



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:34 am GMT

PDB ID : 2IUU  
Title : P. AERUGINOSA FTSK MOTOR DOMAIN, HEXAMER  
Authors : Massey, T.H.; Mercoglian, C.P.; Yates, J.; Sherratt, D.J.; Lowe, J.  
Deposited on : 2006-06-07  
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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

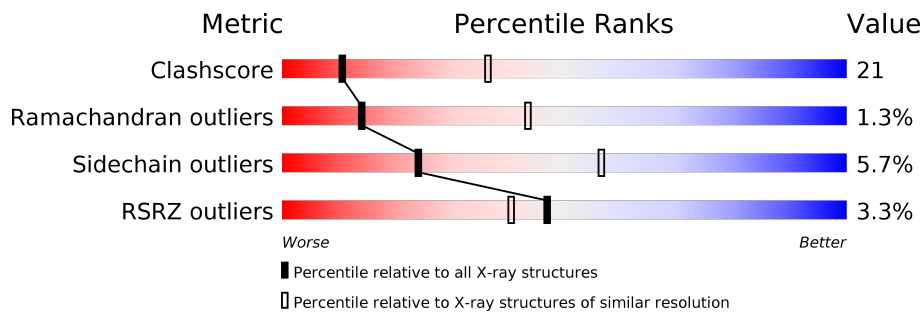
# 1 Overall quality at a glance ⓘ

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)                                      |
| RSRZ outliers         | 101464                      | 1596 (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.

| Mol | Chain | Length | Quality of chain                                                                                   |
|-----|-------|--------|----------------------------------------------------------------------------------------------------|
| 1   | A     | 491    | <div> <div>5%</div> <div> <div>52%</div> <div>29%</div> <div>••</div> <div>17%</div> </div> </div> |
| 1   | B     | 491    | <div> <div>2%</div> <div> <div>51%</div> <div>29%</div> <div>•</div> <div>17%</div> </div> </div>  |
| 1   | C     | 491    | <div> <div>2%</div> <div> <div>51%</div> <div>29%</div> <div>••</div> <div>17%</div> </div> </div> |
| 1   | D     | 491    | <div> <div>0%</div> <div> <div>55%</div> <div>26%</div> <div>••</div> <div>17%</div> </div> </div> |
| 1   | E     | 491    | <div> <div>3%</div> <div> <div>48%</div> <div>32%</div> <div>••</div> <div>17%</div> </div> </div> |
| 1   | F     | 491    | <div> <div>4%</div> <div> <div>52%</div> <div>28%</div> <div>•</div> <div>17%</div> </div> </div>  |

## 2 Entry composition [i](#)

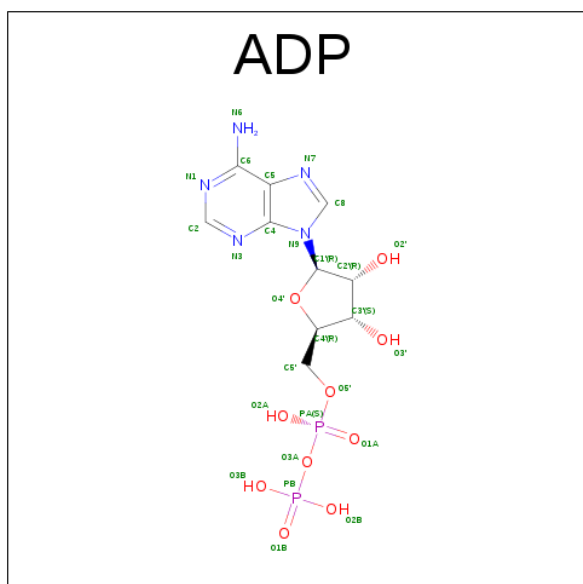
There are 2 unique types of molecules in this entry. The entry contains 18888 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA TRANSLOCASE FTSK.

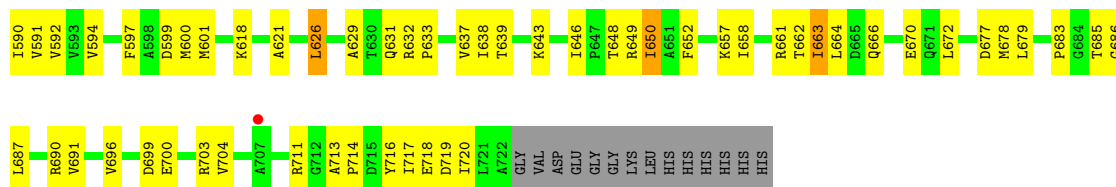
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 408      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3121  | 1983 | 540 | 583 | 15 |         |         |       |
| 1   | B     | 408      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3121  | 1983 | 540 | 583 | 15 |         |         |       |
| 1   | C     | 408      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3121  | 1983 | 540 | 583 | 15 |         |         |       |
| 1   | D     | 408      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3121  | 1983 | 540 | 583 | 15 |         |         |       |
| 1   | E     | 408      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3121  | 1983 | 540 | 583 | 15 |         |         |       |
| 1   | F     | 408      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3121  | 1983 | 540 | 583 | 15 |         |         |       |

