



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:16 am GMT

PDB ID : 1PRT  
Title : THE CRYSTAL STRUCTURE OF PERTUSSIS TOXIN  
Authors : Stein, P.E.; Read, R.J.  
Deposited on : 1993-11-22  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : NOT EXECUTED  
EDS : NOT EXECUTED  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

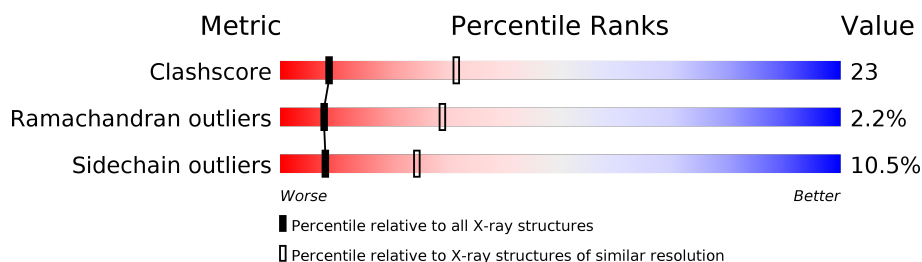
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 112137                      | 1807 (2.90-2.90)                                      |
| Ramachandran outliers | 110173                      | 1768 (2.90-2.90)                                      |
| Sidechain outliers    | 110143                      | 1770 (2.90-2.90)                                      |





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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 234    |                  |
| 1   | G     | 234    |                  |
| 2   | B     | 196    |                  |
| 2   | H     | 196    |                  |
| 3   | C     | 196    |                  |
| 3   | I     | 196    |                  |
| 4   | D     | 110    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 4   | E     | 110    |  54% 40% 5% •  |
| 4   | J     | 110    |  65% 31% 5%    |
| 4   | K     | 110    |  49% 44% 7%    |
| 5   | F     | 98     |  54% 35% 10% • |
| 5   | L     | 98     |  42% 45% 13%   |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14504 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 PERTUSSIS TOXIN (SUBUNIT S1).

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 224      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1769  | 1095 | 318 | 350 | 6 |         |         |       |
| 1   | G     | 224      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1769  | 1095 | 318 | 350 | 6 |         |         |       |

- Molecule 2 is a protein called PERTUSSIS TOXIN (SUBUNIT S2).

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 196      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1522  | 961 | 260 | 292 | 9 |         |         |       |
| 2   | H     | 196      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1522  | 961 | 260 | 292 | 9 |         |         |       |

- Molecule 3 is a protein called PERTUSSIS TOXIN (SUBUNIT S3).

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | C     | 196      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1521  | 969 | 258 | 285 | 9 |         |         |       |
| 3   | I     | 196      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1521  | 969 | 258 | 285 | 9 |         |         |       |

- Molecule 4 is a protein called PERTUSSIS TOXIN (SUBUNIT S4).

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 4   | D     | 110      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 838   | 536 | 143 | 147 | 12 |         |         |       |
| 4   | E     | 110      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 838   | 536 | 143 | 147 | 12 |         |         |       |
| 4   | J     | 110      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 838   | 536 | 143 | 147 | 12 |         |         |       |
| 4   | K     | 110      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 838   | 536 | 143 | 147 | 12 |         |         |       |

- Molecule 5 is a protein called PERTUSSIS TOXIN (SUBUNIT S5).

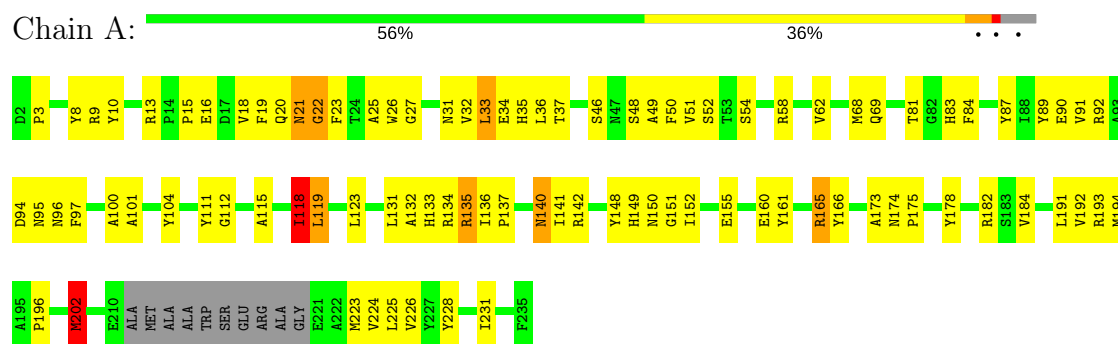
| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | F     | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 764   | 489 | 125 | 144 | 6 |         |         |       |
| 5   | L     | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 764   | 489 | 125 | 144 | 6 |         |         |       |

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

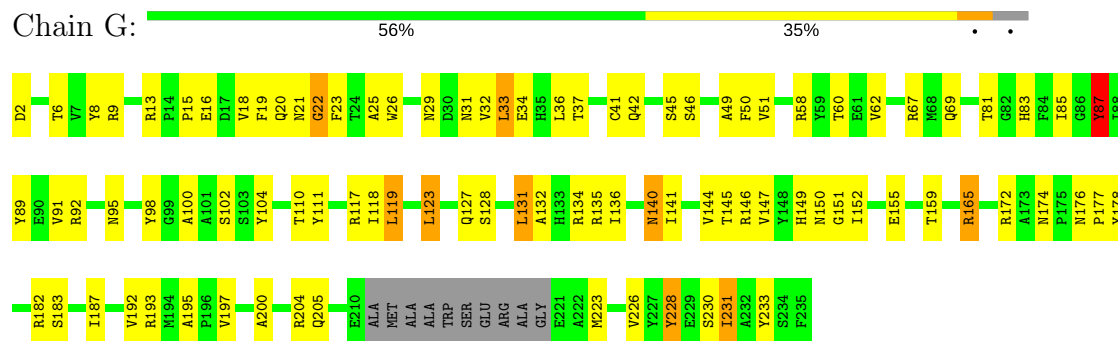
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

Note EDS was not executed.

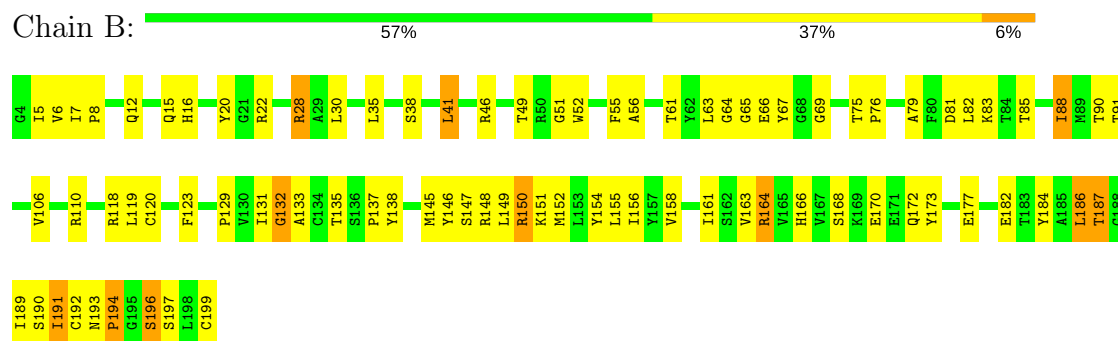
#### • Molecule 1: PERTUSSIS TOXIN (SUBUNIT S1)



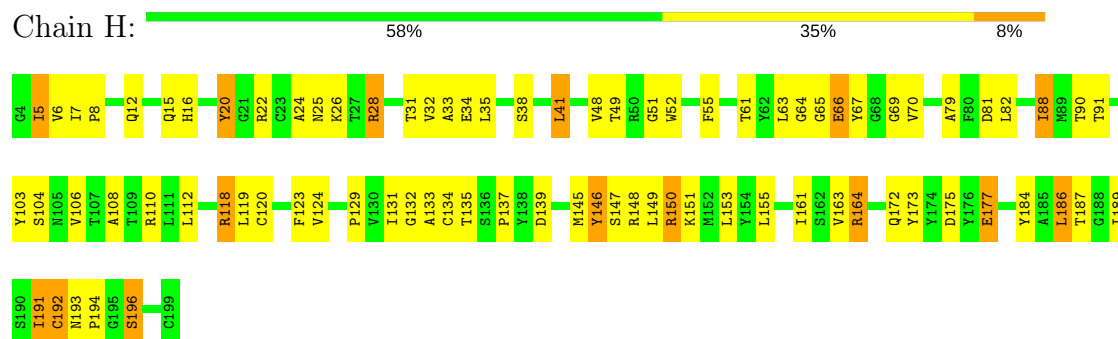
#### • Molecule 1: PERTUSSIS TOXIN (SUBUNIT S1)



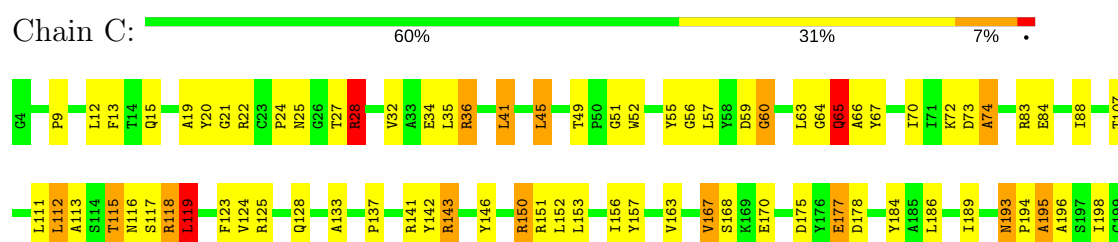
#### • Molecule 2: PERTUSSIS TOXIN (SUBUNIT S2)



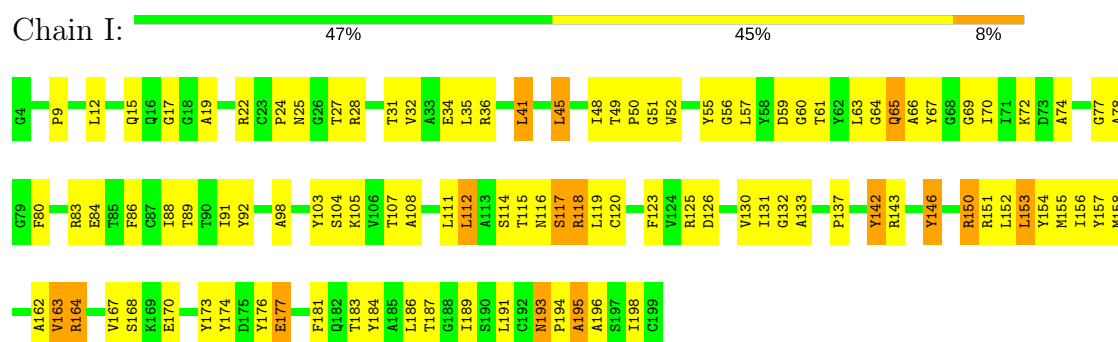
- Molecule 2: PERTUSSIS TOXIN (SUBUNIT S2)



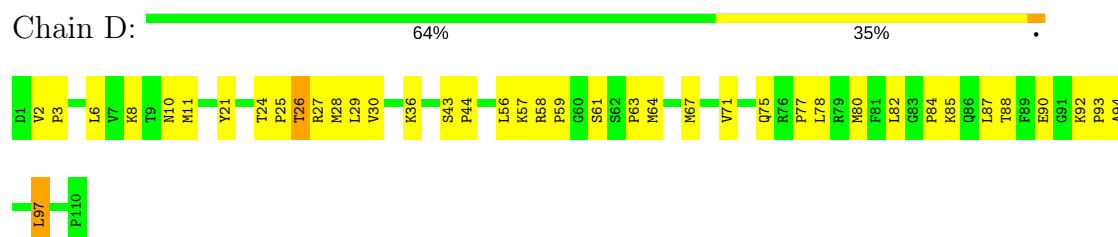
- Molecule 3: PERTUSSIS TOXIN (SUBUNIT S3)



- Molecule 3: PERTUSSIS TOXIN (SUBUNIT S3)

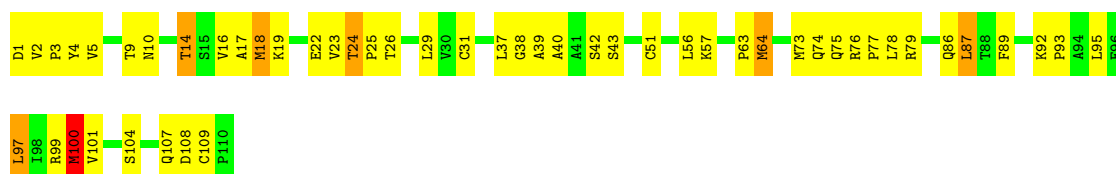


- Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)



- Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)

