |
| 1:D:473:GLU:HG2  | 1:D:497:ALA:HB3  | 1.83                     | 0.60              |
| 2:H:29:VAL:HG22  | 2:H:72:ARG:HD2   | 1.84                     | 0.60              |
| 1:A:52:MET:HG3   | 1:A:114:TYR:HD2  | 1.66                     | 0.60              |
| 1:D:615:ASN:OD1  | 1:D:640:ARG:NH2  | 2.35                     | 0.60              |
| 1:A:351:TYR:HB3  | 1:A:368:VAL:HG23 | 1.84                     | 0.60              |
| 1:B:739:GLY:O    | 1:B:741:ASN:ND2  | 2.34                     | 0.60              |
| 1:E:258:ASP:H    | 1:E:371:ASP:HB2  | 1.67                     | 0.60              |
| 1:F:712:ASN:OD1  | 1:F:734:ARG:NH2  | 2.33                     | 0.60              |
| 2:K:67:ARG:NH2   | 2:K:90:ASP:OD2   | 2.35                     | 0.60              |
| 1:C:429:GLU:HB2  | 1:C:450:VAL:HB   | 1.82                     | 0.60              |
| 1:F:373:ALA:O    | 1:F:377:HIS:ND1  | 2.33                     | 0.60              |
| 1:C:135:ILE:HG12 | 1:C:274:LYS:HZ3  | 1.67                     | 0.60              |
| 2:L:5:VAL:HG13   | 2:L:23:ALA:HB3   | 1.84                     | 0.60              |
| 1:C:709:ASN:HA   | 1:C:732:LYS:HD2  | 1.83                     | 0.60              |
| 1:D:45:LEU:HD21  | 1:D:317:LEU:HD13 | 1.84                     | 0.60              |
| 1:C:412:THR:HG23 | 1:C:415:LYS:H    | 1.67                     | 0.60              |
| 1:D:39:ALA:HB2   | 1:D:129:VAL:HG12 | 1.84                     | 0.60              |
| 1:E:452:LYS:HA   | 1:E:475:TRP:HB2  | 1.84                     | 0.59              |
| 1:F:739:GLY:O    | 1:F:741:ASN:ND2  | 2.35                     | 0.59              |
| 1:B:39:ALA:HB2   | 1:B:129:VAL:HG12 | 1.82                     | 0.59              |
| 1:D:255:GLU:HG3  | 1:D:369:LYS:HB2  | 1.82                     | 0.59              |
| 1:C:504:ASP:OD1  | 1:C:505:ILE:N    | 2.35                     | 0.59              |
| 1:F:251:ARG:HD2  | 1:F:394:LEU:HD11 | 1.84                     | 0.59              |
| 2:J:53:SER:HA    | 2:J:72:ARG:HH22  | 1.67                     | 0.59              |
| 1:A:419:ARG:NH1  | 1:A:431:HIS:O    | 2.34                     | 0.59              |
| 1:B:461:ILE:HB   | 1:B:483:ILE:HG13 | 1.85                     | 0.59              |
| 1:C:615:ASN:HA   | 1:C:640:ARG:HE   | 1.66                     | 0.59              |
| 2:H:29:VAL:O     | 2:H:72:ARG:NH1   | 2.36                     | 0.59              |
| 1:D:357:ARG:NH1  | 1:D:365:ILE:O    | 2.35                     | 0.59              |
| 1:F:39:ALA:HB2   | 1:F:129:VAL:HG12 | 1.85                     | 0.59              |
| 1:C:669:LEU:O    | 1:C:672:ASN:ND2  | 2.36                     | 0.59              |
| 1:E:669:LEU:O    | 1:E:672:ASN:ND2  | 2.36                     | 0.59              |
| 2:J:61:ALA:HB3   | 2:J:64:VAL:HG22  | 1.85                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:91:THR:HG23  | 2:K:112:THR:HA   | 1.85                     | 0.59              |
| 1:D:677:ILE:HD11 | 1:D:697:LEU:HD13 | 1.85                     | 0.58              |
| 1:F:45:LEU:HD21  | 1:F:317:LEU:HD13 | 1.86                     | 0.58              |
| 1:D:408:ASN:ND2  | 1:D:440:ASP:OD2  | 2.36                     | 0.58              |
| 1:E:35:MET:HE2   | 1:E:133:THR:HG22 | 1.85                     | 0.58              |
| 1:E:117:ARG:HG2  | 1:E:295:CYS:HA   | 1.86                     | 0.58              |
| 2:I:35:TYR:HB2   | 2:I:97:TYR:HB3   | 1.85                     | 0.58              |
| 1:A:560:GLN:NE2  | 1:A:564:ASP:OD2  | 2.37                     | 0.58              |
| 1:C:46:GLN:O     | 1:C:50:ASP:HB3   | 2.03                     | 0.58              |
| 1:C:135:ILE:HG23 | 1:C:274:LYS:HZ2  | 1.68                     | 0.58              |
| 1:D:46:GLN:O     | 1:D:50:ASP:HB3   | 2.03                     | 0.58              |
| 1:F:258:ASP:H    | 1:F:371:ASP:HB2  | 1.68                     | 0.58              |
| 2:H:61:ALA:HB3   | 2:H:64:VAL:HG22  | 1.85                     | 0.58              |
| 1:B:370:ASN:OD1  | 1:B:370:ASN:N    | 2.32                     | 0.58              |
| 1:F:370:ASN:OD1  | 1:F:370:ASN:N    | 2.36                     | 0.58              |
| 1:B:46:GLN:O     | 1:B:50:ASP:HB3   | 2.04                     | 0.58              |
| 2:L:6:GLU:O      | 2:L:107:GLN:NE2  | 2.37                     | 0.58              |
| 2:H:5:VAL:HG13   | 2:H:23:ALA:HB3   | 1.86                     | 0.57              |
| 2:L:20:LEU:HB2   | 2:L:81:LEU:HB3   | 1.87                     | 0.57              |
| 1:A:629:ILE:HD13 | 1:A:651:ILE:HD13 | 1.86                     | 0.57              |
| 1:C:646:LEU:O    | 1:C:649:ASN:ND2  | 2.35                     | 0.57              |
| 1:D:52:MET:HG3   | 1:D:114:TYR:HD2  | 1.68                     | 0.57              |
| 1:F:473:GLU:HG2  | 1:F:497:ALA:HB3  | 1.86                     | 0.57              |
| 1:D:303:THR:HG1  | 1:D:308:TYR:HH   | 1.52                     | 0.57              |
| 1:F:258:ASP:HB2  | 1:F:370:ASN:HD22 | 1.68                     | 0.57              |
| 1:A:435:LEU:HB2  | 1:A:456:ILE:HD13 | 1.86                     | 0.57              |
| 1:D:405:LEU:O    | 1:D:409:ASN:ND2  | 2.29                     | 0.57              |
| 1:D:739:GLY:O    | 1:D:741:ASN:ND2  | 2.37                     | 0.57              |
| 1:E:560:GLN:NE2  | 1:E:564:ASP:OD2  | 2.37                     | 0.57              |
| 2:J:20:LEU:HB2   | 2:J:81:LEU:HB3   | 1.85                     | 0.57              |
| 2:J:32:HIS:O     | 2:J:72:ARG:NH1   | 2.37                     | 0.57              |
| 2:L:20:LEU:HD22  | 2:L:81:LEU:HD23  | 1.86                     | 0.57              |
| 1:E:255:GLU:HG2  | 1:E:369:LYS:HB2  | 1.86                     | 0.57              |
| 2:L:61:ALA:HB3   | 2:L:64:VAL:HG22  | 1.85                     | 0.57              |
| 1:A:412:THR:HG23 | 1:A:415:LYS:H    | 1.70                     | 0.57              |
| 2:I:20:LEU:HD12  | 2:I:81:LEU:HD23  | 1.87                     | 0.56              |
| 1:D:258:ASP:HB2  | 1:D:370:ASN:HD22 | 1.69                     | 0.56              |
| 1:D:619:ILE:HG22 | 1:D:641:LEU:HD11 | 1.86                     | 0.56              |
| 1:E:519:GLU:HG2  | 1:E:545:ARG:HG3  | 1.86                     | 0.56              |
| 1:A:615:ASN:HA   | 1:A:640:ARG:HE   | 1.71                     | 0.56              |
| 1:C:19:ILE:HD11  | 1:C:157:VAL:HG23 | 1.87                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:509:PRO:HB2  | 1:C:512:ILE:HG23 | 1.87                     | 0.56              |
| 1:F:567:VAL:O    | 1:F:592:ASN:ND2  | 2.38                     | 0.56              |
| 2:H:2:VAL:HG21   | 2:H:100:VAL:HG21 | 1.88                     | 0.56              |
| 2:H:53:SER:HA    | 2:H:72:ARG:HH22  | 1.70                     | 0.56              |
| 1:A:19:ILE:HD11  | 1:A:157:VAL:HG23 | 1.87                     | 0.56              |
| 1:A:169:THR:HG23 | 1:A:393:PHE:HE1  | 1.70                     | 0.56              |
| 1:D:630:GLU:OE2  | 1:D:653:TYR:OH   | 2.19                     | 0.56              |
| 1:E:714:ALA:HA   | 1:E:737:HIS:HB2  | 1.86                     | 0.56              |
| 2:K:85:SER:O     | 2:K:87:LYS:NZ    | 2.38                     | 0.56              |
| 1:D:452:LYS:HA   | 1:D:475:TRP:HB2  | 1.88                     | 0.56              |
| 1:E:509:PRO:HB2  | 1:E:512:ILE:HG23 | 1.88                     | 0.56              |
| 1:F:615:ASN:OD1  | 1:F:640:ARG:NH2  | 2.39                     | 0.56              |
| 1:F:646:LEU:O    | 1:F:649:ASN:ND2  | 2.39                     | 0.56              |
| 1:E:804:ARG:HH12 | 1:E:808:GLU:HB3  | 1.71                     | 0.56              |
| 1:B:630:GLU:OE2  | 1:B:653:TYR:OH   | 2.18                     | 0.55              |