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

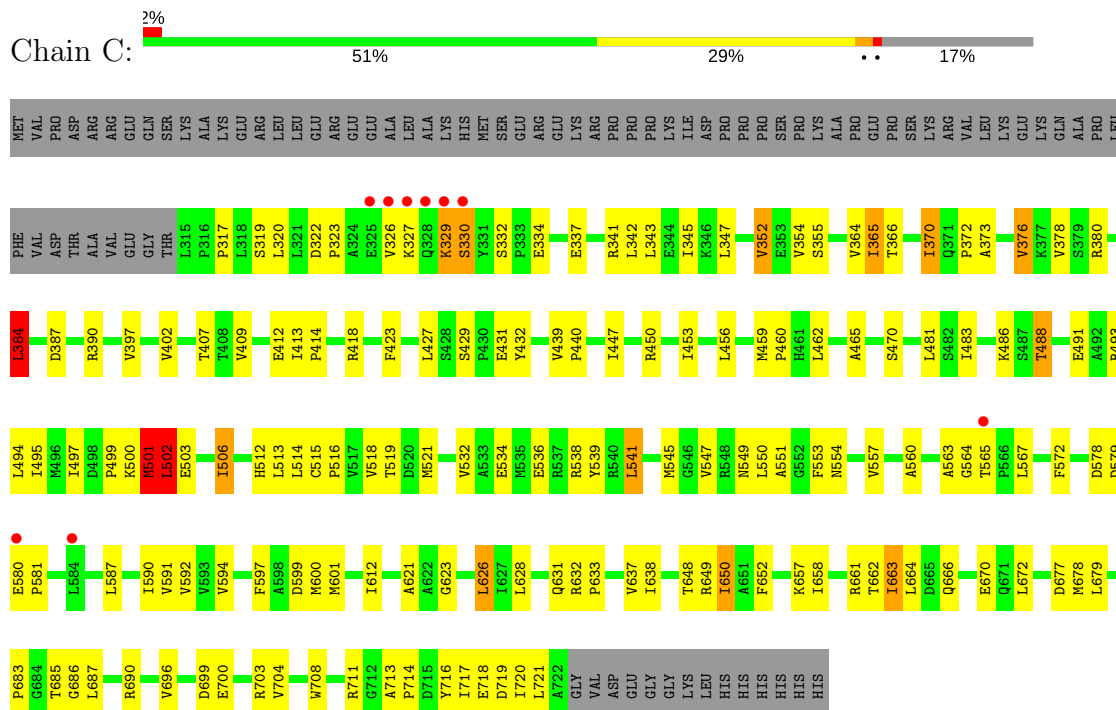


| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |         |
| 2   | B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