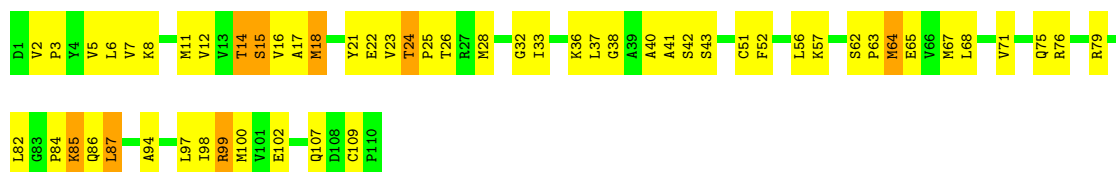




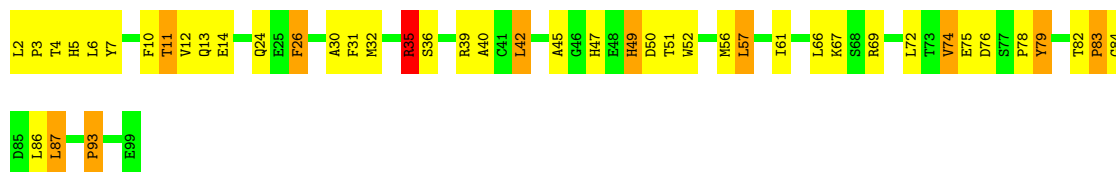
• Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)



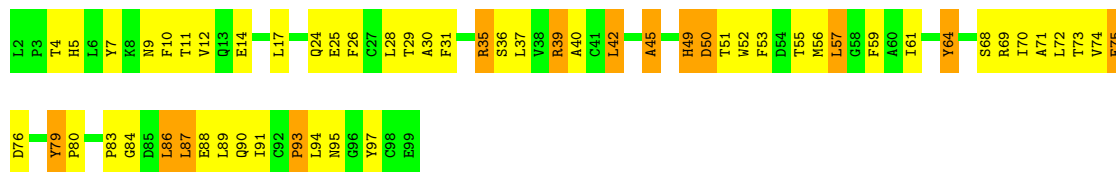
• Molecule 4: PERTUSSIS TOXIN (SUBUNIT S4)



• Molecule 5: PERTUSSIS TOXIN (SUBUNIT S5)



• Molecule 5: PERTUSSIS TOXIN (SUBUNIT S5)





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property   | Value  | Source    |
|--|--|-----------|
| Space group  | P 21 21 21                                     | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 163.80Å 98.20Å 194.50Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)   | 10.00 – 2.90                                   | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (10.00-2.90)                   | Depositor |
| $R_{merge}$  | (Not available)                                | Depositor |
| $R_{sym}$  | (Not available)                                | Depositor |
| Refinement program                                       | X-PLOR   | Depositor |
| R, $R_{free}$  | 0.195 , (Not available)                        | Depositor |
| Estimated twinning fraction                              | No twinning to report.                         | Xtriage   |
| Total number of atoms                                    | 14504  | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 34.0   | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 1   | A     | 0.72         | 2/1809 (0.1%)  | 0.88        | 3/2457 (0.1%)   |
| 1   | G     | 0.55         | 1/1809 (0.1%)  | 0.78        | 3/2457 (0.1%)   |
| 2   | B     | 0.68         | 0/1558         | 0.90        | 2/2115 (0.1%)   |
| 2   | H     | 0.65         | 0/1558         | 0.89        | 2/2115 (0.1%)   |
| 3   | C     | 0.68         | 0/1557         | 0.87        | 1/2115 (0.0%)   |
| 3   | I     | 0.64         | 0/1557         | 0.84        | 1/2115 (0.0%)   |
| 4   | D     | 0.72         | 0/856          | 0.93        | 1/1155 (0.1%)   |
| 4   | E     | 0.88         | 1/856 (0.1%)   | 0.98        | 3/1155 (0.3%)   |
| 4   | J     | 0.66         | 0/856          | 0.89        | 2/1155 (0.2%)   |
| 4   | K     | 0.62         | 0/856          | 0.87        | 1/1155 (0.1%)   |
| 5   | F     | 0.69         | 0/782          | 0.91        | 1/1059 (0.1%)   |
| 5   | L     | 0.61         | 0/782          | 0.88        | 0/1059          |
| All | All   | 0.67         | 4/14836 (0.0%) | 0.88        | 20/20112 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | G     | 0                   | 1                   |
| 2   | B     | 0                   | 1                   |
| 2   | H     | 0                   | 1                   |
| 3   | C     | 0                   | 1                   |
| 3   | I     | 0                   | 2                   |
| 5   | L     | 0                   | 1                   |
| All | All   | 0                   | 7                   |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4   | E     | 100 | MET  | C-N   | 15.84 | 1.70        | 1.34     |
| 1   | A     | 202 | MET  | C-N   | 5.89  | 1.47        | 1.34     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | A     | 135 | ARG  | N-CA  | 5.03 | 1.56        | 1.46     |
| 1   | G     | 134 | ARG  | C-O   | 5.00 | 1.32        | 1.23     |

All (20) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | E     | 100 | MET  | O-C-N     | 11.77 | 141.53      | 122.70   |
| 1   | A     | 135 | ARG  | N-CA-CB   | 9.61  | 127.89      | 110.60   |
| 4   | E     | 100 | MET  | CA-C-N    | -9.22 | 96.92       | 117.20   |
| 1   | G     | 135 | ARG  | NE-CZ-NH2 | 8.11  | 124.36      | 120.30   |
| 1   | G     | 134 | ARG  | NE-CZ-NH2 | 8.03  | 124.31      | 120.30   |
| 2   | H     | 191 | ILE  | N-CA-C    | -6.21 | 94.22       | 111.00   |
| 4   | J     | 18  | MET  | CG-SD-CE  | 6.15  | 110.05      | 100.20   |
| 4   | E     | 100 | MET  | CG-SD-CE  | 6.13  | 110.01      | 100.20   |
| 1   | A     | 202 | MET  | CG-SD-CE  | 6.11  | 109.98      | 100.20   |
| 2   | B     | 191 | ILE  | N-CA-C    | -6.05 | 94.65       | 111.00   |
| 1   | A     | 194 | MET  | CG-SD-CE  | 5.98  | 109.77      | 100.20   |
| 4   | K     | 18  | MET  | CG-SD-CE  | 5.98  | 109.77      | 100.20   |
| 4   | D     | 30  | VAL  | N-CA-C    | -5.90 | 95.07       | 111.00   |
| 2   | B     | 132 | GLY  | N-CA-C    | -5.66 | 98.96       | 113.10   |
| 3   | C     | 119 | LEU  | N-CA-C    | -5.51 | 96.11       | 111.00   |
| 2   | H     | 192 | CYS  | N-CA-C    | 5.51  | 125.89      | 111.00   |
| 3   | I     | 164 | ARG  | N-CA-C    | -5.33 | 96.61       | 111.00   |
| 5   | F     | 35  | ARG  | N-CA-C    | 5.16  | 124.93      | 111.00   |
| 4   | J     | 78  | LEU  | CA-CB-CG  | 5.16  | 127.16      | 115.30   |
| 1   | G     | 134 | ARG  | CA-C-N    | 5.13  | 128.48      | 117.20   |

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | B     | 138 | TYR  | Sidechain |
| 3   | C     | 28  | ARG  | Sidechain |
| 1   | G     | 87  | TYR  | Sidechain |
| 2   | H     | 146 | TYR  | Sidechain |
| 3   | I     | 103 | TYR  | Sidechain |
| 3   | I     | 146 | TYR  | Sidechain |
| 5   | L     | 64  | TYR  | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1769  | 0        | 1655     | 71      | 0            |
| 1   | G     | 1769  | 0        | 1655     | 83      | 0            |
| 2   | B     | 1522  | 0        | 1473     | 72      | 0            |
| 2   | H     | 1522  | 0        | 1473     | 68      | 0            |
| 3   | C     | 1521  | 0        | 1484     | 68      | 0            |
| 3   | I     | 1521  | 0        | 1484     | 92      | 0            |
| 4   | D     | 838   | 0        | 874      | 27      | 0            |
| 4   | E     | 838   | 0        | 873      | 47      | 0            |
| 4   | J     | 838   | 0        | 874      | 34      | 0            |
| 4   | K     | 838   | 0        | 874      | 48      | 0            |
| 5   | F     | 764   | 0        | 747      | 40      | 0            |
| 5   | L     | 764   | 0        | 747      | 65      | 0            |
| All | All   | 14504 | 0        | 14213    | 652     | 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 23.