| 1:C:629:ILE:HD13 | 1:C:651:ILE:HD13 | 1.87                     | 0.55              |
| 1:C:714:ALA:HA   | 1:C:737:HIS:HB2  | 1.88                     | 0.55              |
| 1:F:46:GLN:O     | 1:F:50:ASP:HB3   | 2.06                     | 0.55              |
| 1:E:19:ILE:HD11  | 1:E:157:VAL:HG23 | 1.88                     | 0.55              |
| 1:A:714:ALA:HA   | 1:A:737:HIS:HB2  | 1.89                     | 0.55              |
| 1:C:166:SER:O    | 1:C:169:THR:OG1  | 2.24                     | 0.55              |
| 1:C:760:GLU:HA   | 1:C:785:VAL:HB   | 1.87                     | 0.55              |
| 2:L:29:VAL:HG22  | 2:L:72:ARG:HD2   | 1.89                     | 0.55              |
| 1:A:166:SER:O    | 1:A:169:THR:OG1  | 2.23                     | 0.55              |
| 1:B:322:ALA:O    | 1:B:326:ILE:HG23 | 2.06                     | 0.55              |
| 1:E:129:VAL:O    | 1:E:133:THR:HG23 | 2.06                     | 0.55              |
| 2:H:22:CYS:HB3   | 2:H:79:VAL:HB    | 1.88                     | 0.55              |
| 1:A:789:ASP:N    | 1:A:789:ASP:OD1  | 2.39                     | 0.55              |
| 2:H:6:GLU:O      | 2:H:107:GLN:NE2  | 2.40                     | 0.55              |
| 1:A:117:ARG:HG2  | 1:A:295:CYS:HA   | 1.89                     | 0.55              |
| 2:G:35:TYR:HB2   | 2:G:97:TYR:HB3   | 1.88                     | 0.55              |
| 1:E:258:ASP:O    | 1:E:262:ARG:NH1  | 2.39                     | 0.55              |
| 1:F:251:ARG:HH22 | 1:F:366:PRO:HG2  | 1.72                     | 0.55              |
| 1:A:39:ALA:HB2   | 1:A:129:VAL:HG12 | 1.88                     | 0.54              |
| 1:E:162:LYS:HG3  | 1:E:243:LEU:HD11 | 1.90                     | 0.54              |
| 1:E:164:PHE:O    | 1:E:389:ARG:NH1  | 2.40                     | 0.54              |
| 1:B:576:ASN:HB3  | 1:B:579:THR:HB   | 1.88                     | 0.54              |
| 1:D:322:ALA:O    | 1:D:326:ILE:HG23 | 2.07                     | 0.54              |
| 1:D:710:LEU:HD21 | 1:D:713:LEU:HB2  | 1.89                     | 0.54              |
| 1:C:452:LYS:HA   | 1:C:475:TRP:HB2  | 1.89                     | 0.54              |
| 1:B:251:ARG:HH22 | 1:B:366:PRO:HG2  | 1.72                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:251:ARG:HD2  | 1:D:394:LEU:HD11 | 1.88                     | 0.54              |
| 1:E:629:ILE:HD13 | 1:E:651:ILE:HD13 | 1.90                     | 0.54              |
| 1:E:729:GLN:OE1  | 1:E:731:ARG:NH2  | 2.40                     | 0.54              |
| 2:K:2:VAL:HA     | 2:K:26:GLY:HA3   | 1.90                     | 0.54              |
| 1:A:429:GLU:HB2  | 1:A:450:VAL:HB   | 1.90                     | 0.54              |
| 1:E:606:ILE:HG23 | 1:E:610:ILE:HD12 | 1.90                     | 0.54              |
| 1:B:258:ASP:HB2  | 1:B:370:ASN:HD22 | 1.73                     | 0.53              |
| 1:C:258:ASP:H    | 1:C:371:ASP:HB2  | 1.70                     | 0.53              |
| 1:E:166:SER:O    | 1:E:169:THR:OG1  | 2.26                     | 0.53              |
| 1:F:709:ASN:HA   | 1:F:732:LYS:HD2  | 1.89                     | 0.53              |
| 2:J:83:MET:HE1   | 2:J:111:VAL:HG11 | 1.90                     | 0.53              |
| 2:I:88:PRO:HA    | 2:I:113:VAL:HB   | 1.89                     | 0.53              |
| 1:C:258:ASP:O    | 1:C:262:ARG:NH1  | 2.41                     | 0.53              |
| 1:F:576:ASN:HB3  | 1:F:579:THR:HB   | 1.91                     | 0.53              |
| 1:A:259:ILE:N    | 1:A:371:ASP:OD2  | 2.32                     | 0.53              |
| 1:C:804:ARG:HH12 | 1:C:808:GLU:HB3  | 1.72                     | 0.53              |
| 1:D:712:ASN:OD1  | 1:D:734:ARG:NH2  | 2.41                     | 0.53              |
| 1:E:168:TRP:HH2  | 1:E:398:SER:HB2  | 1.73                     | 0.53              |
| 1:F:419:ARG:NH1  | 1:F:431:HIS:O    | 2.40                     | 0.53              |
| 1:A:316:THR:OG1  | 1:F:115:GLU:OE2  | 2.26                     | 0.53              |
| 1:C:162:LYS:HG3  | 1:C:243:LEU:HD11 | 1.91                     | 0.53              |
| 1:D:370:ASN:OD1  | 1:D:370:ASN:N    | 2.33                     | 0.53              |
| 1:A:162:LYS:HG3  | 1:A:243:LEU:HD11 | 1.91                     | 0.53              |
| 1:D:599:ILE:HG13 | 1:D:622:LYS:HB3  | 1.89                     | 0.53              |
| 1:A:258:ASP:H    | 1:A:371:ASP:HB2  | 1.74                     | 0.53              |
| 1:D:356:ILE:HD12 | 1:D:388:LYS:HG2  | 1.90                     | 0.53              |
| 1:D:646:LEU:O    | 1:D:649:ASN:ND2  | 2.42                     | 0.53              |
| 2:H:83:MET:HE1   | 2:H:111:VAL:HG11 | 1.91                     | 0.53              |
| 2:I:85:SER:O     | 2:I:87:LYS:NZ    | 2.41                     | 0.53              |
| 1:A:102:ASP:OD1  | 1:A:102:ASP:N    | 2.38                     | 0.52              |
| 1:A:400:ASN:OD1  | 1:A:403:ARG:NH1  | 2.40                     | 0.52              |
| 1:E:789:ASP:OD1  | 1:E:789:ASP:N    | 2.41                     | 0.52              |
| 1:B:452:LYS:HA   | 1:B:475:TRP:HB2  | 1.91                     | 0.52              |
| 1:B:709:ASN:HA   | 1:B:732:LYS:HD2  | 1.90                     | 0.52              |
| 1:C:39:ALA:HB2   | 1:C:129:VAL:HG12 | 1.90                     | 0.52              |
| 1:E:580:LYS:HA   | 1:E:602:ASP:HB3  | 1.92                     | 0.52              |
| 1:F:322:ALA:O    | 1:F:326:ILE:HG23 | 2.09                     | 0.52              |
| 1:A:168:TRP:HH2  | 1:A:398:SER:HB2  | 1.75                     | 0.52              |
| 1:B:647:TRP:HE3  | 1:B:670:ASN:HD21 | 1.57                     | 0.52              |
| 1:E:46:GLN:O     | 1:E:50:ASP:HB3   | 2.10                     | 0.52              |
| 1:B:670:ASN:OD1  | 1:B:670:ASN:N    | 2.33                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:519:GLU:HG2  | 1:C:545:ARG:HG3  | 1.90                     | 0.52              |
| 1:D:251:ARG:HH12 | 1:D:366:PRO:HG2  | 1.74                     | 0.52              |
| 1:F:677:ILE:HD11 | 1:F:697:LEU:HD13 | 1.91                     | 0.52              |
| 1:F:647:TRP:HE3  | 1:F:670:ASN:HD21 | 1.58                     | 0.52              |
| 2:G:91:THR:HG23  | 2:G:112:THR:HA   | 1.91                     | 0.52              |
| 1:B:646:LEU:O    | 1:B:649:ASN:ND2  | 2.42                     | 0.52              |
| 1:C:129:VAL:O    | 1:C:133:THR:HG23 | 2.10                     | 0.52              |
| 1:E:520:GLU:HG2  | 1:E:548:VAL:HB   | 1.92                     | 0.52              |
| 1:A:61:THR:O     | 1:A:64:SER:OG    | 2.26                     | 0.51              |
| 1:C:168:TRP:HH2  | 1:C:398:SER:HB2  | 1.75                     | 0.51              |
| 1:E:292:ASP:OD1  | 1:E:292:ASP:N    | 2.41                     | 0.51              |
| 1:E:616:LEU:HB3  | 1:E:638:LEU:HD23 | 1.93                     | 0.51              |
| 1:E:767:GLU:OE2  | 1:F:732:LYS:NZ   | 2.41                     | 0.51              |
| 1:C:420:LEU:HD12 | 1:C:430:LEU:HD13 | 1.93                     | 0.51              |
| 1:E:39:ALA:HB2   | 1:E:129:VAL:HG12 | 1.92                     | 0.51              |
| 1:E:322:ALA:O    | 1:E:326:ILE:HG23 | 2.10                     | 0.51              |
| 1:E:413:LEU:HD11 | 1:E:444:ASP:HB3  | 1.93                     | 0.51              |
| 1:E:400:ASN:OD1  | 1:E:403:ARG:NH1  | 2.39                     | 0.51              |
| 2:J:28:PRO:HB2   | 2:J:31:ARG:HD3   | 1.92                     | 0.51              |
| 1:E:61:THR:O     | 1:E:64:SER:OG    | 2.23                     | 0.51              |
| 1:E:168:TRP:CH2  | 1:E:398:SER:HB2  | 2.46                     | 0.51              |
| 1:F:408:ASN:ND2  | 1:F:440:ASP:OD2  | 2.43                     | 0.51              |