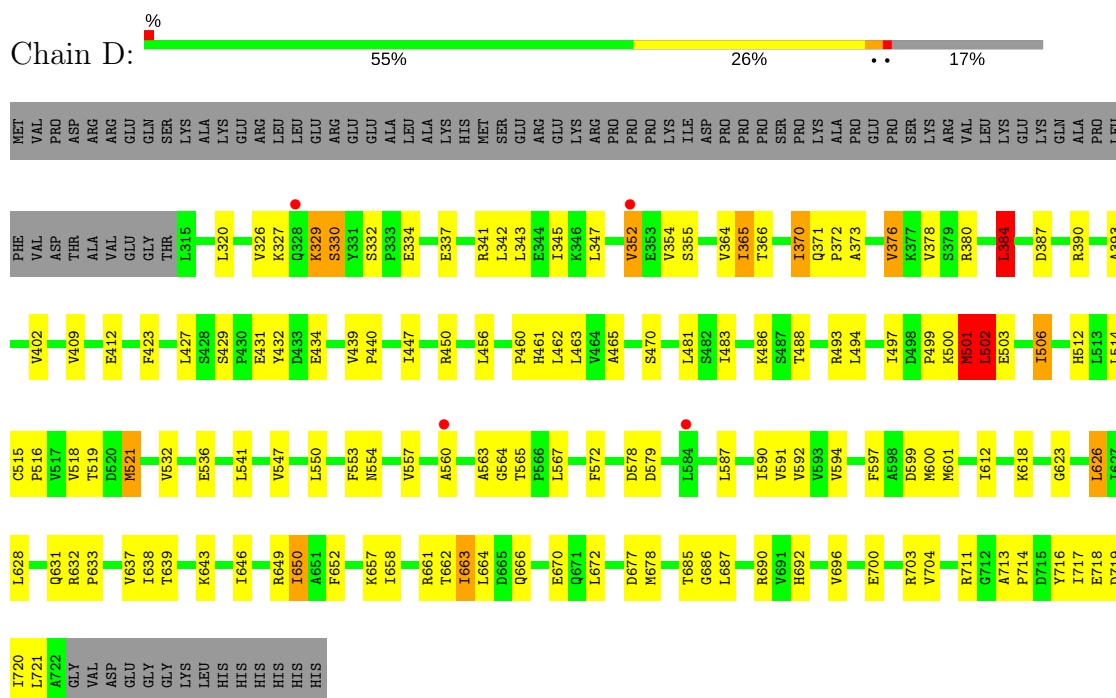




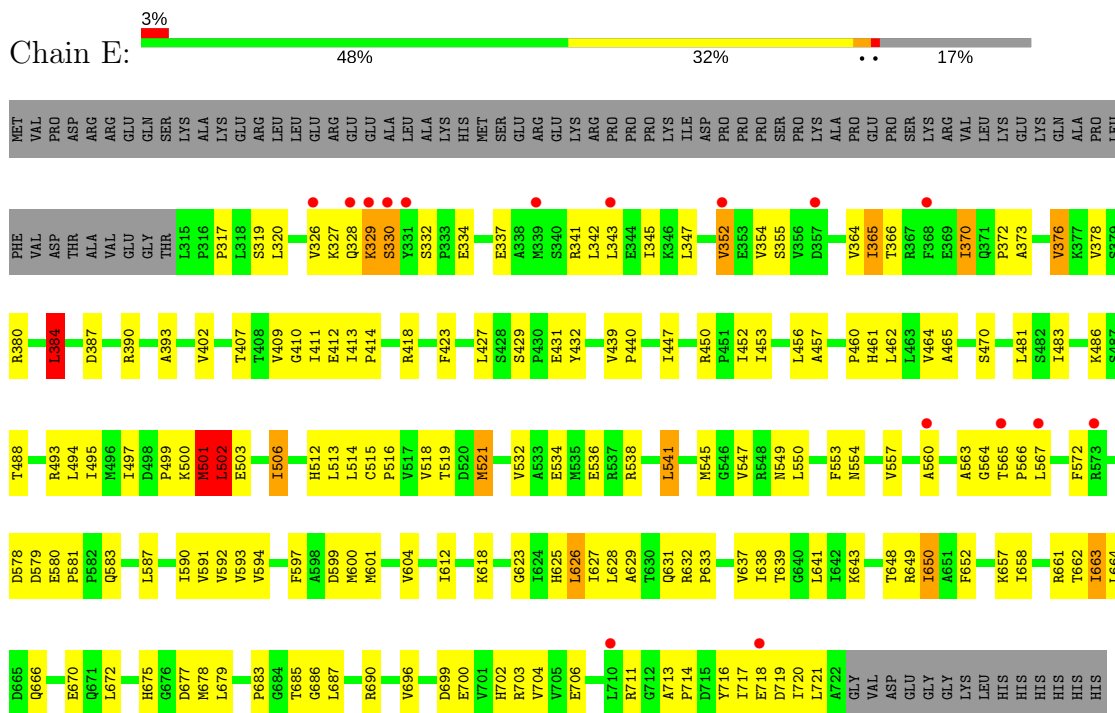
### • Molecule 1: DNA TRANSLOCASE FTSK



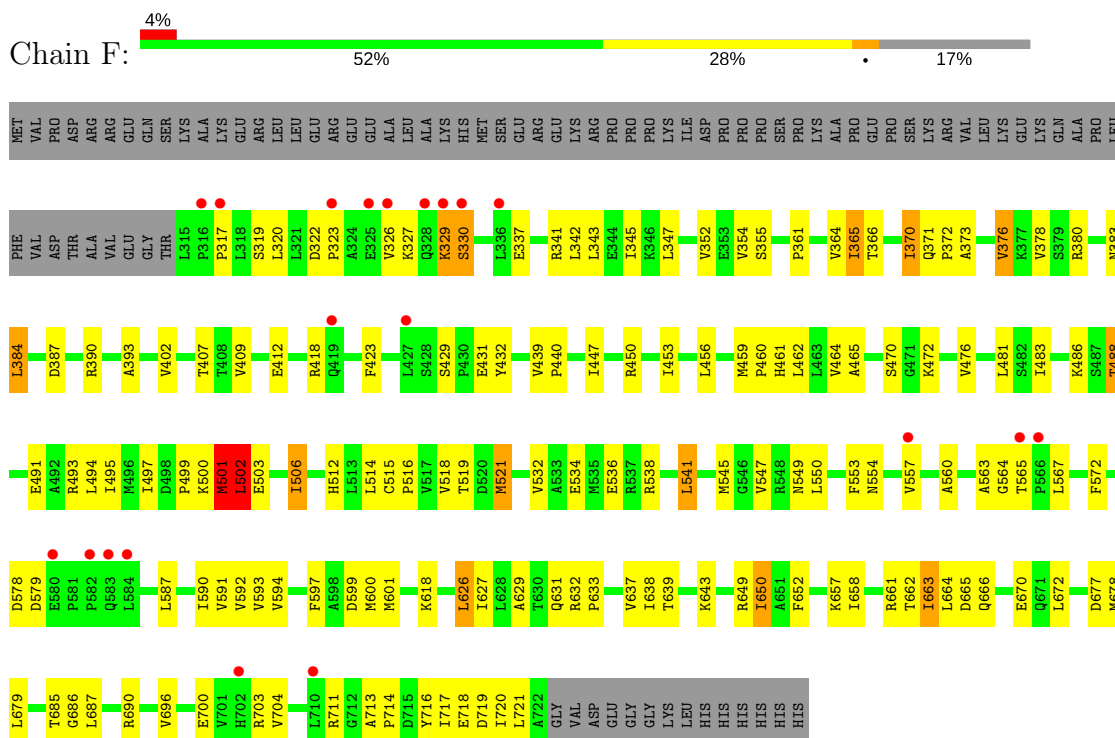
### • Molecule 1: DNA TRANSLOCASE FTSK



- Molecule 1: DNA TRANSLOCASE FTSK



- Molecule 1: DNA TRANSLOCASE FTSK



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 140.01Å 221.76Å 134.07Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 100.00 – 2.90<br>48.11 – 2.90                               | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.6 (100.00-2.90)<br>99.7 (48.11-2.90)                     | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.08                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.83 (at 2.91Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.233 , 0.259<br>0.227 , (Not available)                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                      | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 68.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.292                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 54.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | 0.009 for l,-k,h                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 18888                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 66.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.43         | 0/3177      | 0.70        | 3/4312 (0.1%)   |
| 1   | B     | 0.42         | 0/3177      | 0.70        | 3/4312 (0.1%)   |
| 1   | C     | 0.43         | 0/3177      | 0.70        | 3/4312 (0.1%)   |
| 1   | D     | 0.44         | 0/3177      | 0.71        | 3/4312 (0.1%)   |
| 1   | E     | 0.41         | 0/3177      | 0.70        | 3/4312 (0.1%)   |
| 1   | F     | 0.44         | 0/3177      | 0.70        | 1/4312 (0.0%)   |
| All | All   | 0.43         | 0/19062     | 0.70        | 16/25872 (0.1%) |

There are no bond length outliers.

All (16) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 1   | A     | 384 | LEU  | CA-CB-CG | 6.05 | 129.21      | 115.30   |