All (652) 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) |
|------------------|------------------|--------------------------|-------------------|
| 4:E:100:MET:C    | 4:E:101:VAL:N    | 1.70                     | 1.44              |
| 4:D:2:VAL:HG22   | 4:D:3:PRO:HD2    | 1.35                     | 1.07              |
| 4:J:2:VAL:HG22   | 4:J:3:PRO:HD2    | 1.40                     | 0.99              |
| 1:A:69:GLN:HG3   | 4:E:37:LEU:HD23  | 1.45                     | 0.97              |
| 2:B:163:VAL:HG21 | 2:B:189:ILE:HG23 | 1.49                     | 0.95              |
| 2:B:119:LEU:HB2  | 4:D:63:PRO:HB3   | 1.50                     | 0.92              |
| 2:B:49:THR:HG21  | 2:B:64:GLY:HA3   | 1.55                     | 0.89              |
| 1:G:31:ASN:HD22  | 1:G:34:GLU:HG3   | 1.37                     | 0.88              |
| 4:K:18:MET:HE1   | 5:L:55:THR:CG2   | 2.04                     | 0.88              |
| 1:G:31:ASN:ND2   | 1:G:34:GLU:HG3   | 1.90                     | 0.86              |
| 1:A:54:SER:HB2   | 1:A:202:MET:HE3  | 1.58                     | 0.85              |
| 1:A:152:ILE:H    | 1:A:152:ILE:HD12 | 1.42                     | 0.85              |
| 3:I:119:LEU:HB2  | 4:K:63:PRO:HB3   | 1.58                     | 0.85              |
| 1:G:91:VAL:HG11  | 1:G:136:ILE:HD11 | 1.58                     | 0.85              |
| 4:K:18:MET:HE1   | 5:L:55:THR:HG22  | 1.59                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:50:PHE:CD1   | 1:A:131:LEU:HB3  | 2.13                     | 0.83              |
| 4:E:100:MET:CA   | 4:E:101:VAL:N    | 2.41                     | 0.83              |
| 3:I:49:THR:HG21  | 3:I:64:GLY:HA2   | 1.60                     | 0.83              |
| 1:G:69:GLN:HG3   | 4:K:37:LEU:HD23  | 1.61                     | 0.82              |
| 2:H:49:THR:HG21  | 2:H:64:GLY:HA3   | 1.62                     | 0.82              |
| 1:A:54:SER:HB2   | 1:A:202:MET:CE   | 2.10                     | 0.81              |
| 2:H:163:VAL:HG21 | 2:H:189:ILE:HG23 | 1.62                     | 0.81              |
| 1:G:152:ILE:H    | 1:G:152:ILE:HD12 | 1.47                     | 0.79              |
| 2:H:119:LEU:HB2  | 4:J:63:PRO:HB3   | 1.65                     | 0.77              |
| 3:I:60:GLY:HA2   | 3:I:74:ALA:HB3   | 1.64                     | 0.77              |
| 1:A:92:ARG:HB3   | 1:A:140:ASN:HD22 | 1.50                     | 0.77              |
| 4:E:51:CYS:HB2   | 4:E:87:LEU:HD23  | 1.65                     | 0.77              |
| 1:G:16:GLU:O     | 1:G:20:GLN:HG2   | 1.85                     | 0.77              |
| 2:B:161:ILE:HG21 | 2:B:191:ILE:HD13 | 1.66                     | 0.77              |
| 1:G:92:ARG:HB3   | 1:G:140:ASN:HD22 | 1.50                     | 0.77              |
| 3:I:49:THR:HG23  | 3:I:55:TYR:HE2   | 1.51                     | 0.76              |
| 2:B:145:MET:HA   | 5:F:24:GLN:HE22  | 1.50                     | 0.76              |
| 1:A:111:TYR:CD2  | 1:A:182:ARG:HB2  | 2.20                     | 0.76              |
| 2:H:150:ARG:HG2  | 2:H:150:ARG:HH11 | 1.49                     | 0.75              |
| 4:K:18:MET:CE    | 5:L:55:THR:HG22  | 2.15                     | 0.75              |
| 2:B:166:HIS:O    | 2:B:187:THR:HG22 | 1.85                     | 0.75              |
| 1:G:111:TYR:CD2  | 1:G:182:ARG:HB2  | 2.22                     | 0.75              |
| 2:H:137:PRO:HB3  | 2:H:146:TYR:CD2  | 2.22                     | 0.74              |
| 1:A:91:VAL:HG11  | 1:A:136:ILE:HD11 | 1.69                     | 0.74              |
| 1:G:31:ASN:HD21  | 1:G:183:SER:HB2  | 1.50                     | 0.74              |
| 3:C:25:ASN:ND2   | 3:C:115:THR:HB   | 2.02                     | 0.74              |
| 3:I:63:LEU:HD12  | 3:I:70:ILE:HB    | 1.71                     | 0.73              |
| 1:A:31:ASN:HD22  | 1:A:34:GLU:HG3   | 1.54                     | 0.73              |
| 2:H:148:ARG:HB3  | 5:L:17:LEU:HD21  | 1.70                     | 0.73              |
| 1:A:31:ASN:ND2   | 1:A:34:GLU:HG3   | 2.01                     | 0.73              |
| 2:B:63:LEU:HD12  | 2:B:63:LEU:H     | 1.53                     | 0.72              |
| 2:B:193:ASN:O    | 2:B:196:SER:HB3  | 1.87                     | 0.72              |
| 5:F:42:LEU:HD21  | 5:F:52:TRP:CZ3   | 2.24                     | 0.72              |
| 3:I:173:TYR:HB2  | 3:I:183:THR:HG22 | 1.69                     | 0.72              |
| 2:B:52:TRP:CG    | 4:J:93:PRO:HB3   | 2.24                     | 0.72              |
| 3:C:115:THR:HG22 | 3:C:116:ASN:N    | 2.03                     | 0.72              |
| 3:C:35:LEU:HD13  | 3:C:41:LEU:HD13  | 1.71                     | 0.72              |
| 3:C:119:LEU:HB2  | 4:E:63:PRO:HB3   | 1.70                     | 0.72              |
| 1:A:16:GLU:O     | 1:A:20:GLN:HG2   | 1.89                     | 0.71              |
| 5:L:7:TYR:HB3    | 5:L:10:PHE:CD2   | 2.25                     | 0.71              |
| 2:H:63:LEU:H     | 2:H:63:LEU:HD12  | 1.57                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:K:18:MET:CE    | 5:L:55:THR:CG2   | 2.69                     | 0.70              |
| 1:G:51:VAL:HB    | 1:G:132:ALA:HB3  | 1.73                     | 0.70              |
| 3:C:60:GLY:HA2   | 3:C:74:ALA:HB3   | 1.74                     | 0.70              |
| 1:A:32:VAL:O     | 1:A:36:LEU:HD13  | 1.92                     | 0.70              |
| 4:K:67:MET:O     | 4:K:71:VAL:HG22  | 1.91                     | 0.70              |
| 4:K:62:SER:OG    | 4:K:65:GLU:HB2   | 1.92                     | 0.69              |
| 2:B:28:ARG:HH21  | 2:B:177:GLU:HA   | 1.56                     | 0.69              |
| 3:C:49:THR:HG21  | 3:C:64:GLY:HA2   | 1.74                     | 0.69              |
| 5:F:7:TYR:HB3    | 5:F:10:PHE:CD2   | 2.28                     | 0.69              |
| 3:I:25:ASN:ND2   | 3:I:115:THR:HB   | 2.08                     | 0.69              |
| 1:A:152:ILE:N    | 1:A:152:ILE:HD12 | 2.09                     | 0.68              |
| 1:A:95:ASN:O     | 1:A:174:ASN:HB2  | 1.94                     | 0.68              |
| 1:G:22:GLY:HA2   | 1:G:141:ILE:HD11 | 1.76                     | 0.68              |
| 1:A:83:HIS:CD2   | 1:A:150:ASN:HA   | 2.29                     | 0.67              |
| 3:I:193:ASN:H    | 3:I:198:ILE:HB   | 1.58                     | 0.67              |
| 4:D:2:VAL:CG2    | 4:D:3:PRO:HD2    | 2.18                     | 0.67              |
| 3:C:51:GLY:HA2   | 3:C:65:GLN:OE1   | 1.95                     | 0.67              |
| 2:B:154:TYR:O    | 2:B:158:VAL:HG22 | 1.95                     | 0.66              |
| 5:F:7:TYR:HB2    | 5:F:72:LEU:HD23  | 1.77                     | 0.66              |
| 3:I:56:GLY:O     | 3:I:57:LEU:HD12  | 1.95                     | 0.66              |
| 1:A:165:ARG:HH11 | 1:A:165:ARG:HB3  | 1.59                     | 0.66              |
| 2:B:145:MET:HB3  | 2:B:149:LEU:HD12 | 1.78                     | 0.66              |
| 5:F:56:MET:HE2   | 5:F:86:LEU:HD21  | 1.77                     | 0.66              |
| 1:G:165:ARG:HH11 | 1:G:165:ARG:HB3  | 1.58                     | 0.66              |
| 1:G:195:ALA:HB1  | 4:K:75:GLN:HG2   | 1.77                     | 0.66              |
| 2:H:155:LEU:HD22 | 5:L:61:ILE:HG23  | 1.76                     | 0.65              |
| 5:F:74:VAL:HG23  | 5:F:75:GLU:O     | 1.95                     | 0.65              |
| 2:H:12:GLN:O     | 2:H:88:ILE:HA    | 1.96                     | 0.65              |
| 4:E:1:ASP:HA     | 4:E:86:GLN:HG3   | 1.79                     | 0.65              |
| 2:H:35:LEU:HD12  | 2:H:41:LEU:HB3   | 1.79                     | 0.65              |
| 3:I:194:PRO:HG2  | 3:I:195:ALA:H    | 1.62                     | 0.65              |
| 1:G:83:HIS:CD2   | 1:G:150:ASN:HA   | 2.32                     | 0.64              |
| 2:B:163:VAL:HG21 | 2:B:189:ILE:CG2  | 2.25                     | 0.64              |
| 2:H:28:ARG:HE    | 2:H:177:GLU:HG3  | 1.62                     | 0.64              |
| 3:C:193:ASN:H    | 3:C:198:ILE:HB   | 1.62                     | 0.64              |
| 4:K:86:GLN:HA    | 4:K:94:ALA:O     | 1.96                     | 0.64              |
| 1:A:83:HIS:HD2   | 1:A:150:ASN:HA   | 1.62                     | 0.64              |
| 5:F:6:LEU:HD23   | 5:F:7:TYR:N      | 2.12                     | 0.64              |
| 5:L:69:ARG:HG3   | 5:L:69:ARG:HH11  | 1.62                     | 0.64              |
| 3:I:27:THR:HG22  | 3:I:89:THR:HA    | 1.80                     | 0.64              |
| 3:C:137:PRO:HB3  | 3:C:146:TYR:CD2  | 2.33                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:81:THR:O     | 1:G:152:ILE:HD11 | 1.98                     | 0.63              |
| 3:C:25:ASN:HD21  | 3:C:115:THR:HB   | 1.63                     | 0.63              |
| 2:H:163:VAL:HG21 | 2:H:189:ILE:CG2  | 2.28                     | 0.63              |
| 2:H:5:ILE:HG22   | 2:H:7:ILE:HD12   | 1.81                     | 0.63              |
| 4:J:2:VAL:CG2    | 4:J:3:PRO:HD2    | 2.23                     | 0.63              |
| 2:H:118:ARG:HG3  | 2:H:120:CYS:SG   | 2.39                     | 0.63              |
| 1:A:36:LEU:CD2   | 1:A:104:TYR:HB2  | 2.29                     | 0.63              |
| 3:C:52:TRP:HA    | 3:C:67:TYR:CE2   | 2.34                     | 0.63              |
| 2:B:75:THR:HG23  | 2:B:76:PRO:HD2   | 1.80                     | 0.63              |
| 3:C:9:PRO:HD2    | 3:C:12:LEU:CD1   | 2.29                     | 0.63              |
| 3:I:60:GLY:HA3   | 3:I:72:LYS:O     | 1.98                     | 0.63              |
| 5:L:39:ARG:HB3   | 5:L:83:PRO:HG3   | 1.81                     | 0.63              |
| 2:H:148:ARG:H    | 2:H:148:ARG:HD2  | 1.64                     | 0.62              |
| 2:H:28:ARG:HH21  | 2:H:177:GLU:HA   | 1.63                     | 0.62              |
| 3:I:51:GLY:HA2   | 3:I:65:GLN:OE1   | 1.98                     | 0.62              |
| 1:G:50:PHE:CD1   | 1:G:131:LEU:HB3  | 2.34                     | 0.62              |
| 1:A:51:VAL:HB    | 1:A:132:ALA:HB3  | 1.81                     | 0.62              |
| 1:G:98:TYR:O     | 1:G:131:LEU:HD12 | 1.98                     | 0.62              |
| 2:H:161:ILE:HG21 | 2:H:191:ILE:HD13 | 1.82                     | 0.62              |
| 5:F:10:PHE:CE1   | 5:F:32:MET:HB2   | 2.35                     | 0.62              |
| 1:G:228:TYR:O    | 1:G:231:ILE:HD13 | 1.99                     | 0.62              |
| 2:B:137:PRO:HB3  | 2:B:146:TYR:CD2  | 2.35                     | 0.62              |
| 5:L:75:GLU:HG2   | 5:L:76:ASP:H     | 1.65                     | 0.61              |
| 3:C:9:PRO:HD2    | 3:C:12:LEU:HD11  | 1.80                     | 0.61              |
| 2:B:49:THR:HG22  | 2:B:65:GLY:N     | 2.15                     | 0.61              |
| 5:F:7:TYR:HB3    | 5:F:10:PHE:CE2   | 2.35                     | 0.61              |
| 4:E:79:ARG:HG3   | 4:E:109:CYS:SG   | 2.41                     | 0.61              |
| 3:I:60:GLY:HA2   | 3:I:74:ALA:CB    | 2.30                     | 0.61              |
| 2:H:148:ARG:HB3  | 5:L:17:LEU:CD2   | 2.31                     | 0.61              |
| 3:I:150:ARG:HG3  | 3:I:151:ARG:N    | 2.15                     | 0.61              |
| 3:I:52:TRP:HA    | 3:I:67:TYR:CE2   | 2.36                     | 0.61              |
| 3:C:55:TYR:HD1   | 3:C:84:GLU:HB3   | 1.66                     | 0.60              |
| 1:A:81:THR:O     | 1:A:152:ILE:HD11 | 2.01                     | 0.60              |
| 3:I:137:PRO:HB3  | 3:I:146:TYR:CD2  | 2.36                     | 0.60              |
| 3:I:49:THR:CG2   | 3:I:64:GLY:HA2   | 2.30                     | 0.60              |
| 2:B:145:MET:HG2  | 5:F:24:GLN:OE1   | 2.01                     | 0.60              |
| 4:E:64:MET:CE    | 4:E:100:MET:CE   | 2.79                     | 0.60              |
| 5:L:9:ASN:OD1    | 5:L:97:TYR:HB3   | 2.02                     | 0.60              |
| 1:A:15:PRO:HD3   | 1:A:87:TYR:CE2   | 2.37                     | 0.60              |
| 2:B:150:ARG:HH11 | 2:B:150:ARG:HG2  | 1.67                     | 0.60              |
| 1:G:58:ARG:O     | 1:G:62:VAL:HG23  | 2.01                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:112:LEU:HD12 | 3:C:113:ALA:N    | 2.17                     | 0.60              |
| 3:C:52:TRP:CE2   | 3:C:66:ALA:HB1   | 2.37                     | 0.60              |
| 3:C:63:LEU:HD12  | 3:C:70:ILE:HB    | 1.84                     | 0.59              |
| 1:G:36:LEU:CD2   | 1:G:104:TYR:HB2  | 2.31                     | 0.59              |
| 2:B:156:ILE:CD1  | 2:B:189:ILE:HD13 | 2.33                     | 0.59              |
| 3:C:115:THR:HG22 | 3:C:116:ASN:H    | 1.67                     | 0.59              |
| 4:D:80:MET:HB3   | 4:D:97:LEU:HD21  | 1.84                     | 0.59              |
| 2:B:38:SER:OG    | 2:B:41:LEU:HB2   | 2.03                     | 0.59              |
| 3:C:198:ILE:CD1  | 4:D:90:GLU:HG3   | 2.32                     | 0.59              |
| 1:G:15:PRO:HD3   | 1:G:87:TYR:CE2   | 2.38                     | 0.59              |
| 5:L:69:ARG:HG3   | 5:L:69:ARG:NH1   | 2.15                     | 0.59              |
| 4:E:100:MET:C    | 4:E:101:VAL:CA   | 2.69                     | 0.59              |
| 2:B:28:ARG:NH2   | 2:B:177:GLU:HA   | 2.18                     | 0.59              |
| 4:D:26:THR:HG22  | 4:D:57:LYS:HG3   | 1.85                     | 0.59              |
| 4:K:79:ARG:HG3   | 4:K:109:CYS:SG   | 2.43                     | 0.58              |
| 1:G:18:VAL:HG12  | 1:G:141:ILE:HD13 | 1.85                     | 0.58              |
| 2:H:150:ARG:HG2  | 2:H:150:ARG:NH1  | 2.18                     | 0.58              |
| 1:G:50:PHE:HZ    | 1:G:178:TYR:CE2  | 2.22                     | 0.58              |
| 2:B:49:THR:HG22  | 2:B:65:GLY:H     | 1.68                     | 0.58              |
| 4:K:26:THR:HB    | 4:K:57:LYS:HZ2   | 1.69                     | 0.58              |
| 4:E:64:MET:HE2   | 4:E:100:MET:HE2  | 1.85                     | 0.58              |
| 4:K:26:THR:HB    | 4:K:57:LYS:NZ    | 2.19                     | 0.58              |
| 2:H:137:PRO:HB3  | 2:H:146:TYR:HD2  | 1.68                     | 0.58              |
| 5:F:86:LEU:HD23  | 5:F:86:LEU:O     | 2.04                     | 0.57              |
| 1:G:26:TRP:HZ3   | 1:G:41:CYS:HA    | 1.69                     | 0.57              |
| 2:B:30:LEU:HB2   | 2:B:88:ILE:HD13  | 1.86                     | 0.57              |
| 2:B:51:GLY:O     | 2:B:65:GLY:HA3   | 2.05                     | 0.57              |