| 1:F:590:MET:HE3  | 1:F:593:LEU:HD22 | 1.93                     | 0.51              |
| 1:C:594:THR:HA   | 1:C:616:LEU:HA   | 1.92                     | 0.50              |
| 1:D:777:PRO:HB2  | 1:D:778:LEU:HD12 | 1.92                     | 0.50              |
| 1:F:235:LYS:O    | 1:F:239:GLN:HG2  | 2.11                     | 0.50              |
| 1:A:520:GLU:HG2  | 1:A:548:VAL:HB   | 1.93                     | 0.50              |
| 1:C:171:ARG:HE   | 1:C:232:LEU:HD11 | 1.76                     | 0.50              |
| 1:C:278:ILE:HA   | 1:C:281:TYR:CD2  | 2.47                     | 0.50              |
| 1:D:647:TRP:HE3  | 1:D:670:ASN:HD21 | 1.57                     | 0.50              |
| 1:A:646:LEU:O    | 1:A:649:ASN:ND2  | 2.37                     | 0.50              |
| 1:A:616:LEU:HB3  | 1:A:638:LEU:HD23 | 1.94                     | 0.50              |
| 1:A:46:GLN:O     | 1:A:50:ASP:HB3   | 2.11                     | 0.50              |
| 1:A:583:VAL:HG23 | 1:A:584:LEU:H    | 1.77                     | 0.50              |
| 1:E:518:LEU:HB3  | 1:E:543:LEU:HD22 | 1.94                     | 0.50              |
| 1:F:400:ASN:O    | 1:F:404:GLN:HG2  | 2.12                     | 0.50              |
| 1:A:600:ARG:HG2  | 1:A:623:ASP:HB3  | 1.93                     | 0.50              |
| 1:C:789:ASP:OD1  | 1:C:789:ASP:N    | 2.43                     | 0.50              |
| 1:B:634:SER:OG   | 2:H:59:GLU:OE2   | 2.23                     | 0.50              |
| 1:A:505:ILE:HD12 | 1:A:536:VAL:HG11 | 1.94                     | 0.49              |
| 1:B:251:ARG:HD2  | 1:B:394:LEU:HD11 | 1.94                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:526:ASN:OD1  | 1:B:554:ASN:ND2  | 2.45                     | 0.49              |
| 1:C:580:LYS:HA   | 1:C:602:ASP:HB3  | 1.93                     | 0.49              |
| 1:D:452:LYS:HG2  | 1:D:475:TRP:CG   | 2.46                     | 0.49              |
| 1:A:760:GLU:HA   | 1:A:785:VAL:HB   | 1.93                     | 0.49              |
| 1:A:322:ALA:O    | 1:A:326:ILE:HG23 | 2.12                     | 0.49              |
| 1:B:135:ILE:HG12 | 1:B:274:LYS:HZ2  | 1.78                     | 0.49              |
| 1:B:400:ASN:O    | 1:B:404:GLN:HG2  | 2.12                     | 0.49              |
| 1:B:473:GLU:HG2  | 1:B:497:ALA:HB3  | 1.93                     | 0.49              |
| 1:C:117:ARG:HG2  | 1:C:295:CYS:HA   | 1.94                     | 0.49              |
| 1:D:251:ARG:HH22 | 1:D:366:PRO:HG2  | 1.77                     | 0.49              |
| 1:E:52:MET:HG3   | 1:E:114:TYR:HD2  | 1.78                     | 0.49              |
| 1:A:509:PRO:HB2  | 1:A:512:ILE:HG23 | 1.94                     | 0.49              |
| 1:A:804:ARG:HH12 | 1:A:808:GLU:HB3  | 1.77                     | 0.49              |
| 1:D:518:LEU:HD23 | 1:D:543:LEU:HD13 | 1.93                     | 0.49              |
| 1:E:22:PRO:HD2   | 1:E:25:ASP:HB2   | 1.94                     | 0.49              |
| 2:G:85:SER:O     | 2:G:87:LYS:NZ    | 2.45                     | 0.49              |
| 1:B:677:ILE:HD11 | 1:B:697:LEU:HD13 | 1.94                     | 0.49              |
| 1:D:526:ASN:OD1  | 1:D:554:ASN:ND2  | 2.44                     | 0.49              |
| 1:E:746:LEU:HD23 | 1:E:747:PRO:HD2  | 1.95                     | 0.49              |
| 2:I:91:THR:HG23  | 2:I:112:THR:HA   | 1.94                     | 0.49              |
| 2:K:20:LEU:HD12  | 2:K:81:LEU:HD23  | 1.93                     | 0.49              |
| 1:E:171:ARG:HE   | 1:E:232:LEU:HD11 | 1.77                     | 0.49              |
| 1:F:647:TRP:O    | 1:F:649:ASN:ND2  | 2.45                     | 0.49              |
| 1:A:666:ARG:HG2  | 1:A:689:TYR:HB2  | 1.94                     | 0.49              |
| 1:B:647:TRP:O    | 1:B:649:ASN:ND2  | 2.46                     | 0.49              |
| 1:D:154:GLU:HA   | 1:D:157:VAL:HG12 | 1.95                     | 0.49              |
| 2:J:22:CYS:HB3   | 2:J:79:VAL:HB    | 1.94                     | 0.49              |
| 1:D:135:ILE:HG23 | 1:D:274:LYS:HZ3  | 1.77                     | 0.49              |
| 1:E:450:VAL:HG22 | 1:E:473:GLU:HB2  | 1.95                     | 0.49              |
| 1:A:171:ARG:HE   | 1:A:232:LEU:HD11 | 1.78                     | 0.49              |
| 1:A:356:ILE:HD12 | 1:A:388:LYS:HA   | 1.95                     | 0.49              |
| 1:E:666:ARG:HG2  | 1:E:689:TYR:HB2  | 1.94                     | 0.49              |
| 1:F:154:GLU:HA   | 1:F:157:VAL:HG12 | 1.95                     | 0.49              |
| 2:G:68:PHE:HB3   | 2:G:81:LEU:HD11  | 1.94                     | 0.49              |
| 1:A:353:PHE:CE1  | 1:A:391:ALA:HB2  | 2.47                     | 0.48              |
| 1:D:348:LEU:HD23 | 1:D:348:LEU:H    | 1.77                     | 0.48              |
| 1:E:583:VAL:HG23 | 1:E:584:LEU:H    | 1.78                     | 0.48              |
| 2:K:29:VAL:O     | 2:K:72:ARG:NH1   | 2.46                     | 0.48              |
| 1:A:726:GLU:OE1  | 1:A:726:GLU:N    | 2.40                     | 0.48              |
| 1:B:343:MET:HG3  | 1:B:348:LEU:HD21 | 1.95                     | 0.48              |
| 1:E:760:GLU:HA   | 1:E:785:VAL:HB   | 1.94                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:278:ILE:HA   | 1:A:281:TYR:CD2  | 2.49                     | 0.48              |
| 1:A:709:ASN:HA   | 1:A:732:LYS:HD2  | 1.94                     | 0.48              |
| 1:B:295:CYS:HB2  | 1:B:297:VAL:HG13 | 1.95                     | 0.48              |
| 1:C:413:LEU:HD11 | 1:C:444:ASP:HB3  | 1.95                     | 0.48              |
| 1:C:606:ILE:HG23 | 1:C:610:ILE:HD12 | 1.95                     | 0.48              |
| 1:D:303:THR:OG1  | 1:D:308:TYR:OH   | 2.24                     | 0.48              |
| 1:A:452:LYS:HA   | 1:A:475:TRP:HB2  | 1.94                     | 0.48              |
| 1:A:606:ILE:HG23 | 1:A:610:ILE:HD12 | 1.96                     | 0.48              |
| 1:B:407:LEU:HD11 | 1:B:439:PRO:HG3  | 1.95                     | 0.48              |
| 1:C:168:TRP:CH2  | 1:C:398:SER:HB2  | 2.47                     | 0.48              |
| 1:C:450:VAL:HG22 | 1:C:473:GLU:HB2  | 1.96                     | 0.48              |
| 1:C:547:LYS:HD2  | 1:C:570:GLN:HG3  | 1.94                     | 0.48              |
| 2:G:15:GLY:N     | 2:G:86:LEU:O     | 2.41                     | 0.48              |
| 2:J:29:VAL:HG22  | 2:J:72:ARG:HD2   | 1.94                     | 0.48              |
| 1:A:519:GLU:HA   | 1:A:546:LEU:HA   | 1.95                     | 0.48              |
| 1:B:251:ARG:HH12 | 1:B:366:PRO:HG2  | 1.78                     | 0.48              |
| 2:L:98:VAL:HG12  | 2:L:104:TYR:HB2  | 1.95                     | 0.48              |
| 1:A:323:SER:O    | 1:A:326:ILE:HG12 | 2.14                     | 0.48              |
| 1:B:555:LEU:O    | 1:B:576:ASN:ND2  | 2.47                     | 0.48              |
| 1:C:169:THR:HG23 | 1:C:393:PHE:HE2  | 1.79                     | 0.48              |
| 1:E:348:LEU:HB3  | 1:E:377:HIS:ND1  | 2.29                     | 0.48              |
| 1:E:504:ASP:OD1  | 1:E:505:ILE:N    | 2.44                     | 0.48              |
| 1:B:475:TRP:HA   | 1:B:499:HIS:HB2  | 1.96                     | 0.48              |
| 2:K:60:TYR:HB2   | 2:K:65:LYS:HG3   | 1.96                     | 0.48              |
| 1:B:15:PRO:O     | 1:B:18:ARG:NH1   | 2.46                     | 0.48              |
| 1:B:118:LEU:HD23 | 1:B:123:LYS:HG3  | 1.96                     | 0.48              |
| 1:B:520:GLU:OE2  | 1:B:522:HIS:NE2  | 2.45                     | 0.48              |
| 1:D:400:ASN:O    | 1:D:404:GLN:HG2  | 2.14                     | 0.48              |
| 1:C:518:LEU:HB3  | 1:C:543:LEU:HD22 | 1.95                     | 0.48              |