| 1   | B     | 384 | LEU  | CA-CB-CG | 5.85 | 128.76      | 115.30   |
| 1   | D     | 502 | LEU  | CA-CB-CG | 5.82 | 128.69      | 115.30   |
| 1   | E     | 502 | LEU  | CA-CB-CG | 5.81 | 128.67      | 115.30   |
| 1   | C     | 384 | LEU  | CA-CB-CG | 5.75 | 128.53      | 115.30   |
| 1   | E     | 384 | LEU  | CA-CB-CG | 5.57 | 128.11      | 115.30   |
| 1   | B     | 502 | LEU  | CA-CB-CG | 5.54 | 128.05      | 115.30   |
| 1   | A     | 502 | LEU  | CA-CB-CG | 5.48 | 127.90      | 115.30   |
| 1   | C     | 502 | LEU  | CA-CB-CG | 5.40 | 127.72      | 115.30   |
| 1   | E     | 352 | VAL  | N-CA-C   | 5.32 | 125.37      | 111.00   |
| 1   | D     | 384 | LEU  | CA-CB-CG | 5.31 | 127.52      | 115.30   |
| 1   | F     | 502 | LEU  | CA-CB-CG | 5.30 | 127.50      | 115.30   |
| 1   | B     | 352 | VAL  | N-CA-C   | 5.30 | 125.31      | 111.00   |
| 1   | D     | 352 | VAL  | N-CA-C   | 5.23 | 125.11      | 111.00   |
| 1   | C     | 352 | VAL  | N-CA-C   | 5.16 | 124.93      | 111.00   |
| 1   | A     | 352 | VAL  | N-CA-C   | 5.05 | 124.64      | 111.00   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3121  | 0        | 3238     | 132     | 0            |
| 1   | B     | 3121  | 0        | 3238     | 140     | 1            |
| 1   | C     | 3121  | 0        | 3238     | 134     | 0            |
| 1   | D     | 3121  | 0        | 3238     | 124     | 1            |
| 1   | E     | 3121  | 0        | 3238     | 148     | 0            |
| 1   | F     | 3121  | 0        | 3238     | 133     | 0            |
| 2   | A     | 27    | 0        | 12       | 0       | 0            |
| 2   | B     | 27    | 0        | 12       | 0       | 0            |
| 2   | C     | 27    | 0        | 12       | 0       | 0            |
| 2   | D     | 27    | 0        | 12       | 0       | 0            |
| 2   | E     | 27    | 0        | 12       | 0       | 0            |
| 2   | F     | 27    | 0        | 12       | 0       | 0            |
| All | All   | 18888 | 0        | 19500    | 788     | 1            |

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 21.