| 3:C:119:LEU:CB   | 4:E:63:PRO:HB3   | 2.35                     | 0.57              |
| 3:C:56:GLY:O     | 3:C:57:LEU:HD12  | 2.05                     | 0.57              |
| 3:C:168:SER:OG   | 3:C:170:GLU:HB2  | 2.04                     | 0.57              |
| 1:G:111:TYR:CD1  | 1:G:111:TYR:N    | 2.72                     | 0.57              |
| 1:G:195:ALA:HB1  | 4:K:75:GLN:CG    | 2.34                     | 0.57              |
| 1:A:33:LEU:O     | 1:A:37:THR:HG22  | 2.03                     | 0.57              |
| 3:I:49:THR:HG23  | 3:I:55:TYR:CE2   | 2.36                     | 0.57              |
| 3:C:143:ARG:HH11 | 3:C:143:ARG:HB2  | 1.70                     | 0.56              |
| 3:I:9:PRO:HD2    | 3:I:12:LEU:CD1   | 2.35                     | 0.56              |
| 2:H:20:TYR:HB3   | 4:J:4:TYR:HA     | 1.86                     | 0.56              |
| 1:G:19:PHE:O     | 1:G:165:ARG:HD3  | 2.06                     | 0.56              |
| 4:J:64:MET:CE    | 4:J:97:LEU:HD13  | 2.35                     | 0.56              |
| 3:C:142:TYR:CD1  | 3:C:142:TYR:N    | 2.73                     | 0.56              |
| 3:I:28:ARG:NH1   | 3:I:177:GLU:HA   | 2.20                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:163:VAL:HG22 | 3:I:191:LEU:HA   | 1.85                     | 0.56              |
| 3:I:152:LEU:O    | 3:I:156:ILE:HG12 | 2.05                     | 0.56              |
| 2:B:163:VAL:HG22 | 2:B:164:ARG:H    | 1.70                     | 0.56              |
| 1:A:92:ARG:O     | 1:A:140:ASN:ND2  | 2.38                     | 0.56              |
| 1:G:233:TYR:CZ   | 3:I:155:MET:HG3  | 2.41                     | 0.56              |
| 1:G:233:TYR:CE2  | 3:I:155:MET:HG3  | 2.41                     | 0.56              |
| 1:A:31:ASN:HD22  | 1:A:34:GLU:H     | 1.54                     | 0.55              |
| 2:H:163:VAL:HG22 | 2:H:164:ARG:H    | 1.70                     | 0.55              |
| 1:A:23:PHE:HB2   | 1:A:136:ILE:CG2  | 2.37                     | 0.55              |
| 3:I:28:ARG:CZ    | 3:I:88:ILE:HD11  | 2.36                     | 0.55              |
| 3:C:123:PHE:HE1  | 3:C:133:ALA:HB3  | 1.71                     | 0.55              |
| 1:G:69:GLN:HG3   | 4:K:37:LEU:CD2   | 2.35                     | 0.55              |
| 4:E:14:THR:HG23  | 5:F:93:PRO:HG3   | 1.88                     | 0.55              |
| 1:A:18:VAL:HG11  | 1:A:89:TYR:CE2   | 2.41                     | 0.55              |
| 4:K:52:PHE:CE1   | 4:K:68:LEU:HD22  | 2.42                     | 0.55              |
| 1:A:149:HIS:HA   | 1:A:155:GLU:O    | 2.06                     | 0.55              |
| 3:I:104:SER:O    | 3:I:105:LYS:HB2  | 2.06                     | 0.55              |
| 4:J:37:LEU:N     | 4:J:37:LEU:HD12  | 2.21                     | 0.55              |
| 5:L:57:LEU:HD22  | 5:L:61:ILE:HD11  | 1.89                     | 0.55              |
| 3:C:41:LEU:HD22  | 3:C:45:LEU:HD22  | 1.88                     | 0.55              |
| 4:K:2:VAL:HG13   | 4:K:3:PRO:HD2    | 1.88                     | 0.54              |
| 2:H:145:MET:HA   | 5:L:24:GLN:HE22  | 1.72                     | 0.54              |
| 2:H:106:VAL:HB   | 2:H:123:PHE:HB3  | 1.89                     | 0.54              |
| 4:E:100:MET:HA   | 4:E:101:VAL:N    | 2.21                     | 0.54              |
| 2:H:90:THR:O     | 2:H:173:TYR:HA   | 2.08                     | 0.54              |
| 3:I:24:PRO:HG2   | 3:I:27:THR:OG1   | 2.06                     | 0.54              |
| 4:J:2:VAL:HG12   | 4:J:84:PRO:HA    | 1.88                     | 0.54              |
| 2:H:148:ARG:CB   | 5:L:17:LEU:HD21  | 2.36                     | 0.54              |
| 1:G:26:TRP:CE3   | 1:G:46:SER:HB3   | 2.42                     | 0.54              |
| 3:I:112:LEU:C    | 3:I:112:LEU:HD12 | 2.27                     | 0.54              |
| 5:L:40:ALA:HB1   | 5:L:86:LEU:HB2   | 1.89                     | 0.54              |
| 3:I:117:SER:O    | 4:K:63:PRO:HG2   | 2.08                     | 0.54              |
| 1:A:19:PHE:O     | 1:A:165:ARG:HD3  | 2.08                     | 0.53              |
| 3:I:142:TYR:N    | 3:I:142:TYR:CD1  | 2.75                     | 0.53              |
| 3:I:57:LEU:HD11  | 3:I:86:PHE:CD2   | 2.43                     | 0.53              |
| 3:I:119:LEU:CB   | 4:K:63:PRO:HB3   | 2.36                     | 0.53              |
| 1:G:33:LEU:O     | 1:G:37:THR:HG22  | 2.09                     | 0.53              |
| 1:A:152:ILE:H    | 1:A:152:ILE:CD1  | 2.16                     | 0.53              |
| 2:B:149:LEU:HD22 | 2:B:186:LEU:HD13 | 1.89                     | 0.53              |
| 5:F:75:GLU:HG2   | 5:F:76:ASP:H     | 1.73                     | 0.53              |
| 2:B:12:GLN:O     | 2:B:88:ILE:HA    | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:J:10:ASN:O     | 4:J:36:LYS:HA    | 2.09                     | 0.53              |
| 3:I:50:PRO:HD2   | 3:I:55:TYR:OH    | 2.08                     | 0.53              |
| 4:D:67:MET:O     | 4:D:71:VAL:HG22  | 2.08                     | 0.53              |
| 4:E:64:MET:CE    | 4:E:100:MET:HE3  | 2.39                     | 0.53              |
| 1:G:111:TYR:HD2  | 1:G:182:ARG:HB2  | 1.72                     | 0.53              |
| 3:I:198:ILE:CD1  | 4:J:90:GLU:HG3   | 2.39                     | 0.53              |
| 5:L:7:TYR:HB3    | 5:L:10:PHE:CE2   | 2.43                     | 0.53              |
| 3:I:112:LEU:HD23 | 3:I:176:TYR:CE1  | 2.43                     | 0.53              |
| 3:I:19:ALA:HA    | 3:I:83:ARG:O     | 2.08                     | 0.53              |
| 4:E:51:CYS:SG    | 4:E:89:PHE:HB2   | 2.49                     | 0.53              |
| 1:G:83:HIS:HD2   | 1:G:150:ASN:HA   | 1.74                     | 0.53              |
| 4:E:64:MET:HE1   | 4:E:100:MET:HG2  | 1.90                     | 0.52              |
| 1:G:111:TYR:CE2  | 1:G:182:ARG:HB2  | 2.44                     | 0.52              |
| 2:H:15:GLN:HG3   | 2:H:16:HIS:H     | 1.74                     | 0.52              |
| 3:I:133:ALA:HA   | 3:I:184:TYR:O    | 2.09                     | 0.52              |
| 1:A:22:GLY:HA2   | 1:A:141:ILE:HD11 | 1.91                     | 0.52              |
| 3:C:112:LEU:C    | 3:C:112:LEU:HD12 | 2.30                     | 0.52              |
| 1:G:123:LEU:HD22 | 1:G:127:GLN:HG3  | 1.90                     | 0.52              |
| 3:C:115:THR:CG2  | 3:C:116:ASN:N    | 2.72                     | 0.52              |
| 3:I:193:ASN:O    | 3:I:198:ILE:HB   | 2.10                     | 0.52              |
| 1:A:111:TYR:CE2  | 1:A:182:ARG:HB2  | 2.45                     | 0.52              |
| 1:A:31:ASN:ND2   | 1:A:34:GLU:H     | 2.07                     | 0.52              |
| 2:B:28:ARG:HE    | 2:B:177:GLU:HG3  | 1.74                     | 0.52              |
| 2:H:147:SER:O    | 2:H:151:LYS:HG3  | 2.10                     | 0.52              |
| 1:A:112:GLY:O    | 1:A:115:ALA:HB3  | 2.10                     | 0.52              |
| 2:B:156:ILE:HD13 | 2:B:189:ILE:HD13 | 1.92                     | 0.52              |
| 2:H:35:LEU:CD1   | 2:H:41:LEU:HB3   | 2.39                     | 0.52              |
| 3:I:173:TYR:HB2  | 3:I:183:THR:CG2  | 2.39                     | 0.52              |
| 5:L:25:GLU:HG2   | 5:L:26:PHE:N     | 2.25                     | 0.52              |
| 2:B:163:VAL:HG22 | 2:B:164:ARG:N    | 2.25                     | 0.52              |
| 2:B:163:VAL:HG23 | 2:B:190:SER:O    | 2.10                     | 0.52              |
| 3:C:32:VAL:O     | 3:C:36:ARG:HB2   | 2.09                     | 0.51              |
| 5:F:75:GLU:HB2   | 5:F:87:LEU:HD11  | 1.92                     | 0.51              |
| 3:I:114:SER:HB2  | 3:I:117:SER:HB2  | 1.92                     | 0.51              |
| 1:A:58:ARG:O     | 1:A:62:VAL:HG23  | 2.11                     | 0.51              |
| 2:B:182:GLU:HG2  | 2:B:184:TYR:OH   | 2.11                     | 0.51              |
| 1:G:23:PHE:HB2   | 1:G:136:ILE:CG2  | 2.39                     | 0.51              |
| 2:H:52:TRP:O     | 2:H:67:TYR:HE2   | 1.93                     | 0.51              |
| 5:F:4:THR:HG22   | 5:F:5:HIS:N      | 2.25                     | 0.51              |
| 2:H:55:PHE:N     | 2:H:55:PHE:CD1   | 2.78                     | 0.51              |
| 3:I:163:VAL:HG11 | 3:I:189:ILE:HG23 | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:L:7:TYR:O      | 5:L:71:ALA:HA    | 2.10                     | 0.51              |
| 3:C:24:PRO:O     | 3:C:27:THR:OG1   | 2.27                     | 0.51              |
| 5:F:10:PHE:CD1   | 5:F:32:MET:HB2   | 2.46                     | 0.51              |
| 1:G:149:HIS:HA   | 1:G:155:GLU:O    | 2.11                     | 0.51              |
| 2:B:63:LEU:HD12  | 2:B:63:LEU:N     | 2.24                     | 0.51              |
| 1:G:204:ARG:HA   | 1:G:223:MET:HE1  | 1.92                     | 0.51              |
| 1:A:69:GLN:HG3   | 4:E:37:LEU:CD2   | 2.29                     | 0.51              |
| 4:K:17:ALA:HB2   | 5:L:90:GLN:HB2   | 1.92                     | 0.51              |
| 1:A:84:PHE:O     | 1:A:148:TYR:HA   | 2.11                     | 0.51              |
| 1:A:52:SER:OG    | 1:A:202:MET:HG3  | 2.10                     | 0.51              |
| 3:C:32:VAL:HG12  | 3:C:57:LEU:HD22  | 1.93                     | 0.51              |
| 5:L:68:SER:OG    | 5:L:91:ILE:HG23  | 2.11                     | 0.51              |
| 2:B:135:THR:CG2  | 2:B:146:TYR:HD1  | 2.24                     | 0.51              |
| 4:K:52:PHE:CZ    | 4:K:68:LEU:HD22  | 2.46                     | 0.51              |
| 5:L:64:TYR:CD1   | 5:L:64:TYR:C     | 2.84                     | 0.51              |
| 2:B:135:THR:HG21 | 2:B:146:TYR:HA   | 1.93                     | 0.50              |
| 4:J:37:LEU:H     | 4:J:37:LEU:HD12  | 1.76                     | 0.50              |
| 4:E:74:GLN:OE1   | 4:E:74:GLN:HA    | 2.11                     | 0.50              |
| 2:H:28:ARG:NH2   | 2:H:177:GLU:HA   | 2.25                     | 0.50              |
| 2:H:193:ASN:HB2  | 5:L:14:GLU:OE1   | 2.10                     | 0.50              |
| 5:L:72:LEU:HD23  | 5:L:72:LEU:H     | 1.75                     | 0.50              |
| 2:B:148:ARG:H    | 2:B:148:ARG:HD2  | 1.75                     | 0.50              |
| 1:G:50:PHE:HZ    | 1:G:178:TYR:CD2  | 2.29                     | 0.50              |
| 2:H:5:ILE:HG23   | 2:H:6:VAL:N      | 2.26                     | 0.50              |
| 5:L:9:ASN:HA     | 5:L:69:ARG:HB3   | 1.93                     | 0.50              |
| 1:G:26:TRP:CZ3   | 1:G:41:CYS:HA    | 2.46                     | 0.50              |
| 2:H:119:LEU:HD21 | 2:H:153:LEU:HD23 | 1.94                     | 0.50              |
| 3:I:52:TRP:H     | 3:I:66:ALA:CB    | 2.24                     | 0.50              |
| 1:G:233:TYR:CE1  | 4:J:69:ARG:HD2   | 2.46                     | 0.50              |
| 4:K:11:MET:SD    | 4:K:36:LYS:HB2   | 2.52                     | 0.50              |
| 5:L:49:HIS:O     | 5:L:51:THR:N     | 2.45                     | 0.50              |
| 1:A:174:ASN:OD1  | 1:A:175:PRO:HD2  | 2.11                     | 0.50              |
| 2:B:145:MET:HG2  | 5:F:24:GLN:CD    | 2.32                     | 0.50              |
| 2:B:166:HIS:C    | 2:B:187:THR:HG22 | 2.32                     | 0.50              |
| 2:B:55:PHE:CD1   | 2:B:55:PHE:N     | 2.79                     | 0.50              |
| 5:L:75:GLU:HB2   | 5:L:87:LEU:HD11  | 1.94                     | 0.50              |
| 1:A:118:ILE:HG23 | 1:A:119:LEU:N    | 2.27                     | 0.50              |
| 4:K:18:MET:CE    | 5:L:55:THR:HG21  | 2.41                     | 0.50              |
| 1:G:95:ASN:O     | 1:G:174:ASN:HB2  | 2.12                     | 0.50              |
| 1:G:9:ARG:NH2    | 1:G:205:GLN:HB3  | 2.27                     | 0.50              |
| 3:I:52:TRP:H     | 3:I:66:ALA:HB3   | 1.77                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:82:LEU:HD23  | 4:D:97:LEU:HD23  | 1.94                     | 0.49              |
| 3:I:150:ARG:HG3  | 3:I:151:ARG:H    | 1.76                     | 0.49              |
| 5:F:39:ARG:HB3   | 5:F:83:PRO:HG3   | 1.94                     | 0.49              |
| 3:I:32:VAL:O     | 3:I:36:ARG:HB2   | 2.12                     | 0.49              |
| 4:J:80:MET:HE2   | 4:J:82:LEU:HD21  | 1.94                     | 0.49              |
| 3:I:193:ASN:N    | 3:I:198:ILE:HB   | 2.25                     | 0.49              |
| 1:A:90:GLU:HG2   | 1:A:142:ARG:NH1  | 2.28                     | 0.49              |
| 4:E:9:THR:CG2    | 4:E:10:ASN:N     | 2.75                     | 0.49              |
| 1:G:111:TYR:O    | 1:G:182:ARG:NH2  | 2.46                     | 0.49              |
| 3:C:194:PRO:HG2  | 3:C:195:ALA:H    | 1.77                     | 0.49              |
| 4:D:93:PRO:HB3   | 2:H:52:TRP:CG    | 2.48                     | 0.49              |
| 3:I:91:ILE:HG23  | 3:I:91:ILE:O     | 2.12                     | 0.49              |
| 5:L:11:THR:O     | 5:L:30:ALA:HA    | 2.12                     | 0.49              |
| 3:C:21:GLY:O     | 4:E:5:VAL:HG21   | 2.12                     | 0.49              |
| 3:I:107:THR:O    | 3:I:123:PHE:HA   | 2.13                     | 0.49              |
| 2:B:5:ILE:CG2    | 2:B:6:VAL:N      | 2.75                     | 0.49              |
| 1:G:85:ILE:HA    | 1:G:147:VAL:O    | 2.13                     | 0.49              |
| 3:I:123:PHE:HE2  | 3:I:133:ALA:HB3  | 1.76                     | 0.49              |
| 4:K:5:VAL:HG12   | 4:K:6:LEU:O      | 2.12                     | 0.49              |
| 5:L:70:ILE:CD1   | 5:L:72:LEU:HD22  | 2.43                     | 0.49              |
| 1:A:92:ARG:HB3   | 1:A:140:ASN:ND2  | 2.25                     | 0.49              |
| 4:E:64:MET:HE2   | 4:E:100:MET:CE   | 2.43                     | 0.49              |
| 2:H:147:SER:O    | 2:H:151:LYS:HE2  | 2.12                     | 0.49              |
| 4:K:14:THR:O     | 5:L:93:PRO:HG3   | 2.13                     | 0.49              |
| 4:D:28:MET:HG2   | 4:D:56:LEU:HD21  | 1.94                     | 0.49              |
| 5:F:2:LEU:O      | 5:F:4:THR:N      | 2.46                     | 0.49              |
| 3:I:78:ALA:C     | 3:I:80:PHE:H     | 2.16                     | 0.49              |
| 3:I:77:GLY:O     | 3:I:80:PHE:HB2   | 2.13                     | 0.49              |
| 1:A:96:ASN:OD1   | 1:A:133:HIS:HB3  | 2.13                     | 0.49              |
| 2:B:52:TRP:CD2   | 4:J:93:PRO:HB3   | 2.47                     | 0.49              |