| 1:F:526:ASN:OD1  | 1:F:554:ASN:ND2  | 2.47                     | 0.48              |
| 1:F:599:ILE:HG13 | 1:F:622:LYS:HB3  | 1.95                     | 0.48              |
| 2:G:29:VAL:O     | 2:G:72:ARG:NH1   | 2.47                     | 0.48              |
| 2:G:47:TRP:HE1   | 2:G:50:ALA:HB2   | 1.79                     | 0.48              |
| 2:J:20:LEU:HD22  | 2:J:81:LEU:HD23  | 1.95                     | 0.48              |
| 1:B:357:ARG:HD2  | 1:B:363:SER:HA   | 1.95                     | 0.48              |
| 1:D:475:TRP:HA   | 1:D:499:HIS:HB2  | 1.96                     | 0.48              |
| 1:E:353:PHE:CE1  | 1:E:391:ALA:HB2  | 2.49                     | 0.48              |
| 2:I:6:GLU:OE1    | 2:I:6:GLU:N      | 2.46                     | 0.48              |
| 1:B:774:GLY:O    | 1:B:801:ARG:NH2  | 2.47                     | 0.47              |
| 1:F:278:ILE:HA   | 1:F:281:TYR:CD2  | 2.48                     | 0.47              |
| 1:B:599:ILE:HG13 | 1:B:622:LYS:HB3  | 1.96                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:615:ASN:OD1  | 1:B:640:ARG:NH2  | 2.47                     | 0.47              |
| 1:C:670:ASN:OD1  | 1:C:670:ASN:N    | 2.42                     | 0.47              |
| 1:D:647:TRP:O    | 1:D:649:ASN:ND2  | 2.47                     | 0.47              |
| 1:E:504:ASP:OD2  | 1:E:506:LYS:NZ   | 2.45                     | 0.47              |
| 1:E:646:LEU:O    | 1:E:649:ASN:ND2  | 2.38                     | 0.47              |
| 2:J:6:GLU:O      | 2:J:107:GLN:NE2  | 2.47                     | 0.47              |
| 1:A:168:TRP:CH2  | 1:A:398:SER:HB2  | 2.49                     | 0.47              |
| 1:C:346:ARG:HB3  | 1:C:348:LEU:HG   | 1.97                     | 0.47              |
| 1:F:19:ILE:HD11  | 1:F:157:VAL:HG23 | 1.95                     | 0.47              |
| 1:A:151:SER:O    | 1:A:154:GLU:HG3  | 2.15                     | 0.47              |
| 1:A:395:SER:OG   | 1:A:398:SER:OG   | 2.32                     | 0.47              |
| 1:A:459:VAL:HG23 | 1:A:481:ALA:HA   | 1.96                     | 0.47              |
| 1:A:665:GLU:HA   | 1:A:687:LEU:HA   | 1.96                     | 0.47              |
| 1:B:555:LEU:HD13 | 1:B:559:PRO:HD3  | 1.96                     | 0.47              |
| 1:C:661:LEU:HB3  | 1:C:664:LEU:HG   | 1.96                     | 0.47              |
| 1:D:272:VAL:HG22 | 1:D:336:CYS:HB3  | 1.96                     | 0.47              |
| 1:E:169:THR:HG23 | 1:E:393:PHE:CE2  | 2.49                     | 0.47              |
| 1:E:505:ILE:HD12 | 1:E:536:VAL:HG11 | 1.97                     | 0.47              |
| 1:F:698:THR:HG23 | 1:F:699:PHE:HD1  | 1.79                     | 0.47              |
| 1:A:169:THR:HG23 | 1:A:393:PHE:CE1  | 2.48                     | 0.47              |
| 1:C:233:ASP:O    | 1:C:236:GLU:HG3  | 2.14                     | 0.47              |
| 1:C:323:SER:O    | 1:C:326:ILE:HG12 | 2.14                     | 0.47              |
| 1:C:746:LEU:HD23 | 1:C:747:PRO:HD2  | 1.97                     | 0.47              |
| 1:D:450:VAL:HG22 | 1:D:473:GLU:HB2  | 1.95                     | 0.47              |
| 1:A:519:GLU:HG2  | 1:A:545:ARG:HG3  | 1.97                     | 0.47              |
| 1:A:524:THR:HG23 | 1:A:552:LYS:HD3  | 1.97                     | 0.47              |
| 1:B:272:VAL:HG22 | 1:B:336:CYS:HB3  | 1.97                     | 0.47              |
| 1:C:505:ILE:HD12 | 1:C:536:VAL:HG11 | 1.95                     | 0.47              |
| 1:C:666:ARG:HG2  | 1:C:689:TYR:HB2  | 1.97                     | 0.47              |
| 1:C:782:SER:N    | 1:C:806:ASP:OD2  | 2.37                     | 0.47              |
| 1:D:19:ILE:HD11  | 1:D:157:VAL:HG23 | 1.95                     | 0.47              |
| 1:D:431:HIS:HA   | 1:D:452:LYS:HB2  | 1.96                     | 0.47              |
| 1:E:547:LYS:HD2  | 1:E:570:GLN:HG3  | 1.96                     | 0.47              |
| 1:E:687:LEU:HD21 | 1:E:690:LEU:HD13 | 1.96                     | 0.47              |
| 1:F:356:ILE:HD12 | 1:F:388:LYS:HG2  | 1.96                     | 0.47              |
| 1:F:450:VAL:HG22 | 1:F:473:GLU:HB2  | 1.96                     | 0.47              |
| 1:F:555:LEU:HD13 | 1:F:559:PRO:HD3  | 1.96                     | 0.47              |
| 1:F:711:GLN:OE1  | 1:F:734:ARG:NE   | 2.38                     | 0.47              |
| 2:G:6:GLU:OE1    | 2:G:6:GLU:N      | 2.48                     | 0.47              |
| 2:L:29:VAL:O     | 2:L:72:ARG:NH1   | 2.48                     | 0.47              |
| 1:C:739:GLY:O    | 1:C:741:ASN:ND2  | 2.48                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:278:ILE:HA   | 1:D:281:TYR:CD2  | 2.50                     | 0.47              |
| 1:E:661:LEU:HB3  | 1:E:664:LEU:HG   | 1.97                     | 0.47              |
| 1:C:136:PHE:CE1  | 1:C:274:LYS:HE3  | 2.50                     | 0.47              |
| 1:E:278:ILE:HA   | 1:E:281:TYR:CD2  | 2.49                     | 0.47              |
| 1:E:346:ARG:HB3  | 1:E:348:LEU:HG   | 1.97                     | 0.47              |
| 1:F:303:THR:HG1  | 1:F:308:TYR:HH   | 1.59                     | 0.47              |
| 2:G:67:ARG:NH2   | 2:G:90:ASP:OD2   | 2.47                     | 0.47              |
| 1:F:218:ARG:HG2  | 1:F:223:ILE:HB   | 1.97                     | 0.47              |
| 1:F:290:LYS:HB2  | 1:F:290:LYS:HE3  | 1.70                     | 0.47              |
| 1:F:733:LEU:HD21 | 1:F:736:LEU:HD21 | 1.97                     | 0.47              |
| 2:K:35:TYR:HB2   | 2:K:97:TYR:HB3   | 1.97                     | 0.47              |
| 1:A:129:VAL:O    | 1:A:133:THR:HG23 | 2.15                     | 0.46              |
| 1:A:368:VAL:HG21 | 1:A:376:LEU:HD12 | 1.96                     | 0.46              |
| 1:A:450:VAL:HG22 | 1:A:473:GLU:HB2  | 1.97                     | 0.46              |
| 1:B:591:VAL:O    | 1:B:615:ASN:ND2  | 2.39                     | 0.46              |
| 1:E:154:GLU:HA   | 1:E:157:VAL:HG12 | 1.97                     | 0.46              |
| 1:E:356:ILE:HD13 | 1:E:391:ALA:HB3  | 1.97                     | 0.46              |
| 1:E:665:GLU:OE1  | 1:E:688:ARG:NE   | 2.37                     | 0.46              |
| 1:F:772:GLU:O    | 1:F:775:GLU:HG2  | 2.15                     | 0.46              |
| 2:H:32:HIS:O     | 2:H:72:ARG:NH1   | 2.48                     | 0.46              |
| 1:C:665:GLU:HA   | 1:C:687:LEU:HA   | 1.96                     | 0.46              |
| 1:D:709:ASN:HA   | 1:D:732:LYS:HD2  | 1.96                     | 0.46              |
| 1:F:452:LYS:HG2  | 1:F:475:TRP:CG   | 2.50                     | 0.46              |
| 1:F:771:VAL:HG23 | 1:F:795:PRO:HG2  | 1.97                     | 0.46              |
| 2:K:68:PHE:HB3   | 2:K:81:LEU:HD11  | 1.97                     | 0.46              |
| 1:C:685:ARG:HE   | 1:C:706:LEU:HB3  | 1.80                     | 0.46              |
| 1:D:38:ILE:HD11  | 1:D:325:TYR:HD1  | 1.81                     | 0.46              |
| 1:F:168:TRP:CZ3  | 1:F:172:ALA:HB2  | 2.50                     | 0.46              |
| 2:H:91:THR:HG23  | 2:H:112:THR:HA   | 1.98                     | 0.46              |
| 2:I:4:LEU:HD11   | 2:I:98:VAL:HG12  | 1.97                     | 0.46              |
| 1:A:661:LEU:HB3  | 1:A:664:LEU:HG   | 1.97                     | 0.46              |
| 1:B:154:GLU:HA   | 1:B:157:VAL:HG12 | 1.98                     | 0.46              |
| 2:I:15:GLY:HA2   | 2:I:85:SER:HA    | 1.97                     | 0.46              |
| 1:A:580:LYS:HA   | 1:A:602:ASP:HB3  | 1.98                     | 0.46              |
| 1:A:594:THR:HA   | 1:A:616:LEU:HA   | 1.97                     | 0.46              |
| 1:A:622:LYS:HB2  | 1:A:647:TRP:NE1  | 2.30                     | 0.46              |