All (788) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:502:LEU:HD13 | 1:D:503:GLU:HG2  | 1.53                     | 0.91              |
| 1:E:502:LEU:HD13 | 1:E:503:GLU:HG2  | 1.49                     | 0.91              |
| 1:F:502:LEU:HD13 | 1:F:503:GLU:HG2  | 1.51                     | 0.90              |
| 1:B:502:LEU:HD13 | 1:B:503:GLU:HG2  | 1.54                     | 0.88              |
| 1:A:502:LEU:HD13 | 1:A:503:GLU:HG2  | 1.55                     | 0.87              |
| 1:B:521:MET:HE3  | 1:B:600:MET:HG3  | 1.55                     | 0.86              |
| 1:D:506:ILE:HD13 | 1:D:506:ILE:O    | 1.75                     | 0.86              |
| 1:C:506:ILE:HD13 | 1:C:506:ILE:O    | 1.76                     | 0.85              |
| 1:C:502:LEU:HD13 | 1:C:503:GLU:HG2  | 1.56                     | 0.85              |
| 1:F:506:ILE:O    | 1:F:506:ILE:HD13 | 1.77                     | 0.85              |
| 1:D:521:MET:HE3  | 1:D:600:MET:HG3  | 1.56                     | 0.85              |
| 1:C:521:MET:HE3  | 1:C:600:MET:HG3  | 1.58                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:506:ILE:O    | 1:E:506:ILE:HD13 | 1.79                     | 0.83              |
| 1:B:506:ILE:HD13 | 1:B:506:ILE:O    | 1.78                     | 0.83              |
| 1:D:497:ILE:HG21 | 1:D:600:MET:HE2  | 1.60                     | 0.82              |
| 1:A:497:ILE:HG21 | 1:A:600:MET:HE2  | 1.60                     | 0.82              |
| 1:B:497:ILE:HG21 | 1:B:600:MET:HE2  | 1.59                     | 0.81              |
| 1:D:329:LYS:HG2  | 1:D:330:SER:H    | 1.46                     | 0.81              |
| 1:A:329:LYS:HG2  | 1:A:330:SER:H    | 1.46                     | 0.81              |
| 1:E:497:ILE:HG21 | 1:E:600:MET:HE1  | 1.64                     | 0.80              |
| 1:D:500:LYS:O    | 1:D:502:LEU:N    | 2.12                     | 0.80              |
| 1:A:500:LYS:O    | 1:A:502:LEU:N    | 2.15                     | 0.80              |
| 1:E:329:LYS:HG2  | 1:E:330:SER:H    | 1.46                     | 0.80              |
| 1:C:500:LYS:O    | 1:C:502:LEU:N    | 2.15                     | 0.79              |
| 1:B:500:LYS:O    | 1:B:502:LEU:N    | 2.15                     | 0.79              |
| 1:D:554:ASN:HD21 | 1:D:587:LEU:H    | 1.28                     | 0.79              |
| 1:C:329:LYS:HG2  | 1:C:330:SER:H    | 1.47                     | 0.79              |
| 1:C:497:ILE:HG21 | 1:C:600:MET:HE2  | 1.64                     | 0.78              |
| 1:C:554:ASN:HD21 | 1:C:587:LEU:H    | 1.30                     | 0.78              |
| 1:A:663:ILE:HD13 | 1:A:663:ILE:O    | 1.84                     | 0.78              |
| 1:B:554:ASN:HD21 | 1:B:587:LEU:H    | 1.32                     | 0.77              |
| 1:E:658:ILE:HD12 | 1:E:658:ILE:H    | 1.50                     | 0.77              |
| 1:D:638:ILE:HD12 | 1:D:662:THR:HG22 | 1.67                     | 0.77              |
| 1:B:658:ILE:HD12 | 1:B:658:ILE:H    | 1.47                     | 0.77              |
| 1:B:329:LYS:HG2  | 1:B:330:SER:H    | 1.48                     | 0.76              |
| 1:E:521:MET:HE3  | 1:E:600:MET:HG3  | 1.67                     | 0.76              |
| 1:F:329:LYS:HG2  | 1:F:330:SER:H    | 1.49                     | 0.76              |
| 1:A:547:VAL:HG11 | 1:A:553:PHE:N    | 2.01                     | 0.76              |
| 1:F:554:ASN:HD21 | 1:F:587:LEU:H    | 1.33                     | 0.76              |
| 1:A:554:ASN:HD21 | 1:A:587:LEU:H    | 1.34                     | 0.76              |
| 1:F:658:ILE:HD12 | 1:F:658:ILE:H    | 1.51                     | 0.76              |
| 1:F:521:MET:HE3  | 1:F:600:MET:HG3  | 1.67                     | 0.75              |
| 1:E:380:ARG:O    | 1:E:384:LEU:HD22 | 1.87                     | 0.75              |
| 1:A:658:ILE:HD12 | 1:A:658:ILE:H    | 1.51                     | 0.75              |
| 1:E:554:ASN:HD21 | 1:E:587:LEU:H    | 1.34                     | 0.75              |
| 1:A:506:ILE:O    | 1:A:506:ILE:HD13 | 1.86                     | 0.74              |
| 1:B:547:VAL:HG11 | 1:B:553:PHE:N    | 2.01                     | 0.74              |
| 1:E:500:LYS:O    | 1:E:502:LEU:N    | 2.19                     | 0.74              |
| 1:F:499:PRO:HB3  | 1:F:521:MET:CE   | 2.19                     | 0.73              |
| 1:C:658:ILE:H    | 1:C:658:ILE:HD12 | 1.53                     | 0.73              |
| 1:C:440:PRO:HG3  | 1:C:486:LYS:HD2  | 1.70                     | 0.73              |