| 4:D:26:THR:O     | 4:D:27:ARG:HG2   | 2.13                     | 0.49              |
| 5:F:56:MET:CE    | 5:F:86:LEU:HD21  | 2.41                     | 0.49              |
| 4:K:107:GLN:H    | 4:K:107:GLN:CD   | 2.17                     | 0.49              |
| 1:A:26:TRP:CE3   | 1:A:46:SER:HB3   | 2.48                     | 0.48              |
| 1:G:100:ALA:HA   | 1:G:131:LEU:HD11 | 1.95                     | 0.48              |
| 2:H:112:LEU:HD21 | 2:H:175:ASP:HB3  | 1.94                     | 0.48              |
| 2:H:52:TRP:C     | 2:H:67:TYR:HE2   | 2.16                     | 0.48              |
| 3:I:92:TYR:HB2   | 3:I:174:TYR:HE2  | 1.79                     | 0.48              |
| 3:I:177:GLU:CD   | 4:K:79:ARG:HH22  | 2.17                     | 0.48              |
| 3:C:150:ARG:HG3  | 3:C:151:ARG:N    | 2.28                     | 0.48              |
| 4:D:64:MET:CE    | 4:D:97:LEU:HD13  | 2.43                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:25:ASN:HD21  | 3:I:115:THR:HB   | 1.78                     | 0.48              |
| 4:K:32:GLY:C     | 4:K:33:ILE:HD12  | 2.34                     | 0.48              |
| 4:D:87:LEU:O     | 4:D:94:ALA:N     | 2.40                     | 0.48              |
| 4:J:86:GLN:HA    | 4:J:94:ALA:O     | 2.14                     | 0.48              |
| 2:B:15:GLN:HG3   | 2:B:16:HIS:H     | 1.78                     | 0.48              |
| 2:B:52:TRP:HE1   | 4:J:88:THR:HG23  | 1.78                     | 0.48              |
| 3:C:49:THR:HG23  | 3:C:55:TYR:HE2   | 1.78                     | 0.48              |
| 2:B:118:ARG:HG3  | 2:B:120:CYS:SG   | 2.53                     | 0.48              |
| 2:H:63:LEU:HD13  | 2:H:70:VAL:HB    | 1.96                     | 0.48              |
| 1:A:224:VAL:HG12 | 1:A:224:VAL:O    | 2.12                     | 0.48              |
| 3:I:104:SER:HA   | 3:I:164:ARG:HA   | 1.96                     | 0.48              |
| 3:I:115:THR:HG22 | 3:I:116:ASN:N    | 2.28                     | 0.48              |
| 3:I:9:PRO:HD2    | 3:I:12:LEU:HD11  | 1.95                     | 0.48              |
| 4:E:2:VAL:HG12   | 4:E:4:TYR:H      | 1.78                     | 0.47              |
| 1:A:50:PHE:HD1   | 1:A:131:LEU:HB3  | 1.75                     | 0.47              |
| 1:A:111:TYR:HD2  | 1:A:182:ARG:HB2  | 1.76                     | 0.47              |
| 2:B:168:SER:OG   | 2:B:170:GLU:HG3  | 2.14                     | 0.47              |
| 3:C:73:ASP:O     | 3:C:74:ALA:HB2   | 2.14                     | 0.47              |
| 2:H:149:LEU:HD22 | 2:H:186:LEU:HD13 | 1.95                     | 0.47              |
| 4:E:26:THR:HB    | 4:E:57:LYS:NZ    | 2.30                     | 0.47              |
| 2:H:193:ASN:O    | 2:H:196:SER:HB3  | 2.13                     | 0.47              |
| 2:H:25:ASN:O     | 2:H:26:LYS:HB2   | 2.14                     | 0.47              |
| 4:K:98:ILE:O     | 4:K:99:ARG:HB2   | 2.14                     | 0.47              |
| 1:A:8:TYR:N      | 1:A:8:TYR:CD1    | 2.83                     | 0.47              |
| 4:K:51:CYS:HB2   | 4:K:87:LEU:HD23  | 1.97                     | 0.47              |
| 5:L:73:THR:HB    | 5:L:88:GLU:HB3   | 1.96                     | 0.47              |
| 4:E:107:GLN:H    | 4:E:107:GLN:CD   | 2.17                     | 0.47              |
| 5:F:32:MET:HE1   | 5:F:35:ARG:NH1   | 2.29                     | 0.47              |
| 1:G:149:HIS:CD2  | 1:G:151:GLY:HA2  | 2.49                     | 0.47              |
| 5:L:56:MET:HE2   | 5:L:86:LEU:HD21  | 1.96                     | 0.47              |
| 1:A:94:ASP:O     | 1:A:173:ALA:HA   | 2.13                     | 0.47              |
| 3:C:25:ASN:ND2   | 3:C:115:THR:CB   | 2.77                     | 0.47              |
| 1:G:31:ASN:HD22  | 1:G:34:GLU:CG    | 2.16                     | 0.47              |
| 2:H:145:MET:HG2  | 5:L:24:GLN:CD    | 2.34                     | 0.47              |
| 4:K:12:VAL:HG13  | 4:K:37:LEU:HG    | 1.96                     | 0.47              |
| 2:B:164:ARG:CZ   | 2:B:199:CYS:HB3  | 2.44                     | 0.47              |
| 1:G:87:TYR:N     | 1:G:87:TYR:CD1   | 2.81                     | 0.47              |
| 2:H:148:ARG:N    | 2:H:148:ARG:HD2  | 2.27                     | 0.47              |
| 3:I:133:ALA:HB1  | 3:I:186:LEU:HB2  | 1.96                     | 0.47              |
| 2:H:108:ALA:HB2  | 2:H:123:PHE:CE2  | 2.49                     | 0.47              |
| 3:I:111:LEU:HG   | 3:I:157:TYR:CE1  | 2.50                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:J:16:VAL:O     | 4:J:17:ALA:HB2   | 2.13                     | 0.47              |
| 4:K:57:LYS:HG3   | 5:L:49:HIS:NE2   | 2.30                     | 0.47              |
| 5:L:75:GLU:HG2   | 5:L:76:ASP:N     | 2.29                     | 0.47              |
| 3:C:152:LEU:O    | 3:C:156:ILE:HG12 | 2.15                     | 0.47              |
| 4:D:43:SER:HA    | 4:D:44:PRO:HD3   | 1.77                     | 0.47              |
| 3:I:32:VAL:HG12  | 3:I:57:LEU:HD23  | 1.97                     | 0.47              |
| 4:K:24:THR:HA    | 4:K:25:PRO:HD2   | 1.81                     | 0.47              |
| 5:L:29:THR:HG23  | 5:L:37:LEU:HB3   | 1.97                     | 0.47              |
| 3:C:107:THR:O    | 3:C:123:PHE:HA   | 2.15                     | 0.46              |
| 1:G:92:ARG:CZ    | 1:G:140:ASN:ND2  | 2.78                     | 0.46              |
| 2:B:41:LEU:HD12  | 2:B:41:LEU:HA    | 1.80                     | 0.46              |
| 1:G:2:ASP:HB3    | 1:G:172:ARG:NH1  | 2.30                     | 0.46              |
| 5:L:57:LEU:HD22  | 5:L:61:ILE:CD1   | 2.44                     | 0.46              |
| 5:L:75:GLU:CG    | 5:L:76:ASP:H     | 2.27                     | 0.46              |
| 1:A:50:PHE:HZ    | 1:A:178:TYR:CD2  | 2.33                     | 0.46              |
| 1:G:32:VAL:O     | 1:G:36:LEU:HD13  | 2.15                     | 0.46              |
| 2:H:51:GLY:O     | 2:H:65:GLY:HA3   | 2.14                     | 0.46              |
| 3:C:167:VAL:HG22 | 3:C:184:TYR:HB2  | 1.96                     | 0.46              |
| 5:F:35:ARG:HB2   | 5:F:36:SER:H     | 1.46                     | 0.46              |
| 4:E:99:ARG:O     | 4:E:100:MET:HB3  | 2.16                     | 0.46              |
| 5:F:7:TYR:HB2    | 5:F:72:LEU:CD2   | 2.46                     | 0.46              |
| 3:C:60:GLY:HA3   | 3:C:72:LYS:O     | 2.16                     | 0.46              |
| 5:F:78:PRO:HG2   | 5:F:79:TYR:CE2   | 2.51                     | 0.46              |
| 1:G:8:TYR:CD1    | 1:G:8:TYR:N      | 2.84                     | 0.46              |
| 5:L:7:TYR:HE1    | 5:L:74:VAL:HG22  | 1.81                     | 0.46              |
| 5:F:57:LEU:O     | 5:F:61:ILE:HG13  | 2.16                     | 0.46              |
| 3:I:154:TYR:CE1  | 3:I:158:MET:HG3  | 2.51                     | 0.46              |
| 3:C:13:PHE:CD2   | 3:C:41:LEU:HD21  | 2.52                     | 0.46              |
| 1:G:19:PHE:HZ    | 1:G:144:VAL:HG12 | 1.81                     | 0.46              |
| 4:K:18:MET:HE1   | 5:L:55:THR:HG21  | 1.91                     | 0.46              |
| 5:L:14:GLU:O     | 5:L:28:LEU:HA    | 2.16                     | 0.45              |
| 5:F:69:ARG:HH11  | 5:F:69:ARG:HG3   | 1.81                     | 0.45              |
| 1:G:200:ALA:O    | 1:G:204:ARG:HB2  | 2.16                     | 0.45              |
| 3:I:45:LEU:HA    | 3:I:48:ILE:HG22  | 1.98                     | 0.45              |
| 3:I:63:LEU:O     | 3:I:69:GLY:HA2   | 2.16                     | 0.45              |
| 3:I:12:LEU:HD22  | 3:I:89:THR:O     | 2.17                     | 0.45              |
| 2:B:145:MET:HB3  | 2:B:149:LEU:CD1  | 2.43                     | 0.45              |
| 2:B:52:TRP:O     | 2:B:67:TYR:HE2   | 2.00                     | 0.45              |
| 4:J:87:LEU:O     | 4:J:94:ALA:N     | 2.50                     | 0.45              |
| 3:C:28:ARG:NH1   | 3:C:177:GLU:HA   | 2.31                     | 0.45              |
| 4:E:97:LEU:HD11  | 4:E:100:MET:SD   | 2.55                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:E:17:ALA:N     | 4:E:31:CYS:O     | 2.49                     | 0.45              |
| 4:E:40:ALA:C     | 4:E:42:SER:N     | 2.68                     | 0.45              |
| 4:J:64:MET:HE1   | 4:J:97:LEU:HD13  | 1.98                     | 0.45              |
| 5:L:26:PHE:CE1   | 5:L:42:LEU:HB3   | 2.52                     | 0.45              |
| 5:L:53:PHE:O     | 5:L:57:LEU:HB2   | 2.16                     | 0.45              |
| 1:A:25:ALA:HB1   | 1:A:48:SER:O     | 2.16                     | 0.45              |
| 2:B:131:ILE:HG13 | 2:B:132:GLY:H    | 1.82                     | 0.45              |
| 2:B:90:THR:O     | 2:B:173:TYR:HA   | 2.16                     | 0.45              |
| 3:C:52:TRP:H     | 3:C:66:ALA:HB3   | 1.82                     | 0.45              |
| 1:G:6:THR:HA     | 1:G:91:VAL:O     | 2.17                     | 0.45              |
| 2:B:155:LEU:HD22 | 5:F:61:ILE:HG23  | 1.99                     | 0.45              |
| 1:G:110:THR:HB   | 1:G:111:TYR:CD1  | 2.52                     | 0.45              |
| 3:I:28:ARG:NH2   | 3:I:34:GLU:OE1   | 2.50                     | 0.45              |
| 1:A:191:LEU:HA   | 1:A:191:LEU:HD23 | 1.71                     | 0.45              |
| 2:B:156:ILE:HD11 | 2:B:189:ILE:HD13 | 1.98                     | 0.45              |
| 5:F:49:HIS:O     | 5:F:51:THR:N     | 2.50                     | 0.45              |
| 1:A:27:GLY:O     | 1:A:49:ALA:HA    | 2.17                     | 0.45              |
| 2:H:193:ASN:HB2  | 5:L:14:GLU:CD    | 2.37                     | 0.45              |
| 1:A:68:MET:HB2   | 1:A:84:PHE:CE2   | 2.52                     | 0.44              |
| 3:C:141:ARG:HB3  | 3:C:142:TYR:CD1  | 2.52                     | 0.44              |
| 2:H:145:MET:HB2  | 2:H:149:LEU:HD12 | 1.98                     | 0.44              |
| 3:I:118:ARG:HG3  | 3:I:120:CYS:SG   | 2.57                     | 0.44              |
| 2:B:131:ILE:HD12 | 2:B:131:ILE:HA   | 1.85                     | 0.44              |
| 4:E:64:MET:CE    | 4:E:100:MET:HE2  | 2.45                     | 0.44              |
| 5:F:75:GLU:N     | 5:F:87:LEU:HD11  | 2.32                     | 0.44              |
| 3:I:153:LEU:HA   | 3:I:153:LEU:HD23 | 1.76                     | 0.44              |
| 4:J:28:MET:SD    | 4:J:56:LEU:HD21  | 2.57                     | 0.44              |
| 3:C:28:ARG:CZ    | 3:C:88:ILE:HD11  | 2.47                     | 0.44              |
| 2:H:52:TRP:CH2   | 2:H:66:GLU:HB3   | 2.52                     | 0.44              |
| 2:H:79:ALA:C     | 2:H:81:ASP:H     | 2.19                     | 0.44              |
| 4:J:11:MET:SD    | 4:J:36:LYS:HB2   | 2.58                     | 0.44              |
| 4:K:64:MET:HE1   | 4:K:100:MET:HG2  | 1.99                     | 0.44              |
| 1:A:149:HIS:CD2  | 1:A:151:GLY:HA2  | 2.53                     | 0.44              |
| 1:A:111:TYR:CD1  | 1:A:111:TYR:N    | 2.86                     | 0.44              |
| 4:E:40:ALA:O     | 4:E:42:SER:N     | 2.50                     | 0.44              |
| 1:G:102:SER:HB3  | 1:G:177:PRO:HG3  | 2.00                     | 0.44              |
| 2:H:7:ILE:HA     | 2:H:8:PRO:HD3    | 1.85                     | 0.44              |
| 3:I:31:THR:HG21  | 3:I:177:GLU:HB2  | 2.00                     | 0.44              |
| 3:I:35:LEU:HD13  | 3:I:41:LEU:HD13  | 1.99                     | 0.44              |
| 5:L:88:GLU:HG2   | 5:L:89:LEU:N     | 2.32                     | 0.44              |
| 3:C:167:VAL:CG2  | 3:C:184:TYR:HB2  | 2.47                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:34:GLU:HG3   | 3:C:178:ASP:OD1  | 2.18                     | 0.44              |
| 5:L:74:VAL:O     | 5:L:74:VAL:HG23  | 2.18                     | 0.44              |
| 2:B:56:ALA:O     | 2:B:85:THR:HA    | 2.18                     | 0.44              |
| 3:C:118:ARG:H    | 3:C:118:ARG:HG2  | 1.57                     | 0.44              |
| 4:D:92:LYS:HB3   | 4:D:93:PRO:HD2   | 1.98                     | 0.44              |
| 4:E:24:THR:HA    | 4:E:25:PRO:HD2   | 1.82                     | 0.44              |
| 1:G:144:VAL:HG22 | 1:G:145:THR:N    | 2.33                     | 0.44              |
| 1:G:25:ALA:HB1   | 1:G:49:ALA:HA    | 1.98                     | 0.44              |
| 4:J:37:LEU:H     | 4:J:37:LEU:CD1   | 2.31                     | 0.44              |
| 4:J:81:PHE:CD1   | 4:J:81:PHE:N     | 2.85                     | 0.44              |
| 4:E:40:ALA:C     | 4:E:42:SER:H     | 2.21                     | 0.44              |
| 4:E:76:ARG:HA    | 4:E:77:PRO:HD3   | 1.71                     | 0.44              |
| 5:F:40:ALA:HA    | 5:F:84:GLY:O     | 2.18                     | 0.44              |
| 2:H:133:ALA:HA   | 2:H:184:TYR:O    | 2.17                     | 0.44              |
| 1:A:142:ARG:HB2  | 1:A:166:TYR:CE1  | 2.53                     | 0.43              |
| 2:B:35:LEU:HD12  | 2:B:41:LEU:HB3   | 2.00                     | 0.43              |
| 4:K:18:MET:HE2   | 5:L:55:THR:HG22  | 1.99                     | 0.43              |
| 1:A:13:ARG:HH11  | 1:A:13:ARG:HG3   | 1.83                     | 0.43              |
| 4:D:75:GLN:NE2   | 4:D:75:GLN:HA    | 2.33                     | 0.43              |
| 4:K:8:LYS:HG2    | 4:K:82:LEU:HD12  | 1.99                     | 0.43              |
| 4:K:15:SER:OG    | 5:L:93:PRO:HD3   | 2.17                     | 0.43              |
| 2:B:133:ALA:HA   | 2:B:184:TYR:O    | 2.19                     | 0.43              |
| 4:J:10:ASN:ND2   | 4:J:109:CYS:HB3  | 2.33                     | 0.43              |
| 5:L:94:LEU:O     | 5:L:95:ASN:HB2   | 2.19                     | 0.43              |
| 1:A:34:GLU:HA    | 1:A:37:THR:HG22  | 2.00                     | 0.43              |
| 4:D:11:MET:O     | 4:D:78:LEU:N     | 2.48                     | 0.43              |
| 4:E:18:MET:HE2   | 4:E:18:MET:HB3   | 1.84                     | 0.43              |
| 3:I:78:ALA:O     | 3:I:80:PHE:N     | 2.51                     | 0.43              |
| 5:L:10:PHE:O     | 5:L:70:ILE:HG12  | 2.19                     | 0.43              |
| 4:D:24:THR:HA    | 4:D:25:PRO:HD3   | 1.70                     | 0.43              |
| 5:F:4:THR:HG22   | 5:F:5:HIS:H      | 1.84                     | 0.43              |
| 1:A:20:GLN:HB2   | 1:A:21:ASN:OD1   | 2.19                     | 0.43              |
| 3:C:177:GLU:CD   | 4:E:79:ARG:HH22  | 2.21                     | 0.43              |