| 1:D:159:ILE:HA   | 1:D:162:LYS:HG2  | 1.98                     | 0.46              |
| 1:E:739:GLY:O    | 1:E:741:ASN:ND2  | 2.49                     | 0.46              |
| 2:K:15:GLY:HA2   | 2:K:85:SER:HA    | 1.97                     | 0.46              |
| 1:A:233:ASP:O    | 1:A:236:GLU:HG3  | 2.16                     | 0.46              |
| 1:B:19:ILE:HD11  | 1:B:157:VAL:HG23 | 1.96                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:56:PRO:HG2   | 1:B:99:TYR:CD1   | 2.51                     | 0.46              |
| 1:D:168:TRP:CZ3  | 1:D:172:ALA:HB2  | 2.51                     | 0.46              |
| 1:E:294:ASP:OD1  | 1:E:309:ARG:NH1  | 2.47                     | 0.46              |
| 2:K:47:TRP:HE1   | 2:K:50:ALA:HB2   | 1.79                     | 0.46              |
| 2:L:73:ASP:OD1   | 2:L:73:ASP:N     | 2.48                     | 0.46              |
| 1:A:566:GLY:HA2  | 1:A:569:LEU:HD12 | 1.97                     | 0.46              |
| 1:A:782:SER:N    | 1:A:806:ASP:OD2  | 2.47                     | 0.46              |
| 1:C:583:VAL:HG23 | 1:C:584:LEU:H    | 1.81                     | 0.46              |
| 1:C:627:LYS:HG2  | 1:C:650:HIS:HB2  | 1.98                     | 0.46              |
| 2:K:73:ASP:OD1   | 2:K:78:THR:OG1   | 2.28                     | 0.46              |
| 1:B:46:GLN:NE2   | 1:B:114:TYR:OH   | 2.48                     | 0.46              |
| 2:I:96:CYS:O     | 2:I:106:GLY:N    | 2.48                     | 0.46              |
| 2:K:6:GLU:OE2    | 2:K:96:CYS:N     | 2.43                     | 0.46              |
| 1:E:357:ARG:HB2  | 1:E:362:TYR:O    | 2.16                     | 0.46              |
| 1:F:489:ALA:O    | 1:F:493:GLU:HG2  | 2.16                     | 0.46              |
| 2:I:47:TRP:HE1   | 2:I:50:ALA:HB2   | 1.81                     | 0.46              |
| 1:A:511:TRP:O    | 1:A:514:SER:OG   | 2.31                     | 0.46              |
| 1:B:168:TRP:CZ3  | 1:B:172:ALA:HB2  | 2.51                     | 0.46              |
| 1:B:590:MET:HE3  | 1:B:593:LEU:HD22 | 1.98                     | 0.46              |
| 1:D:537:ILE:HG13 | 1:D:561:VAL:HG11 | 1.98                     | 0.46              |
| 1:F:520:GLU:OE2  | 1:F:522:HIS:NE2  | 2.46                     | 0.46              |
| 1:F:595:GLU:HG2  | 1:F:618:GLU:HB2  | 1.97                     | 0.46              |
| 2:J:98:VAL:HG12  | 2:J:104:TYR:HB2  | 1.98                     | 0.46              |
| 2:K:6:GLU:N      | 2:K:6:GLU:OE1    | 2.48                     | 0.46              |
| 1:B:152:LYS:NZ   | 1:B:257:GLY:HA3  | 2.30                     | 0.45              |
| 1:B:729:GLN:OE1  | 1:B:749:ARG:NH2  | 2.41                     | 0.45              |
| 1:C:243:LEU:HD23 | 1:C:393:PHE:CZ   | 2.52                     | 0.45              |
| 1:C:251:ARG:O    | 1:C:255:GLU:HB2  | 2.15                     | 0.45              |
| 1:E:159:ILE:O    | 1:E:162:LYS:HG2  | 2.17                     | 0.45              |
| 2:K:88:PRO:HA    | 2:K:113:VAL:HB   | 1.97                     | 0.45              |
| 1:E:243:LEU:HD23 | 1:E:393:PHE:CZ   | 2.50                     | 0.45              |
| 1:E:323:SER:O    | 1:E:326:ILE:HG12 | 2.14                     | 0.45              |
| 1:A:56:PRO:HG2   | 1:A:99:TYR:CD1   | 2.51                     | 0.45              |
| 1:B:278:ILE:HA   | 1:B:281:TYR:CD2  | 2.51                     | 0.45              |
| 1:E:233:ASP:O    | 1:E:236:GLU:HG3  | 2.15                     | 0.45              |
| 1:A:504:ASP:OD1  | 1:A:505:ILE:N    | 2.45                     | 0.45              |
| 1:D:634:SER:OG   | 2:J:59:GLU:OE2   | 2.25                     | 0.45              |
| 1:E:511:TRP:O    | 1:E:514:SER:OG   | 2.29                     | 0.45              |
| 1:F:461:ILE:HB   | 1:F:483:ILE:HG13 | 1.98                     | 0.45              |
| 1:A:173:LEU:O    | 1:A:176:THR:OG1  | 2.34                     | 0.45              |
| 1:A:611:PHE:CE1  | 1:A:634:SER:HB2  | 2.52                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:537:ILE:HG13 | 1:B:561:VAL:HG11 | 1.98                     | 0.45              |
| 1:B:710:LEU:HD21 | 1:B:713:LEU:HB2  | 1.99                     | 0.45              |
| 1:D:290:LYS:HB2  | 1:D:290:LYS:HE3  | 1.68                     | 0.45              |
| 1:D:555:LEU:HD13 | 1:D:559:PRO:HD3  | 1.97                     | 0.45              |
| 1:E:154:GLU:HG3  | 1:E:155:HIS:N    | 2.32                     | 0.45              |
| 1:C:543:LEU:HD13 | 1:C:546:LEU:HD13 | 1.98                     | 0.45              |
| 1:C:780:LYS:HD2  | 1:C:806:ASP:HA   | 1.98                     | 0.45              |
| 1:A:159:ILE:O    | 1:A:162:LYS:HG2  | 2.17                     | 0.45              |
| 1:A:546:LEU:HB3  | 1:A:568:HIS:HE1  | 1.82                     | 0.45              |
| 1:B:499:HIS:NE2  | 1:B:522:HIS:HD2  | 2.14                     | 0.45              |
| 1:C:356:ILE:HD12 | 1:C:388:LYS:HA   | 1.99                     | 0.45              |
| 1:F:248:LYS:NZ   | 1:F:399:GLU:OE2  | 2.36                     | 0.45              |
| 1:F:669:LEU:O    | 1:F:672:ASN:ND2  | 2.50                     | 0.45              |
| 1:A:543:LEU:HD13 | 1:A:546:LEU:HD13 | 1.99                     | 0.45              |
| 1:A:547:LYS:HD2  | 1:A:570:GLN:HG3  | 1.99                     | 0.45              |
| 1:F:431:HIS:HA   | 1:F:452:LYS:HB2  | 1.99                     | 0.45              |
| 1:B:159:ILE:HA   | 1:B:162:LYS:HG2  | 1.99                     | 0.45              |
| 1:B:772:GLU:O    | 1:B:775:GLU:HG2  | 2.17                     | 0.45              |
| 1:F:24:TRP:CG    | 1:F:339:THR:HG1  | 2.34                     | 0.45              |
| 1:B:492:ARG:NH2  | 1:B:516:LYS:HD2  | 2.32                     | 0.45              |
| 1:C:500:ILE:HB   | 1:C:523:LEU:HD23 | 1.98                     | 0.45              |
| 1:C:605:ARG:HD2  | 2:I:54:TYR:CZ    | 2.52                     | 0.45              |
| 1:D:495:LEU:HD23 | 1:D:515:LEU:HD13 | 1.97                     | 0.45              |
| 1:D:715:VAL:O    | 1:D:718:ASN:ND2  | 2.50                     | 0.45              |
| 2:L:53:SER:HA    | 2:L:72:ARG:HH22  | 1.82                     | 0.45              |
| 1:A:348:LEU:HB3  | 1:A:377:HIS:ND1  | 2.32                     | 0.44              |
| 1:C:772:GLU:O    | 1:C:775:GLU:HG2  | 2.17                     | 0.44              |
| 1:D:771:VAL:HG23 | 1:D:795:PRO:HG2  | 1.99                     | 0.44              |
| 1:E:782:SER:N    | 1:E:806:ASP:OD2  | 2.42                     | 0.44              |
| 2:I:40:ALA:HB3   | 2:I:43:LYS:HD2   | 1.99                     | 0.44              |
| 1:C:290:LYS:HE3  | 1:C:290:LYS:HB2  | 1.69                     | 0.44              |
| 1:C:461:ILE:HB   | 1:C:483:ILE:HG13 | 1.99                     | 0.44              |
| 1:D:772:GLU:O    | 1:D:775:GLU:HG2  | 2.17                     | 0.44              |
| 1:F:159:ILE:HA   | 1:F:162:LYS:HG2  | 1.99                     | 0.44              |
| 1:F:425:GLN:N    | 1:F:425:GLN:OE1  | 2.50                     | 0.44              |
| 2:G:88:PRO:HA    | 2:G:113:VAL:HB   | 2.00                     | 0.44              |
| 2:H:87:LYS:N     | 2:H:90:ASP:OD2   | 2.39                     | 0.44              |
| 1:E:169:THR:HG23 | 1:E:393:PHE:HE2  | 1.83                     | 0.44              |
| 1:F:152:LYS:NZ   | 1:F:257:GLY:HA3  | 2.33                     | 0.44              |
| 2:K:15:GLY:N     | 2:K:86:LEU:O     | 2.49                     | 0.44              |
| 1:A:704:ILE:HD13 | 1:A:727:LEU:HD13 | 2.00                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:746:LEU:HD23 | 1:A:747:PRO:HD2  | 1.99                     | 0.44              |