| 1:E:499:PRO:HB3  | 1:E:521:MET:CE   | 2.18                     | 0.73              |
| 1:A:521:MET:HE3  | 1:A:600:MET:HG3  | 1.69                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:380:ARG:O    | 1:D:384:LEU:HD22 | 1.88                     | 0.73              |
| 1:E:440:PRO:HG3  | 1:E:486:LYS:HD2  | 1.71                     | 0.73              |
| 1:A:685:THR:HG22 | 1:A:686:GLY:N    | 2.04                     | 0.73              |
| 1:C:365:ILE:HG13 | 1:C:412:GLU:HB3  | 1.71                     | 0.73              |
| 1:F:500:LYS:O    | 1:F:502:LEU:N    | 2.20                     | 0.73              |
| 1:E:547:VAL:HG11 | 1:E:553:PHE:N    | 2.03                     | 0.72              |
| 1:F:365:ILE:HG13 | 1:F:412:GLU:HB3  | 1.70                     | 0.72              |
| 1:B:685:THR:HG22 | 1:B:686:GLY:N    | 2.05                     | 0.72              |
| 1:F:497:ILE:HG21 | 1:F:600:MET:HE2  | 1.71                     | 0.72              |
| 1:F:638:ILE:HD12 | 1:F:662:THR:HG22 | 1.72                     | 0.72              |
| 1:A:365:ILE:HG13 | 1:A:412:GLU:HB3  | 1.71                     | 0.72              |
| 1:E:685:THR:HG22 | 1:E:686:GLY:N    | 2.03                     | 0.72              |
| 1:B:380:ARG:O    | 1:B:384:LEU:HD22 | 1.89                     | 0.71              |
| 1:A:638:ILE:HD12 | 1:A:662:THR:HG22 | 1.72                     | 0.71              |
| 1:B:500:LYS:C    | 1:B:502:LEU:H    | 1.94                     | 0.71              |
| 1:D:658:ILE:H    | 1:D:658:ILE:HD12 | 1.56                     | 0.71              |
| 1:F:685:THR:HG22 | 1:F:686:GLY:N    | 2.06                     | 0.71              |
| 1:F:500:LYS:C    | 1:F:502:LEU:H    | 1.94                     | 0.70              |
| 1:F:547:VAL:HG11 | 1:F:553:PHE:N    | 2.07                     | 0.70              |
| 1:C:717:ILE:O    | 1:C:720:ILE:HG22 | 1.91                     | 0.70              |
| 1:A:380:ARG:O    | 1:A:384:LEU:HD22 | 1.90                     | 0.70              |
| 1:B:663:ILE:O    | 1:B:663:ILE:HD13 | 1.91                     | 0.70              |
| 1:F:717:ILE:HG22 | 1:F:719:ASP:HB3  | 1.74                     | 0.70              |
| 1:D:500:LYS:C    | 1:D:502:LEU:H    | 1.94                     | 0.70              |
| 1:C:500:LYS:C    | 1:C:502:LEU:H    | 1.94                     | 0.70              |
| 1:F:711:ARG:HH21 | 1:F:711:ARG:HG3  | 1.55                     | 0.69              |
| 1:A:500:LYS:C    | 1:A:502:LEU:H    | 1.95                     | 0.69              |
| 1:E:500:LYS:C    | 1:E:502:LEU:H    | 1.95                     | 0.69              |
| 1:A:440:PRO:HG3  | 1:A:486:LYS:HD2  | 1.73                     | 0.69              |
| 1:B:500:LYS:HE3  | 1:B:599:ASP:OD2  | 1.93                     | 0.69              |
| 1:D:663:ILE:HD13 | 1:D:663:ILE:O    | 1.93                     | 0.69              |
| 1:E:493:ARG:HD2  | 1:E:512:HIS:O    | 1.93                     | 0.69              |
| 1:F:717:ILE:O    | 1:F:720:ILE:HG22 | 1.92                     | 0.69              |
| 1:B:717:ILE:HG22 | 1:B:719:ASP:HB3  | 1.75                     | 0.69              |
| 1:D:685:THR:HG22 | 1:D:686:GLY:N    | 2.07                     | 0.69              |
| 1:C:685:THR:HG22 | 1:C:686:GLY:N    | 2.06                     | 0.68              |
| 1:D:547:VAL:HG11 | 1:D:553:PHE:N    | 2.08                     | 0.68              |
| 1:F:380:ARG:O    | 1:F:384:LEU:HD22 | 1.93                     | 0.68              |
| 1:B:711:ARG:HH21 | 1:B:711:ARG:HG3  | 1.59                     | 0.68              |
| 1:F:601:MET:CE   | 1:F:637:VAL:HG13 | 2.23                     | 0.68              |
| 1:A:717:ILE:HG22 | 1:A:719:ASP:HB3  | 1.73                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:717:ILE:HG22 | 1:D:719:ASP:HB3  | 1.74                     | 0.68              |
| 1:F:500:LYS:HE3  | 1:F:599:ASP:OD2  | 1.94                     | 0.68              |
| 1:C:387:ASP:OD2  | 1:D:378:VAL:HG23 | 1.93                     | 0.68              |
| 1:C:380:ARG:O    | 1:C:384:LEU:HD22 | 1.92                     | 0.68              |
| 1:B:497:ILE:HG21 | 1:B:600:MET:CE   | 2.24                     | 0.68              |
| 1:C:711:ARG:HH21 | 1:C:711:ARG:HG3  | 1.58                     | 0.68              |
| 1:A:499:PRO:HB3  | 1:A:521:MET:CE   | 2.24                     | 0.68              |
| 1:B:601:MET:CE   | 1:B:637:VAL:HG13 | 2.24                     | 0.68              |