| 4:E:92:LYS:HB3   | 4:E:93:PRO:HD2   | 2.00                     | 0.43              |
| 1:G:92:ARG:CZ    | 1:G:140:ASN:HD21 | 2.31                     | 0.43              |
| 2:H:38:SER:OG    | 2:H:41:LEU:HB2   | 2.17                     | 0.43              |
| 2:B:193:ASN:HB2  | 5:F:14:GLU:OE1   | 2.19                     | 0.43              |
| 2:B:79:ALA:C     | 2:B:81:ASP:H     | 2.21                     | 0.43              |
| 4:D:8:LYS:HG3    | 4:D:82:LEU:HD12  | 2.00                     | 0.43              |
| 4:D:85:LYS:HB3   | 4:D:85:LYS:HE3   | 1.67                     | 0.43              |
| 2:H:119:LEU:O    | 2:H:134:CYS:HA   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:107:THR:HG22 | 3:I:108:ALA:N    | 2.34                     | 0.43              |
| 3:C:111:LEU:HG   | 3:C:157:TYR:CE2  | 2.54                     | 0.43              |
| 4:D:11:MET:SD    | 4:D:36:LYS:HB2   | 2.59                     | 0.43              |
| 2:H:5:ILE:HG22   | 2:H:7:ILE:CD1    | 2.48                     | 0.43              |
| 4:K:21:TYR:HB3   | 4:K:24:THR:O     | 2.19                     | 0.43              |
| 3:C:141:ARG:HG2  | 3:C:142:TYR:CE1  | 2.54                     | 0.43              |
| 2:H:32:VAL:HG12  | 2:H:33:ALA:N     | 2.33                     | 0.43              |
| 5:L:40:ALA:HA    | 5:L:84:GLY:O     | 2.19                     | 0.43              |
| 3:C:198:ILE:HD12 | 4:D:90:GLU:HG3   | 1.99                     | 0.42              |
| 4:D:28:MET:SD    | 4:D:56:LEU:HD21  | 2.59                     | 0.42              |
| 4:E:26:THR:O     | 4:E:56:LEU:HB2   | 2.19                     | 0.42              |
| 1:G:13:ARG:O     | 1:G:89:TYR:OH    | 2.30                     | 0.42              |
| 3:I:181:PHE:CD1  | 3:I:181:PHE:C    | 2.92                     | 0.42              |
| 3:I:167:VAL:CG2  | 3:I:184:TYR:HB2  | 2.49                     | 0.42              |
| 3:I:32:VAL:HG12  | 3:I:57:LEU:CD2   | 2.49                     | 0.42              |
| 4:J:104:SER:HB3  | 4:J:108:ASP:OD1  | 2.19                     | 0.42              |
| 4:K:21:TYR:N     | 4:K:28:MET:HA    | 2.33                     | 0.42              |
| 2:H:131:ILE:HG13 | 2:H:132:GLY:H    | 1.84                     | 0.42              |
| 3:I:12:LEU:HD11  | 3:I:174:TYR:CE2  | 2.54                     | 0.42              |
| 3:I:45:LEU:HD12  | 3:I:45:LEU:HA    | 1.66                     | 0.42              |
| 4:E:107:GLN:CD   | 4:E:107:GLN:N    | 2.72                     | 0.42              |
| 1:G:176:ASN:HA   | 1:G:177:PRO:HD3  | 1.83                     | 0.42              |
| 1:G:195:ALA:HB2  | 5:L:94:LEU:HD12  | 2.01                     | 0.42              |
| 5:L:35:ARG:HB2   | 5:L:36:SER:H     | 1.54                     | 0.42              |
| 1:A:3:PRO:HB3    | 1:A:173:ALA:HB3  | 2.01                     | 0.42              |
| 2:B:75:THR:CG2   | 2:B:76:PRO:HD2   | 2.48                     | 0.42              |
| 3:C:186:LEU:HD21 | 3:C:189:ILE:HD11 | 2.01                     | 0.42              |
| 4:D:10:ASN:O     | 4:D:36:LYS:HA    | 2.19                     | 0.42              |
| 2:H:31:THR:OG1   | 2:H:34:GLU:HB2   | 2.20                     | 0.42              |
| 3:I:142:TYR:CE2  | 3:I:187:THR:HG22 | 2.54                     | 0.42              |
| 4:K:76:ARG:HD2   | 4:K:102:GLU:OE2  | 2.19                     | 0.42              |
| 2:B:15:GLN:HG3   | 2:B:16:HIS:N     | 2.34                     | 0.42              |
| 3:C:19:ALA:HA    | 3:C:83:ARG:O     | 2.20                     | 0.42              |
| 3:C:60:GLY:HA2   | 3:C:74:ALA:CB    | 2.47                     | 0.42              |
| 4:D:11:MET:O     | 4:D:77:PRO:HA    | 2.20                     | 0.42              |
| 1:G:152:ILE:HA   | 4:K:41:ALA:HB3   | 2.02                     | 0.42              |
| 1:G:18:VAL:HG11  | 1:G:89:TYR:CE2   | 2.54                     | 0.42              |
| 1:G:193:ARG:O    | 1:G:197:VAL:HA   | 2.20                     | 0.42              |
| 2:H:5:ILE:CG2    | 2:H:6:VAL:N      | 2.81                     | 0.42              |
| 3:I:162:ALA:O    | 3:I:163:VAL:HG23 | 2.19                     | 0.42              |
| 4:J:10:ASN:HB3   | 4:J:37:LEU:HD13  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 4:K:28:MET:SD    | 4:K:56:LEU:HD21 | 2.60                     | 0.42              |
| 2:B:147:SER:O    | 2:B:151:LYS:HG3 | 2.20                     | 0.42              |
| 3:I:194:PRO:C    | 3:I:196:ALA:H   | 2.22                     | 0.42              |
| 1:A:95:ASN:C     | 1:A:97:PHE:H    | 2.23                     | 0.42              |
| 4:E:74:GLN:O     | 4:E:75:GLN:HB2  | 2.20                     | 0.42              |
| 3:I:142:TYR:HD1  | 3:I:142:TYR:N   | 2.15                     | 0.42              |
| 3:I:193:ASN:HA   | 3:I:194:PRO:HD2 | 1.90                     | 0.42              |
| 4:J:50:PHE:CD1   | 4:J:50:PHE:N    | 2.86                     | 0.42              |
| 5:F:11:THR:O     | 5:F:30:ALA:HA   | 2.20                     | 0.42              |
| 1:G:117:ARG:HD3  | 1:G:117:ARG:HA  | 1.89                     | 0.42              |
| 4:J:82:LEU:HB3   | 4:J:95:LEU:HB3  | 2.01                     | 0.42              |
| 1:A:54:SER:CB    | 1:A:202:MET:CE  | 2.92                     | 0.42              |
| 3:C:25:ASN:HD21  | 3:C:115:THR:CB  | 2.29                     | 0.42              |
| 1:G:87:TYR:HB2   | 1:G:89:TYR:CE1  | 2.55                     | 0.42              |
| 3:I:131:ILE:HG13 | 3:I:132:GLY:H   | 1.85                     | 0.42              |
| 5:L:4:THR:HG22   | 5:L:5:HIS:N     | 2.35                     | 0.42              |
| 2:B:106:VAL:HB   | 2:B:123:PHE:HB3 | 2.00                     | 0.42              |
| 2:B:182:GLU:HB3  | 2:B:184:TYR:CE2 | 2.55                     | 0.42              |
| 2:B:46:ARG:HH11  | 2:B:46:ARG:HG3  | 1.85                     | 0.42              |
| 4:E:2:VAL:HG13   | 4:E:3:PRO:HD2   | 2.02                     | 0.42              |
| 3:C:45:LEU:HA    | 3:C:45:LEU:HD12 | 1.72                     | 0.41              |
| 5:F:10:PHE:CE1   | 5:F:32:MET:CB   | 3.01                     | 0.41              |
| 1:G:13:ARG:HH11  | 1:G:13:ARG:HG3  | 1.85                     | 0.41              |
| 2:H:41:LEU:HD12  | 2:H:41:LEU:HA   | 1.94                     | 0.41              |
| 4:J:51:CYS:SG    | 4:J:89:PHE:HB2  | 2.59                     | 0.41              |
| 4:J:40:ALA:O     | 4:J:46:ALA:HB2  | 2.19                     | 0.41              |
| 1:A:225:LEU:HD23 | 1:A:225:LEU:HA  | 1.86                     | 0.41              |
| 1:A:32:VAL:HG12  | 1:A:32:VAL:O    | 2.21                     | 0.41              |
| 2:B:118:ARG:NH1  | 2:B:173:TYR:CE1 | 2.89                     | 0.41              |
| 2:B:83:LYS:HE3   | 4:J:2:VAL:O     | 2.20                     | 0.41              |
| 2:H:103:TYR:N    | 2:H:103:TYR:CD1 | 2.88                     | 0.41              |
| 2:H:106:VAL:HA   | 2:H:124:VAL:O   | 2.20                     | 0.41              |
| 5:L:50:ASP:C     | 5:L:52:TRP:N    | 2.72                     | 0.41              |
| 1:A:69:GLN:HE21  | 4:E:38:GLY:H    | 1.67                     | 0.41              |
| 2:B:38:SER:CB    | 2:B:41:LEU:HB2  | 2.51                     | 0.41              |
| 3:C:25:ASN:ND2   | 3:C:115:THR:CG2 | 2.84                     | 0.41              |
| 3:C:194:PRO:C    | 3:C:196:ALA:H   | 2.24                     | 0.41              |
| 3:C:20:TYR:CD1   | 3:C:83:ARG:HA   | 2.55                     | 0.41              |
| 2:H:15:GLN:HG3   | 2:H:16:HIS:N    | 2.36                     | 0.41              |
| 3:I:55:TYR:HD1   | 3:I:84:GLU:HB3  | 1.84                     | 0.41              |
| 4:K:85:LYS:H     | 4:K:85:LYS:HD3  | 1.84                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:L:59:PHE:CE2   | 5:L:91:ILE:HG13  | 2.55                     | 0.41              |
| 5:L:74:VAL:O     | 5:L:74:VAL:CG2   | 2.69                     | 0.41              |
| 1:A:100:ALA:HA   | 1:A:131:LEU:HD11 | 2.02                     | 0.41              |
| 3:C:21:GLY:C     | 4:E:5:VAL:HG21   | 2.41                     | 0.41              |
| 3:I:168:SER:C    | 3:I:170:GLU:H    | 2.24                     | 0.41              |
| 2:B:52:TRP:CD1   | 4:J:93:PRO:HB3   | 2.54                     | 0.41              |
| 4:K:87:LEU:O     | 4:K:94:ALA:N     | 2.53                     | 0.41              |
| 5:L:39:ARG:HB3   | 5:L:83:PRO:CG    | 2.50                     | 0.41              |
| 3:C:56:GLY:C     | 3:C:57:LEU:HD12  | 2.41                     | 0.41              |
| 2:H:175:ASP:O    | 4:J:99:ARG:NH2   | 2.54                     | 0.41              |
| 1:A:50:PHE:HZ    | 1:A:178:TYR:CE2  | 2.39                     | 0.41              |
| 1:A:35:HIS:ND1   | 1:A:50:PHE:HB2   | 2.35                     | 0.41              |
| 3:C:28:ARG:HD2   | 3:C:175:ASP:O    | 2.21                     | 0.41              |
| 1:G:110:THR:CG2  | 1:G:111:TYR:CE1  | 3.04                     | 0.41              |
| 1:G:152:ILE:HD12 | 1:G:152:ILE:N    | 2.26                     | 0.41              |
| 1:G:37:THR:HG21  | 1:G:187:ILE:HD13 | 2.02                     | 0.41              |
| 5:L:97:TYR:CD1   | 5:L:97:TYR:N     | 2.88                     | 0.41              |
| 2:B:152:MET:O    | 2:B:156:ILE:HG12 | 2.21                     | 0.41              |
| 3:C:125:ARG:O    | 3:C:128:GLN:HG2  | 2.20                     | 0.41              |
| 3:C:63:LEU:CD1   | 3:C:70:ILE:HB    | 2.48                     | 0.41              |
| 5:F:26:PHE:HE1   | 5:F:42:LEU:HD12  | 1.85                     | 0.41              |
| 1:G:119:LEU:HD12 | 1:G:119:LEU:HA   | 1.81                     | 0.41              |
| 1:G:146:ARG:HB3  | 1:G:159:THR:OG1  | 2.21                     | 0.41              |
| 1:G:98:TYR:CE2   | 1:G:174:ASN:ND2  | 2.89                     | 0.41              |
| 3:I:125:ARG:HB2  | 3:I:130:VAL:HG21 | 2.03                     | 0.41              |
| 4:K:107:GLN:N    | 4:K:107:GLN:CD   | 2.74                     | 0.41              |
| 1:A:160:GLU:C    | 1:A:161:TYR:CD1  | 2.94                     | 0.41              |
| 1:A:193:ARG:HH11 | 1:A:223:MET:HG3  | 1.86                     | 0.41              |
| 4:E:2:VAL:HG21   | 4:E:95:LEU:HD21  | 2.03                     | 0.41              |
| 5:F:79:TYR:O     | 5:F:82:THR:HB    | 2.21                     | 0.41              |
| 2:H:131:ILE:HD11 | 2:H:184:TYR:CD2  | 2.56                     | 0.41              |
| 4:K:40:ALA:O     | 4:K:42:SER:N     | 2.54                     | 0.41              |
| 4:E:19:LYS:CG    | 4:E:29:LEU:HB2   | 2.51                     | 0.41              |
| 1:G:127:GLN:O    | 1:G:128:SER:C    | 2.60                     | 0.41              |
| 3:C:124:VAL:HG13 | 3:C:128:GLN:O    | 2.21                     | 0.40              |
| 4:E:104:SER:OG   | 4:E:108:ASP:OD1  | 2.39                     | 0.40              |
| 4:E:64:MET:HB3   | 4:E:64:MET:HE2   | 1.76                     | 0.40              |
| 1:G:149:HIS:HE1  | 4:K:38:GLY:O     | 2.04                     | 0.40              |
| 5:L:51:THR:HG22  | 5:L:55:THR:OG1   | 2.21                     | 0.40              |
| 3:C:168:SER:C    | 3:C:170:GLU:H    | 2.24                     | 0.40              |
| 1:G:152:ILE:CD1  | 1:G:152:ILE:H    | 2.23                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:42:GLN:HB3   | 1:G:45:SER:HB3   | 2.04                     | 0.40              |
| 2:H:177:GLU:CD   | 4:J:79:ARG:NH2   | 2.74                     | 0.40              |
| 3:I:112:LEU:HD23 | 3:I:176:TYR:CD1  | 2.56                     | 0.40              |
| 3:I:131:ILE:HG13 | 3:I:132:GLY:N    | 2.37                     | 0.40              |
| 3:I:167:VAL:HG22 | 3:I:184:TYR:HB2  | 2.03                     | 0.40              |
| 5:L:79:TYR:HA    | 5:L:80:PRO:HD2   | 1.89                     | 0.40              |
| 2:B:7:ILE:HA     | 2:B:8:PRO:HD3    | 1.83                     | 0.40              |
| 4:D:2:VAL:HG12   | 4:D:84:PRO:HA    | 2.02                     | 0.40              |
| 4:E:73:MET:CE    | 5:F:66:LEU:HD11  | 2.51                     | 0.40              |
| 5:F:66:LEU:O     | 5:F:67:LYS:HB2   | 2.22                     | 0.40              |
| 1:G:67:ARG:HD2   | 1:G:67:ARG:HA    | 1.91                     | 0.40              |
| 2:H:104:SER:O    | 2:H:106:VAL:HG13 | 2.20                     | 0.40              |
| 3:I:108:ALA:HB2  | 3:I:123:PHE:CE1  | 2.56                     | 0.40              |
| 5:L:45:ALA:HB3   | 5:L:50:ASP:OD2   | 2.21                     | 0.40              |
| 2:B:193:ASN:HB2  | 5:F:14:GLU:CD    | 2.42                     | 0.40              |
| 5:F:78:PRO:HG2   | 5:F:79:TYR:CZ    | 2.56                     | 0.40              |
| 1:G:204:ARG:HA   | 1:G:223:MET:CE   | 2.51                     | 0.40              |
| 3:I:153:LEU:HD23 | 3:I:156:ILE:HD11 | 2.04                     | 0.40              |
| 5:L:26:PHE:HE1   | 5:L:42:LEU:HD13  | 1.86                     | 0.40              |
| 1:A:101:ALA:O    | 1:A:104:TYR:N    | 2.54                     | 0.40              |
| 4:D:58:ARG:HA    | 4:D:59:PRO:HD3   | 1.83                     | 0.40              |
| 3:I:48:ILE:HG13  | 3:I:48:ILE:O     | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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     | 220/234 (94%) | 197 (90%) | 20 (9%)  | 3 (1%)   | 13          | 41 |
| 1   | G     | 220/234 (94%) | 194 (88%) | 24 (11%) | 2 (1%)   | 20          | 54 |
| 2   | B     | 194/196 (99%) | 176 (91%) | 15 (8%)  | 3 (2%)   | 12          | 39 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2   | H     | 194/196 (99%)   | 173 (89%)  | 17 (9%)  | 4 (2%)   | 8           | 30  |
| 3   | C     | 194/196 (99%)   | 168 (87%)  | 21 (11%) | 5 (3%)   | 6           | 24  |
| 3   | I     | 194/196 (99%)   | 171 (88%)  | 18 (9%)  | 5 (3%)   | 6           | 24  |
| 4   | D     | 108/110 (98%)   | 99 (92%)   | 9 (8%)   | 0        | 100         | 100 |
| 4   | E     | 108/110 (98%)   | 95 (88%)   | 9 (8%)   | 4 (4%)   | 4           | 16  |
| 4   | J     | 108/110 (98%)   | 98 (91%)   | 10 (9%)  | 0        | 100         | 100 |
| 4   | K     | 108/110 (98%)   | 97 (90%)   | 5 (5%)   | 6 (6%)   | 2           | 6   |
| 5   | F     | 96/98 (98%)     | 83 (86%)   | 8 (8%)   | 5 (5%)   | 2           | 8   |
| 5   | L     | 96/98 (98%)     | 81 (84%)   | 11 (12%) | 4 (4%)   | 3           | 12  |
| All | All   | 1840/1888 (98%) | 1632 (89%) | 167 (9%) | 41 (2%)  | 8           | 29  |