| 1:B:354:GLU:O    | 1:B:358:GLU:HB2  | 2.18                     | 0.44              |
| 1:E:627:LYS:HG2  | 1:E:650:HIS:HB2  | 2.00                     | 0.44              |
| 1:C:56:PRO:HG2   | 1:C:99:TYR:CD1   | 2.53                     | 0.44              |
| 1:C:443:PHE:CE1  | 1:C:465:ILE:HG22 | 2.53                     | 0.44              |
| 1:D:669:LEU:O    | 1:D:672:ASN:ND2  | 2.50                     | 0.44              |
| 1:E:791:PHE:CE2  | 1:E:799:LYS:HE3  | 2.52                     | 0.44              |
| 2:H:73:ASP:N     | 2:H:73:ASP:OD1   | 2.50                     | 0.44              |
| 2:H:73:ASP:OD1   | 2:H:78:THR:OG1   | 2.30                     | 0.44              |
| 1:A:518:LEU:HB3  | 1:A:543:LEU:HD22 | 2.00                     | 0.44              |
| 1:F:135:ILE:HG12 | 1:F:274:LYS:HZ3  | 1.82                     | 0.44              |
| 1:F:593:LEU:HD23 | 1:F:613:LEU:HD13 | 1.99                     | 0.44              |
| 1:F:603:LEU:HD13 | 1:F:607:PRO:HD3  | 2.00                     | 0.44              |
| 1:A:413:LEU:HD11 | 1:A:444:ASP:HB3  | 1.98                     | 0.44              |
| 1:B:109:VAL:HG21 | 1:B:308:TYR:CE2  | 2.52                     | 0.44              |
| 1:B:502:PHE:CE1  | 1:B:508:ILE:HD11 | 2.52                     | 0.44              |
| 1:B:728:PHE:HA   | 1:B:753:LEU:HD21 | 1.99                     | 0.44              |
| 1:D:663:ASN:HA   | 1:D:686:LYS:HD2  | 1.99                     | 0.44              |
| 1:E:56:PRO:HG2   | 1:E:99:TYR:CD1   | 2.53                     | 0.44              |
| 1:F:19:ILE:HD12  | 1:F:379:ILE:HD11 | 1.98                     | 0.44              |
| 1:B:135:ILE:HG23 | 1:B:274:LYS:NZ   | 2.33                     | 0.44              |
| 1:E:620:ASP:HA   | 1:E:645:LYS:HB2  | 1.99                     | 0.44              |
| 1:A:154:GLU:HA   | 1:A:157:VAL:HG12 | 2.00                     | 0.44              |
| 1:A:500:ILE:HB   | 1:A:523:LEU:HD23 | 1.99                     | 0.44              |
| 1:A:622:LYS:HB2  | 1:A:647:TRP:HE1  | 1.83                     | 0.44              |
| 1:B:24:TRP:CG    | 1:B:339:THR:HG1  | 2.36                     | 0.44              |
| 1:B:425:GLN:N    | 1:B:425:GLN:OE1  | 2.51                     | 0.44              |
| 1:C:353:PHE:CE1  | 1:C:391:ALA:HB2  | 2.53                     | 0.44              |
| 1:C:590:MET:HE2  | 1:C:593:LEU:HD13 | 1.99                     | 0.44              |
| 1:C:791:PHE:CE2  | 1:C:799:LYS:HE3  | 2.53                     | 0.44              |
| 1:D:780:LYS:HG2  | 1:D:805:ALA:HB1  | 1.99                     | 0.44              |
| 2:H:5:VAL:HG23   | 2:H:107:GLN:HG2  | 1.99                     | 0.44              |
| 2:L:36:TRP:CE2   | 2:L:81:LEU:HB2   | 2.52                     | 0.44              |
| 1:A:356:ILE:HD13 | 1:A:391:ALA:HB3  | 2.00                     | 0.43              |
| 1:A:728:PHE:O    | 1:A:731:ARG:NH1  | 2.50                     | 0.43              |
| 1:E:356:ILE:HD12 | 1:E:388:LYS:HA   | 2.00                     | 0.43              |
| 1:F:251:ARG:HH12 | 1:F:366:PRO:HG2  | 1.82                     | 0.43              |
| 2:G:15:GLY:HA2   | 2:G:85:SER:HA    | 2.00                     | 0.43              |
| 1:D:647:TRP:CD1  | 1:D:647:TRP:H    | 2.36                     | 0.43              |
| 1:F:56:PRO:HG2   | 1:F:99:TYR:CD1   | 2.54                     | 0.43              |
| 1:F:468:LEU:HB3  | 1:F:471:LEU:HB2  | 1.99                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:475:TRP:HA   | 1:F:499:HIS:HB2  | 1.99                     | 0.43              |
| 1:F:781:ARG:HH12 | 1:F:786:VAL:HG12 | 1.83                     | 0.43              |
| 2:L:22:CYS:HB2   | 2:L:36:TRP:CH2   | 2.52                     | 0.43              |
| 1:C:322:ALA:O    | 1:C:326:ILE:HG23 | 2.17                     | 0.43              |
| 1:C:587:LEU:HD21 | 1:C:596:LEU:HD21 | 2.00                     | 0.43              |
| 1:D:647:TRP:CD1  | 1:D:647:TRP:N    | 2.85                     | 0.43              |
| 2:L:2:VAL:HG21   | 2:L:100:VAL:HG21 | 2.00                     | 0.43              |
| 1:C:52:MET:HG3   | 1:C:114:TYR:HD2  | 1.82                     | 0.43              |
| 1:C:348:LEU:HB3  | 1:C:377:HIS:ND1  | 2.34                     | 0.43              |
| 1:D:56:PRO:HG2   | 1:D:99:TYR:CD1   | 2.53                     | 0.43              |
| 1:D:248:LYS:NZ   | 1:D:399:GLU:OE2  | 2.39                     | 0.43              |
| 1:F:647:TRP:N    | 1:F:647:TRP:CD1  | 2.85                     | 0.43              |
| 2:K:34:MET:HE2   | 2:K:79:VAL:HG21  | 1.99                     | 0.43              |
| 1:B:32:SER:HA    | 1:B:35:MET:HE2   | 1.99                     | 0.43              |
| 1:B:685:ARG:HH21 | 1:B:706:LEU:HD13 | 1.83                     | 0.43              |
| 1:B:800:GLU:OE1  | 1:C:688:ARG:NH1  | 2.49                     | 0.43              |
| 1:D:135:ILE:HD13 | 1:D:274:LYS:HD3  | 2.00                     | 0.43              |
| 1:D:235:LYS:O    | 1:D:239:GLN:HG2  | 2.19                     | 0.43              |
| 1:F:129:VAL:HG13 | 1:F:325:TYR:CE1  | 2.53                     | 0.43              |
| 2:H:69:THR:HB    | 2:H:82:GLN:HB3   | 2.00                     | 0.43              |
| 1:B:160:LEU:HD11 | 1:B:386:TYR:HB3  | 2.01                     | 0.43              |
| 1:B:734:ARG:O    | 1:B:757:THR:N    | 2.44                     | 0.43              |
| 1:E:780:LYS:HD2  | 1:E:806:ASP:HA   | 2.00                     | 0.43              |
| 1:B:647:TRP:CD1  | 1:B:647:TRP:N    | 2.86                     | 0.43              |
| 1:B:797:GLU:HG2  | 1:C:688:ARG:HD3  | 2.01                     | 0.43              |
| 1:C:296:THR:HG23 | 1:C:307:THR:HG22 | 2.00                     | 0.43              |
| 1:C:452:LYS:HE2  | 1:C:475:TRP:CZ3  | 2.54                     | 0.43              |
| 1:C:520:GLU:HG2  | 1:C:548:VAL:HB   | 1.99                     | 0.43              |
| 1:D:115:GLU:OE2  | 1:E:316:THR:OG1  | 2.32                     | 0.43              |
| 1:D:510:LEU:HD12 | 1:D:510:LEU:HA   | 1.83                     | 0.43              |
| 1:E:129:VAL:HG13 | 1:E:325:TYR:CE1  | 2.54                     | 0.43              |
| 1:F:728:PHE:HA   | 1:F:753:LEU:HD21 | 2.00                     | 0.43              |
| 1:B:679:THR:OG1  | 1:B:703:ASP:OD2  | 2.31                     | 0.43              |
| 1:B:780:LYS:HG2  | 1:B:805:ALA:HB1  | 1.99                     | 0.43              |
| 1:D:670:ASN:OD1  | 1:D:670:ASN:N    | 2.34                     | 0.43              |
| 1:B:290:LYS:HE3  | 1:B:290:LYS:HB2  | 1.76                     | 0.43              |
| 1:B:419:ARG:NH1  | 1:B:431:HIS:O    | 2.51                     | 0.43              |
| 1:F:685:ARG:HH21 | 1:F:706:LEU:HD13 | 1.84                     | 0.43              |
| 1:A:698:THR:HG22 | 1:A:719:ARG:HB2  | 2.01                     | 0.42              |
| 1:C:400:ASN:OD1  | 1:C:403:ARG:NH1  | 2.52                     | 0.42              |
| 1:C:519:GLU:HA   | 1:C:546:LEU:HA   | 2.01                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:87:LYS:HB3   | 2:G:89:GLU:OE1   | 2.19                     | 0.42              |
| 1:A:173:LEU:HD13 | 1:A:173:LEU:HA   | 1.89                     | 0.42              |
| 1:A:235:LYS:O    | 1:A:239:GLN:HG2  | 2.19                     | 0.42              |
| 1:B:348:LEU:H    | 1:B:348:LEU:HD23 | 1.83                     | 0.42              |
| 1:B:499:HIS:CE1  | 1:B:522:HIS:HD2  | 2.37                     | 0.42              |
| 1:C:169:THR:HG23 | 1:C:393:PHE:CE2  | 2.53                     | 0.42              |
| 1:C:302:LEU:HD11 | 1:D:309:ARG:HD3  | 2.01                     | 0.42              |
| 1:C:616:LEU:HB3  | 1:C:638:LEU:HD23 | 2.00                     | 0.42              |