| 1:C:717:ILE:HG22 | 1:C:719:ASP:HB3  | 1.75                     | 0.67              |
| 1:C:663:ILE:O    | 1:C:663:ILE:HD13 | 1.95                     | 0.67              |
| 1:E:365:ILE:HG13 | 1:E:412:GLU:HB3  | 1.75                     | 0.67              |
| 1:E:717:ILE:O    | 1:E:720:ILE:HG22 | 1.94                     | 0.67              |
| 1:E:497:ILE:HD13 | 1:E:600:MET:HE1  | 1.77                     | 0.67              |
| 1:F:554:ASN:HA   | 1:F:557:VAL:HG12 | 1.77                     | 0.67              |
| 1:C:547:VAL:HG11 | 1:C:553:PHE:N    | 2.11                     | 0.66              |
| 1:E:429:SER:HB2  | 1:E:431:GLU:OE2  | 1.94                     | 0.66              |
| 1:D:601:MET:CE   | 1:D:637:VAL:HG13 | 2.26                     | 0.66              |
| 1:E:601:MET:CE   | 1:E:637:VAL:HG13 | 2.25                     | 0.66              |
| 1:E:717:ILE:HG22 | 1:E:719:ASP:HB3  | 1.77                     | 0.66              |
| 1:F:440:PRO:HG3  | 1:F:486:LYS:HD2  | 1.78                     | 0.66              |
| 1:A:497:ILE:HG21 | 1:A:600:MET:CE   | 2.25                     | 0.66              |
| 1:E:341:ARG:O    | 1:E:345:ILE:HG12 | 1.96                     | 0.65              |
| 1:B:572:PHE:HZ   | 1:B:579:ASP:HB3  | 1.61                     | 0.65              |
| 1:A:717:ILE:O    | 1:A:720:ILE:HG22 | 1.95                     | 0.65              |
| 1:F:499:PRO:HB3  | 1:F:521:MET:HE1  | 1.78                     | 0.65              |
| 1:A:700:GLU:O    | 1:A:704:VAL:HG23 | 1.95                     | 0.65              |
| 1:B:440:PRO:HG3  | 1:B:486:LYS:HD2  | 1.78                     | 0.65              |
| 1:D:462:LEU:HD11 | 1:D:650:ILE:HD13 | 1.79                     | 0.65              |
| 1:F:423:PHE:HE1  | 1:F:481:LEU:HB3  | 1.62                     | 0.65              |
| 1:A:402:VAL:HG13 | 1:A:687:LEU:HD11 | 1.78                     | 0.65              |
| 1:E:663:ILE:HD13 | 1:E:663:ILE:O    | 1.97                     | 0.65              |
| 1:C:497:ILE:HD13 | 1:C:600:MET:HE2  | 1.78                     | 0.65              |
| 1:E:439:VAL:HG12 | 1:E:483:ILE:HD12 | 1.78                     | 0.65              |
| 1:D:365:ILE:HG13 | 1:D:412:GLU:HB3  | 1.78                     | 0.65              |
| 1:D:493:ARG:HD2  | 1:D:512:HIS:O    | 1.97                     | 0.65              |
| 1:D:554:ASN:HA   | 1:D:557:VAL:HG12 | 1.79                     | 0.65              |
| 1:C:499:PRO:HB3  | 1:C:521:MET:CE   | 2.27                     | 0.64              |
| 1:D:717:ILE:O    | 1:D:720:ILE:HG22 | 1.97                     | 0.64              |
| 1:E:554:ASN:HA   | 1:E:557:VAL:HG12 | 1.80                     | 0.64              |
| 1:C:638:ILE:HD12 | 1:C:662:THR:HG22 | 1.79                     | 0.64              |
| 1:F:663:ILE:O    | 1:F:663:ILE:HD13 | 1.98                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:717:ILE:O    | 1:B:720:ILE:HG22 | 1.97                     | 0.64              |
| 1:C:497:ILE:HG21 | 1:C:600:MET:CE   | 2.28                     | 0.64              |
| 1:E:462:LEU:HD11 | 1:E:650:ILE:CD1  | 2.27                     | 0.64              |
| 1:A:499:PRO:HB3  | 1:A:521:MET:HE1  | 1.78                     | 0.64              |
| 1:B:439:VAL:HG12 | 1:B:483:ILE:HD12 | 1.79                     | 0.64              |
| 1:E:327:LYS:O    | 1:E:327:LYS:HG3  | 1.98                     | 0.64              |
| 1:B:499:PRO:HB3  | 1:B:521:MET:CE   | 2.28                     | 0.64              |
| 1:B:499:PRO:HB3  | 1:B:521:MET:HE1  | 1.79                     | 0.64              |
| 1:E:572:PHE:HZ   | 1:E:579:ASP:HB3  | 1.62                     | 0.64              |
| 1:E:638:ILE:HD12 | 1:E:662:THR:HG22 | 1.79                     | 0.64              |
| 1:F:402:VAL:HG13 | 1:F:687:LEU:HD11 | 1.79                     | 0.64              |
| 1:A:387:ASP:OD2  | 1:B:378:VAL:HG23 | 1.98                     | 0.64              |
| 1:B:365:ILE:HG13 | 1:B:412:GLU:HB3  | 1.78                     | 0.64              |
| 1:D:329:LYS:HG2  | 1:D:330:SER:N    | 2.13                     | 0.64              |
| 1:D:700:GLU:O    | 1:D:704:VAL:HG23 | 1.98                     | 0.64              |
| 1:A:493:ARG:HD2  | 1:A:512:HIS:O    | 1.97                     | 0.63              |
| 1:D:327:LYS:HG3  | 1:D:327:LYS:O    | 1.98                     | 0.63              |
| 1:B:327:LYS:HG3  | 1:B:327:LYS:O    | 1.99                     | 0.63              |
| 1:C:329:LYS:HG2  | 1:C:330:SER:N    | 2.13                     | 0.63              |