All (41) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F     | 45  | ALA  |
| 5   | F     | 49  | HIS  |
| 5   | L     | 49  | HIS  |
| 5   | L     | 50  | ASP  |
| 2   | B     | 110 | ARG  |
| 3   | C     | 65  | GLN  |
| 4   | E     | 22  | GLU  |
| 5   | F     | 47  | HIS  |
| 5   | F     | 50  | ASP  |
| 1   | G     | 22  | GLY  |
| 1   | G     | 29  | ASN  |
| 2   | H     | 48  | VAL  |
| 2   | H     | 69  | GLY  |
| 3   | I     | 126 | ASP  |
| 4   | K     | 22  | GLU  |
| 4   | K     | 85  | LYS  |
| 2   | B     | 69  | GLY  |
| 3   | C     | 59  | ASP  |
| 4   | E     | 100 | MET  |
| 2   | H     | 24  | ALA  |
| 3   | I     | 98  | ALA  |
| 1   | A     | 135 | ARG  |
| 3   | C     | 195 | ALA  |
| 2   | H     | 110 | ARG  |
| 3   | I     | 59  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | L     | 45  | ALA  |
| 5   | L     | 75  | GLU  |
| 2   | B     | 194 | PRO  |
| 3   | C     | 60  | GLY  |
| 4   | E     | 39  | ALA  |
| 3   | I     | 195 | ALA  |
| 3   | I     | 17  | GLY  |
| 4   | K     | 99  | ARG  |
| 4   | E     | 23  | VAL  |
| 1   | A     | 22  | GLY  |
| 1   | A     | 118 | ILE  |
| 5   | F     | 3   | PRO  |
| 4   | K     | 7   | VAL  |
| 4   | K     | 23  | VAL  |
| 3   | C     | 74  | ALA  |
| 4   | K     | 84  | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A     | 185/190 (97%)  | 167 (90%) | 18 (10%) | 9           | 29 |
| 1   | G     | 185/190 (97%)  | 170 (92%) | 15 (8%)  | 14          | 38 |
| 2   | B     | 163/163 (100%) | 144 (88%) | 19 (12%) | 6           | 18 |
| 2   | H     | 163/163 (100%) | 140 (86%) | 23 (14%) | 4           | 12 |
| 3   | C     | 155/155 (100%) | 136 (88%) | 19 (12%) | 5           | 16 |
| 3   | I     | 155/155 (100%) | 139 (90%) | 16 (10%) | 8           | 25 |
| 4   | D     | 94/94 (100%)   | 87 (93%)  | 7 (7%)   | 16          | 42 |
| 4   | E     | 94/94 (100%)   | 85 (90%)  | 9 (10%)  | 10          | 29 |
| 4   | J     | 94/94 (100%)   | 88 (94%)  | 6 (6%)   | 20          | 50 |
| 4   | K     | 94/94 (100%)   | 86 (92%)  | 8 (8%)   | 12          | 35 |
| 5   | F     | 83/83 (100%)   | 70 (84%)  | 13 (16%) | 3           | 9  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 5   | L     | 83/83 (100%)    | 73 (88%)   | 10 (12%)  | 6           | 17 |
| All | All   | 1548/1558 (99%) | 1385 (90%) | 163 (10%) | 8           | 24 |