| 1:D:132:HIS:HA   | 1:D:135:ILE:HG22 | 2.01                     | 0.42              |
| 1:D:223:ILE:HA   | 1:D:483:ILE:O    | 2.18                     | 0.42              |
| 1:D:275:PHE:CE1  | 1:D:333:GLY:HA3  | 2.54                     | 0.42              |
| 1:F:348:LEU:HD23 | 1:F:348:LEU:H    | 1.84                     | 0.42              |
| 1:F:679:THR:OG1  | 1:F:703:ASP:OD2  | 2.33                     | 0.42              |
| 1:B:35:MET:HE3   | 1:B:133:THR:HG22 | 2.01                     | 0.42              |
| 1:B:669:LEU:O    | 1:B:672:ASN:ND2  | 2.53                     | 0.42              |
| 1:F:278:ILE:HA   | 1:F:281:TYR:HD2  | 1.84                     | 0.42              |
| 1:F:422:LYS:HG2  | 1:F:428:LEU:HD23 | 2.01                     | 0.42              |
| 1:B:117:ARG:HG2  | 1:B:295:CYS:HA   | 2.00                     | 0.42              |
| 1:B:235:LYS:O    | 1:B:239:GLN:HG2  | 2.20                     | 0.42              |
| 1:B:275:PHE:CE1  | 1:B:333:GLY:HA3  | 2.54                     | 0.42              |
| 1:B:768:CYS:HB2  | 1:B:793:THR:HG21 | 2.01                     | 0.42              |
| 1:C:430:LEU:HB3  | 1:C:448:LEU:HD21 | 2.02                     | 0.42              |
| 1:C:450:VAL:HG13 | 1:C:473:GLU:HB2  | 2.01                     | 0.42              |
| 1:F:715:VAL:O    | 1:F:718:ASN:ND2  | 2.50                     | 0.42              |
| 1:A:270:ILE:O    | 1:A:273:ILE:HG13 | 2.19                     | 0.42              |
| 1:A:443:PHE:CE1  | 1:A:465:ILE:HG22 | 2.55                     | 0.42              |
| 1:B:510:LEU:HD12 | 1:B:510:LEU:HA   | 1.82                     | 0.42              |
| 1:C:710:LEU:HG   | 1:C:733:LEU:HD13 | 2.02                     | 0.42              |
| 1:D:531:ASN:H    | 1:D:533:ARG:NH2  | 2.16                     | 0.42              |
| 1:E:109:VAL:HG21 | 1:E:308:TYR:CE2  | 2.54                     | 0.42              |
| 2:H:28:PRO:HG2   | 2:H:31:ARG:HB2   | 2.01                     | 0.42              |
| 1:A:407:LEU:HD12 | 1:A:407:LEU:HA   | 1.87                     | 0.42              |
| 1:A:590:MET:HE2  | 1:A:593:LEU:HD13 | 2.02                     | 0.42              |
| 1:C:115:GLU:OE2  | 1:D:316:THR:OG1  | 2.38                     | 0.42              |
| 1:D:135:ILE:HG23 | 1:D:274:LYS:NZ   | 2.34                     | 0.42              |
| 1:E:243:LEU:HD12 | 1:E:243:LEU:HA   | 1.85                     | 0.42              |
| 1:E:297:VAL:HG23 | 1:E:299:ILE:HG12 | 2.01                     | 0.42              |
| 1:E:709:ASN:HA   | 1:E:732:LYS:HD2  | 2.01                     | 0.42              |
| 1:D:520:GLU:OE2  | 1:D:522:HIS:NE2  | 2.34                     | 0.42              |
| 1:D:733:LEU:HD21 | 1:D:736:LEU:HD21 | 2.00                     | 0.42              |
| 1:E:136:PHE:CE1  | 1:E:274:LYS:HE3  | 2.55                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:259:ILE:N    | 1:E:371:ASP:OD2  | 2.38                     | 0.42              |
| 1:E:420:LEU:HD12 | 1:E:430:LEU:HD13 | 2.00                     | 0.42              |
| 1:E:575:ASN:HA   | 1:E:599:ILE:O    | 2.20                     | 0.42              |
| 1:F:441:THR:O    | 1:F:441:THR:OG1  | 2.38                     | 0.42              |
| 1:B:248:LYS:NZ   | 1:B:399:GLU:OE2  | 2.40                     | 0.42              |
| 1:B:452:LYS:HG2  | 1:B:475:TRP:CG   | 2.54                     | 0.42              |
| 1:C:431:HIS:HA   | 1:C:452:LYS:HB2  | 2.01                     | 0.42              |
| 1:D:147:PRO:HA   | 1:D:150:SER:HB3  | 2.00                     | 0.42              |
| 1:D:774:GLY:O    | 1:D:801:ARG:NH2  | 2.53                     | 0.42              |
| 1:E:303:THR:OG1  | 1:E:308:TYR:OH   | 2.30                     | 0.42              |
| 1:F:648:TYR:CE2  | 1:F:671:ARG:HG3  | 2.55                     | 0.42              |
| 1:A:149:THR:O    | 1:A:153:LEU:HG   | 2.20                     | 0.42              |
| 1:B:647:TRP:CD1  | 1:B:647:TRP:H    | 2.38                     | 0.42              |
| 1:E:600:ARG:HG2  | 1:E:623:ASP:HB3  | 2.02                     | 0.42              |
| 1:F:384:PRO:O    | 1:F:387:SER:OG   | 2.28                     | 0.42              |
| 1:B:52:MET:HG3   | 1:B:114:TYR:HD2  | 1.84                     | 0.42              |
| 1:D:600:ARG:HG2  | 1:D:623:ASP:CB   | 2.50                     | 0.42              |
| 1:F:275:PHE:CE1  | 1:F:333:GLY:HA3  | 2.55                     | 0.42              |
| 1:F:500:ILE:HG21 | 1:F:508:ILE:HG12 | 2.02                     | 0.42              |
| 2:J:91:THR:HG23  | 2:J:112:THR:HA   | 2.02                     | 0.42              |
| 1:A:585:ASN:OD1  | 1:A:588:LYS:NZ   | 2.31                     | 0.41              |
| 1:C:154:GLU:HA   | 1:C:157:VAL:HG12 | 2.01                     | 0.41              |
| 1:F:135:ILE:HG23 | 1:F:274:LYS:NZ   | 2.35                     | 0.41              |
| 1:F:311:ALA:O    | 1:F:313:PRO:HD3  | 2.20                     | 0.41              |
| 1:F:780:LYS:HG2  | 1:F:805:ALA:HB1  | 2.02                     | 0.41              |
| 2:G:73:ASP:OD1   | 2:G:73:ASP:N     | 2.53                     | 0.41              |
| 1:A:290:LYS:HE3  | 1:A:290:LYS:HB2  | 1.66                     | 0.41              |
| 1:A:791:PHE:CE2  | 1:A:799:LYS:HE3  | 2.54                     | 0.41              |
| 1:B:715:VAL:O    | 1:B:718:ASN:ND2  | 2.53                     | 0.41              |
| 1:D:233:ASP:OD1  | 1:D:234:LYS:N    | 2.54                     | 0.41              |
| 1:E:443:PHE:CE1  | 1:E:465:ILE:HG22 | 2.55                     | 0.41              |
| 1:F:531:ASN:H    | 1:F:533:ARG:NH2  | 2.19                     | 0.41              |
| 2:L:22:CYS:HB3   | 2:L:79:VAL:HB    | 2.01                     | 0.41              |
| 1:C:41:PHE:O     | 1:C:44:THR:HG22  | 2.20                     | 0.41              |
| 1:C:311:ALA:O    | 1:C:313:PRO:HD3  | 2.20                     | 0.41              |
| 1:D:300:GLU:CD   | 1:D:306:ARG:HD2  | 2.45                     | 0.41              |
| 1:E:476:LEU:HB2  | 1:E:500:ILE:HD13 | 2.01                     | 0.41              |
| 1:A:316:THR:O    | 1:A:320:ILE:HG12 | 2.20                     | 0.41              |
| 1:A:780:LYS:HD2  | 1:A:806:ASP:HA   | 2.02                     | 0.41              |
| 1:B:648:TYR:CE2  | 1:B:671:ARG:HG3  | 2.56                     | 0.41              |
| 1:C:159:ILE:O    | 1:C:162:LYS:HG2  | 2.20                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:575:ASN:HA   | 1:C:599:ILE:O    | 2.20                     | 0.41              |
| 1:E:290:LYS:HB2  | 1:E:290:LYS:HE3  | 1.68                     | 0.41              |
| 1:E:430:LEU:HB3  | 1:E:448:LEU:HD21 | 2.02                     | 0.41              |
| 1:E:527:LEU:HG   | 1:E:553:SER:HB3  | 2.02                     | 0.41              |
| 1:F:19:ILE:HG13  | 1:F:20:LEU:HD22  | 2.02                     | 0.41              |
| 2:G:40:ALA:HB3   | 2:G:43:LYS:HD2   | 2.03                     | 0.41              |
| 1:A:34:VAL:O     | 1:A:38:ILE:HG23  | 2.20                     | 0.41              |
| 1:A:500:ILE:HG22 | 1:A:502:PHE:HD1  | 1.85                     | 0.41              |
| 1:B:439:PRO:HB2  | 1:B:442:VAL:HG13 | 2.03                     | 0.41              |
| 1:E:173:LEU:HD13 | 1:E:173:LEU:HA   | 1.89                     | 0.41              |
| 1:E:251:ARG:O    | 1:E:255:GLU:HB2  | 2.21                     | 0.41              |
| 1:E:270:ILE:O    | 1:E:273:ILE:HG13 | 2.20                     | 0.41              |
| 1:F:529:ALA:O    | 1:F:533:ARG:HB3  | 2.20                     | 0.41              |
| 2:H:36:TRP:CE2   | 2:H:81:LEU:HB2   | 2.55                     | 0.41              |
| 1:A:302:LEU:HD11 | 1:B:309:ARG:HD3  | 2.02                     | 0.41              |
| 1:D:135:ILE:HG12 | 1:D:274:LYS:HZ3  | 1.86                     | 0.41              |
| 1:D:300:GLU:OE2  | 1:D:306:ARG:NH1  | 2.52                     | 0.41              |
| 1:D:509:PRO:HB3  | 1:D:511:TRP:NE1  | 2.35                     | 0.41              |
| 1:E:736:LEU:HD23 | 1:E:736:LEU:HA   | 1.90                     | 0.41              |
| 1:F:710:LEU:HD21 | 1:F:713:LEU:HB2  | 2.02                     | 0.41              |
| 1:A:710:LEU:HG   | 1:A:733:LEU:HD13 | 2.03                     | 0.41              |
| 1:B:297:VAL:HG23 | 1:B:299:ILE:HG12 | 2.03                     | 0.41              |
| 1:C:243:LEU:HD12 | 1:C:243:LEU:HA   | 1.86                     | 0.41              |
| 1:C:255:GLU:HG2  | 1:C:369:LYS:HB2  | 2.02                     | 0.41              |
| 1:F:109:VAL:HG21 | 1:F:308:TYR:CE2  | 2.55                     | 0.41              |
| 1:F:151:SER:O    | 1:F:154:GLU:HG3  | 2.20                     | 0.41              |
| 1:A:164:PHE:O    | 1:A:389:ARG:NH1  | 2.53                     | 0.41              |
| 1:A:611:PHE:CD1  | 1:A:634:SER:HB2  | 2.56                     | 0.41              |
| 1:A:687:LEU:HD21 | 1:A:690:LEU:HD13 | 2.02                     | 0.41              |
| 1:D:364:ASP:HB2  | 1:D:397:VAL:HG23 | 2.03                     | 0.41              |
| 1:F:647:TRP:CD1  | 1:F:647:TRP:H    | 2.37                     | 0.41              |
| 1:B:468:LEU:HB3  | 1:B:471:LEU:HB2  | 2.03                     | 0.41              |
| 1:B:489:ALA:O    | 1:B:493:GLU:HG2  | 2.21                     | 0.41              |
| 1:B:649:ASN:HB2  | 1:B:651:ILE:HG13 | 2.03                     | 0.41              |
| 1:C:704:ILE:HD13 | 1:C:727:LEU:HD13 | 2.02                     | 0.41              |
| 1:D:413:LEU:HD12 | 1:D:413:LEU:HA   | 1.91                     | 0.41              |
| 1:D:588:LYS:HE2  | 1:D:588:LYS:HB3  | 1.96                     | 0.41              |
| 1:D:648:TYR:CE1  | 1:D:671:ARG:HG3  | 2.56                     | 0.41              |
| 1:E:500:ILE:HB   | 1:E:523:LEU:HD23 | 2.02                     | 0.41              |
| 1:E:594:THR:HA   | 1:E:616:LEU:HA   | 2.02                     | 0.41              |
| 1:E:772:GLU:O    | 1:E:775:GLU:HG2  | 2.20                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:233:ASP:OD1  | 1:F:234:LYS:N    | 2.54                     | 0.41              |
| 1:F:354:GLU:O    | 1:F:358:GLU:HB2  | 2.21                     | 0.41              |
| 1:F:357:ARG:HD2  | 1:F:363:SER:HA   | 2.01                     | 0.41              |
| 2:L:17:SER:HB3   | 2:L:82:GLN:NE2   | 2.36                     | 0.41              |
| 1:A:685:ARG:HE   | 1:A:706:LEU:HB3  | 1.84                     | 0.41              |
| 1:B:233:ASP:OD1  | 1:B:234:LYS:N    | 2.54                     | 0.41              |
| 1:B:518:LEU:HD23 | 1:B:543:LEU:HD13 | 2.02                     | 0.41              |
| 1:F:634:SER:OG   | 2:L:59:GLU:OE2   | 2.25                     | 0.41              |
| 1:D:502:PHE:CE1  | 1:D:508:ILE:HD11 | 2.56                     | 0.40              |
| 2:K:40:ALA:HB3   | 2:K:43:LYS:HB3   | 2.03                     | 0.40              |
| 1:A:377:HIS:O    | 1:A:381:GLN:HG2  | 2.21                     | 0.40              |
| 1:A:420:LEU:HD12 | 1:A:430:LEU:HD13 | 2.03                     | 0.40              |
| 1:A:688:ARG:HD3  | 1:F:797:GLU:HG2  | 2.03                     | 0.40              |
| 1:C:263:LEU:HD23 | 1:C:263:LEU:HA   | 1.85                     | 0.40              |
| 1:C:270:ILE:O    | 1:C:273:ILE:HG13 | 2.21                     | 0.40              |
| 1:E:422:LYS:HE2  | 1:E:422:LYS:HB3  | 1.85                     | 0.40              |
| 1:E:519:GLU:HA   | 1:E:546:LEU:HA   | 2.02                     | 0.40              |
| 1:F:135:ILE:HD13 | 1:F:274:LYS:HD3  | 2.04                     | 0.40              |
| 1:F:575:ASN:HA   | 1:F:599:ILE:O    | 2.20                     | 0.40              |
| 2:K:34:MET:HG3   | 2:K:79:VAL:HG21  | 2.02                     | 0.40              |
| 2:L:83:MET:HE1   | 2:L:111:VAL:HG11 | 2.02                     | 0.40              |
| 1:B:294:ASP:OD1  | 1:B:309:ARG:NH1  | 2.54                     | 0.40              |
| 1:C:303:THR:HG1  | 1:C:308:TYR:HH   | 1.63                     | 0.40              |
| 1:D:129:VAL:HG13 | 1:D:325:TYR:CE1  | 2.56                     | 0.40              |
| 1:D:354:GLU:O    | 1:D:358:GLU:HB2  | 2.21                     | 0.40              |
| 1:E:316:THR:O    | 1:E:320:ILE:HG12 | 2.21                     | 0.40              |
| 1:F:453:LEU:HD22 | 1:F:456:ILE:HD12 | 2.02                     | 0.40              |
| 2:K:40:ALA:HB3   | 2:K:43:LYS:HD2   | 2.04                     | 0.40              |
| 1:B:151:SER:O    | 1:B:154:GLU:HG3  | 2.20                     | 0.40              |
| 1:C:250:PHE:CZ   | 1:C:254:VAL:HG21 | 2.57                     | 0.40              |
| 1:C:611:PHE:CE1  | 1:C:634:SER:HB2  | 2.56                     | 0.40              |
| 1:D:551:LEU:HD11 | 1:D:562:VAL:HG21 | 2.02                     | 0.40              |
| 1:E:670:ASN:OD1  | 1:E:670:ASN:N    | 2.40                     | 0.40              |
| 1:E:704:ILE:HD13 | 1:E:727:LEU:HD13 | 2.03                     | 0.40              |
| 1:F:52:MET:HG3   | 1:F:114:TYR:HB2  | 2.04                     | 0.40              |
| 1:F:223:ILE:HA   | 1:F:483:ILE:O    | 2.20                     | 0.40              |
| 1:A:688:ARG:NH1  | 1:F:800:GLU:OE1  | 2.55                     | 0.40              |
| 1:B:356:ILE:HD12 | 1:B:388:LYS:HG2  | 2.03                     | 0.40              |
| 1:B:631:GLU:HG3  | 2:H:52:TYR:CE2   | 2.57                     | 0.40              |
| 1:C:129:VAL:HG13 | 1:C:325:TYR:CE1  | 2.56                     | 0.40              |
| 1:C:622:LYS:HB2  | 1:C:647:TRP:NE1  | 2.36                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:160:LEU:HD11 | 1:D:386:TYR:HB3 | 2.04                     | 0.40              |
| 1:F:794:LEU:O    | 1:F:799:LYS:NZ  | 2.55                     | 0.40              |
| 2:I:15:GLY:N     | 2:I:86:LEU:O    | 2.52                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 473/810 (58%)   | 454 (96%)  | 19 (4%)  | 0        | 100         | 100 |
| 1   | B     | 726/810 (90%)   | 699 (96%)  | 27 (4%)  | 0        | 100         | 100 |
| 1   | C     | 712/810 (88%)   | 685 (96%)  | 27 (4%)  | 0        | 100         | 100 |
| 1   | D     | 726/810 (90%)   | 700 (96%)  | 26 (4%)  | 0        | 100         | 100 |
| 1   | E     | 712/810 (88%)   | 687 (96%)  | 25 (4%)  | 0        | 100         | 100 |
| 1   | F     | 726/810 (90%)   | 699 (96%)  | 27 (4%)  | 0        | 100         | 100 |
| 2   | G     | 112/144 (78%)   | 111 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 2   | H     | 112/144 (78%)   | 109 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 2   | I     | 112/144 (78%)   | 109 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 2   | J     | 112/144 (78%)   | 110 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 2   | K     | 112/144 (78%)   | 109 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 2   | L     | 112/144 (78%)   | 110 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| All | All   | 4747/5724 (83%) | 4582 (96%) | 165 (4%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13202. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

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

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

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

## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

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

## 8 Fourier-Shell correlation

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

## 9 Map-model fit

This section was not generated.