All (163) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 9   | ARG  |
| 1   | A     | 10  | TYR  |
| 1   | A     | 21  | ASN  |
| 1   | A     | 33  | LEU  |
| 1   | A     | 118 | ILE  |
| 1   | A     | 119 | LEU  |
| 1   | A     | 123 | LEU  |
| 1   | A     | 134 | ARG  |
| 1   | A     | 137 | PRO  |
| 1   | A     | 140 | ASN  |
| 1   | A     | 165 | ARG  |
| 1   | A     | 184 | VAL  |
| 1   | A     | 192 | VAL  |
| 1   | A     | 196 | PRO  |
| 1   | A     | 202 | MET  |
| 1   | A     | 226 | VAL  |
| 1   | A     | 228 | TYR  |
| 1   | A     | 231 | ILE  |
| 2   | B     | 20  | TYR  |
| 2   | B     | 22  | ARG  |
| 2   | B     | 28  | ARG  |
| 2   | B     | 41  | LEU  |
| 2   | B     | 61  | THR  |
| 2   | B     | 66  | GLU  |
| 2   | B     | 82  | LEU  |
| 2   | B     | 88  | ILE  |
| 2   | B     | 91  | THR  |
| 2   | B     | 129 | PRO  |
| 2   | B     | 150 | ARG  |
| 2   | B     | 164 | ARG  |
| 2   | B     | 172 | GLN  |
| 2   | B     | 186 | LEU  |
| 2   | B     | 187 | THR  |
| 2   | B     | 192 | CYS  |
| 2   | B     | 194 | PRO  |
| 2   | B     | 196 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 197 | SER  |
| 3   | C     | 15  | GLN  |
| 3   | C     | 22  | ARG  |
| 3   | C     | 28  | ARG  |
| 3   | C     | 36  | ARG  |
| 3   | C     | 41  | LEU  |
| 3   | C     | 45  | LEU  |
| 3   | C     | 65  | GLN  |
| 3   | C     | 112 | LEU  |
| 3   | C     | 115 | THR  |
| 3   | C     | 117 | SER  |
| 3   | C     | 118 | ARG  |
| 3   | C     | 119 | LEU  |
| 3   | C     | 143 | ARG  |
| 3   | C     | 150 | ARG  |
| 3   | C     | 153 | LEU  |
| 3   | C     | 163 | VAL  |
| 3   | C     | 167 | VAL  |
| 3   | C     | 177 | GLU  |
| 3   | C     | 193 | ASN  |
| 4   | D     | 6   | LEU  |
| 4   | D     | 21  | TYR  |
| 4   | D     | 26  | THR  |
| 4   | D     | 29  | LEU  |
| 4   | D     | 61  | SER  |
| 4   | D     | 88  | THR  |
| 4   | D     | 97  | LEU  |
| 4   | E     | 14  | THR  |
| 4   | E     | 16  | VAL  |
| 4   | E     | 18  | MET  |
| 4   | E     | 24  | THR  |
| 4   | E     | 43  | SER  |
| 4   | E     | 64  | MET  |
| 4   | E     | 78  | LEU  |
| 4   | E     | 87  | LEU  |
| 4   | E     | 97  | LEU  |
| 5   | F     | 11  | THR  |
| 5   | F     | 12  | VAL  |
| 5   | F     | 13  | GLN  |
| 5   | F     | 26  | PHE  |
| 5   | F     | 31  | PHE  |
| 5   | F     | 35  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F     | 42  | LEU  |
| 5   | F     | 57  | LEU  |
| 5   | F     | 74  | VAL  |
| 5   | F     | 79  | TYR  |
| 5   | F     | 83  | PRO  |
| 5   | F     | 87  | LEU  |
| 5   | F     | 93  | PRO  |
| 1   | G     | 21  | ASN  |
| 1   | G     | 33  | LEU  |
| 1   | G     | 60  | THR  |
| 1   | G     | 87  | TYR  |
| 1   | G     | 118 | ILE  |
| 1   | G     | 119 | LEU  |
| 1   | G     | 123 | LEU  |
| 1   | G     | 131 | LEU  |
| 1   | G     | 140 | ASN  |
| 1   | G     | 165 | ARG  |
| 1   | G     | 192 | VAL  |
| 1   | G     | 226 | VAL  |
| 1   | G     | 228 | TYR  |
| 1   | G     | 230 | SER  |
| 1   | G     | 231 | ILE  |
| 2   | H     | 5   | ILE  |
| 2   | H     | 20  | TYR  |
| 2   | H     | 22  | ARG  |
| 2   | H     | 28  | ARG  |
| 2   | H     | 41  | LEU  |
| 2   | H     | 61  | THR  |
| 2   | H     | 66  | GLU  |
| 2   | H     | 82  | LEU  |
| 2   | H     | 88  | ILE  |
| 2   | H     | 91  | THR  |
| 2   | H     | 118 | ARG  |
| 2   | H     | 129 | PRO  |
| 2   | H     | 135 | THR  |
| 2   | H     | 139 | ASP  |
| 2   | H     | 150 | ARG  |
| 2   | H     | 164 | ARG  |
| 2   | H     | 172 | GLN  |
| 2   | H     | 177 | GLU  |
| 2   | H     | 186 | LEU  |
| 2   | H     | 187 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 192 | CYS  |
| 2   | H     | 194 | PRO  |
| 2   | H     | 196 | SER  |
| 3   | I     | 15  | GLN  |
| 3   | I     | 22  | ARG  |
| 3   | I     | 41  | LEU  |
| 3   | I     | 45  | LEU  |
| 3   | I     | 61  | THR  |
| 3   | I     | 65  | GLN  |
| 3   | I     | 112 | LEU  |
| 3   | I     | 117 | SER  |
| 3   | I     | 118 | ARG  |
| 3   | I     | 142 | TYR  |
| 3   | I     | 143 | ARG  |
| 3   | I     | 150 | ARG  |
| 3   | I     | 153 | LEU  |
| 3   | I     | 163 | VAL  |
| 3   | I     | 177 | GLU  |
| 3   | I     | 193 | ASN  |
| 4   | J     | 2   | VAL  |
| 4   | J     | 10  | ASN  |
| 4   | J     | 26  | THR  |
| 4   | J     | 79  | ARG  |
| 4   | J     | 88  | THR  |
| 4   | J     | 97  | LEU  |
| 4   | K     | 14  | THR  |
| 4   | K     | 15  | SER  |
| 4   | K     | 16  | VAL  |
| 4   | K     | 24  | THR  |
| 4   | K     | 43  | SER  |
| 4   | K     | 64  | MET  |
| 4   | K     | 87  | LEU  |
| 4   | K     | 97  | LEU  |
| 5   | L     | 12  | VAL  |
| 5   | L     | 31  | PHE  |
| 5   | L     | 35  | ARG  |
| 5   | L     | 39  | ARG  |
| 5   | L     | 42  | LEU  |
| 5   | L     | 57  | LEU  |
| 5   | L     | 79  | TYR  |
| 5   | L     | 86  | LEU  |
| 5   | L     | 87  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | L     | 93  | PRO  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 31  | ASN  |
| 1   | A     | 42  | GLN  |
| 1   | A     | 66  | HIS  |
| 1   | A     | 95  | ASN  |
| 1   | A     | 140 | ASN  |
| 2   | B     | 12  | GLN  |
| 2   | B     | 15  | GLN  |
| 2   | B     | 105 | ASN  |
| 2   | B     | 172 | GLN  |
| 3   | C     | 25  | ASN  |
| 4   | D     | 10  | ASN  |
| 4   | D     | 75  | GLN  |
| 4   | E     | 47  | HIS  |
| 5   | F     | 24  | GLN  |
| 1   | G     | 31  | ASN  |
| 1   | G     | 42  | GLN  |
| 1   | G     | 66  | HIS  |
| 1   | G     | 83  | HIS  |
| 1   | G     | 95  | ASN  |
| 1   | G     | 140 | ASN  |
| 1   | G     | 149 | HIS  |
| 2   | H     | 12  | GLN  |
| 2   | H     | 15  | GLN  |
| 2   | H     | 93  | ASN  |
| 2   | H     | 172 | GLN  |
| 3   | I     | 25  | ASN  |
| 3   | I     | 172 | GLN  |
| 4   | J     | 10  | ASN  |
| 4   | K     | 47  | HIS  |
| 5   | L     | 24  | GLN  |

### 5.3.3 RNA ⓘ

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 carbohydrates 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 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.