| 1:E:329:LYS:CG   | 1:E:330:SER:H    | 2.11                     | 0.63              |
| 1:A:572:PHE:HZ   | 1:A:579:ASP:HB3  | 1.63                     | 0.63              |
| 1:E:500:LYS:HE3  | 1:E:599:ASP:OD2  | 1.98                     | 0.63              |
| 1:F:327:LYS:HG3  | 1:F:327:LYS:O    | 1.98                     | 0.63              |
| 1:F:493:ARG:HD2  | 1:F:512:HIS:O    | 1.99                     | 0.63              |
| 1:A:711:ARG:HH21 | 1:A:711:ARG:HG3  | 1.63                     | 0.63              |
| 1:C:327:LYS:HG3  | 1:C:327:LYS:O    | 1.97                     | 0.63              |
| 1:D:440:PRO:HG3  | 1:D:486:LYS:HD2  | 1.80                     | 0.63              |
| 1:A:329:LYS:HG2  | 1:A:330:SER:N    | 2.13                     | 0.63              |
| 1:B:638:ILE:HD12 | 1:B:662:THR:HG22 | 1.80                     | 0.63              |
| 1:E:499:PRO:HB3  | 1:E:521:MET:HE1  | 1.81                     | 0.63              |
| 1:F:462:LEU:HD11 | 1:F:650:ILE:HD13 | 1.80                     | 0.63              |
| 1:B:514:LEU:HD11 | 1:B:590:ILE:HD12 | 1.80                     | 0.63              |
| 1:F:572:PHE:HZ   | 1:F:579:ASP:HB3  | 1.64                     | 0.63              |
| 1:A:354:VAL:HG23 | 1:A:372:PRO:HA   | 1.81                     | 0.62              |
| 1:E:711:ARG:HH21 | 1:E:711:ARG:HG3  | 1.64                     | 0.62              |
| 1:B:329:LYS:HG2  | 1:B:330:SER:N    | 2.14                     | 0.62              |
| 1:C:370:ILE:HD13 | 1:C:409:VAL:O    | 1.99                     | 0.62              |
| 1:C:601:MET:CE   | 1:C:637:VAL:HG13 | 2.30                     | 0.62              |
| 1:E:387:ASP:OD2  | 1:F:378:VAL:HG23 | 2.00                     | 0.62              |
| 1:D:370:ILE:HD13 | 1:D:409:VAL:O    | 1.99                     | 0.62              |
| 1:F:370:ILE:HD13 | 1:F:409:VAL:O    | 1.99                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:429:SER:HB2  | 1:A:431:GLU:OE2  | 1.99                     | 0.62              |
| 1:B:658:ILE:HD12 | 1:B:658:ILE:N    | 2.14                     | 0.62              |
| 1:B:685:THR:HG22 | 1:B:686:GLY:H    | 1.65                     | 0.62              |
| 1:C:514:LEU:HD11 | 1:C:590:ILE:HD12 | 1.80                     | 0.62              |
| 1:A:494:LEU:HD23 | 1:A:591:VAL:HB   | 1.81                     | 0.62              |
| 1:D:572:PHE:HZ   | 1:D:579:ASP:HB3  | 1.65                     | 0.62              |
| 1:C:554:ASN:HA   | 1:C:557:VAL:HG12 | 1.82                     | 0.62              |
| 1:F:370:ILE:H    | 1:F:370:ILE:HD13 | 1.65                     | 0.62              |
| 1:E:354:VAL:HG23 | 1:E:372:PRO:HA   | 1.80                     | 0.62              |
| 1:D:439:VAL:HG12 | 1:D:483:ILE:HD12 | 1.82                     | 0.61              |
| 1:D:711:ARG:HH21 | 1:D:711:ARG:HG3  | 1.65                     | 0.61              |
| 1:B:341:ARG:O    | 1:B:345:ILE:HG12 | 2.01                     | 0.61              |
| 1:B:497:ILE:HD12 | 1:B:594:VAL:HG22 | 1.82                     | 0.61              |
| 1:C:370:ILE:HD13 | 1:C:370:ILE:H    | 1.66                     | 0.61              |
| 1:D:499:PRO:HB3  | 1:D:521:MET:HE1  | 1.83                     | 0.61              |
| 1:C:541:LEU:O    | 1:C:545:MET:HG2  | 2.01                     | 0.61              |
| 1:F:329:LYS:HG2  | 1:F:330:SER:N    | 2.15                     | 0.61              |
| 1:F:462:LEU:HD11 | 1:F:650:ILE:CD1  | 2.30                     | 0.61              |
| 1:A:423:PHE:HE1  | 1:A:481:LEU:HB3  | 1.63                     | 0.61              |
| 1:A:631:GLN:O    | 1:A:633:PRO:HD3  | 2.01                     | 0.61              |
| 1:E:497:ILE:HG21 | 1:E:600:MET:CE   | 2.31                     | 0.61              |
| 1:B:429:SER:HB2  | 1:B:431:GLU:OE2  | 2.00                     | 0.61              |
| 1:C:439:VAL:HG12 | 1:C:483:ILE:HD12 | 1.82                     | 0.61              |
| 1:E:497:ILE:HD12 | 1:E:594:VAL:HG22 | 1.83                     | 0.61              |
| 1:F:429:SER:HB2  | 1:F:431:GLU:OE2  | 2.00                     | 0.61              |
| 1:A:327:LYS:HG3  | 1:A:327:LYS:O    | 2.01                     | 0.60              |
| 1:D:500:LYS:HE3  | 1:D:599:ASP:OD2  | 2.01                     | 0.60              |
| 1:A:341:ARG:O    | 1:A:345:ILE:HG12 | 2.01                     | 0.60              |
| 1:A:370:ILE:HD13 | 1:A:409:VAL:O    | 2.02                     | 0.60              |
| 1:C:465:ALA:HB3  | 1:C:663:ILE:HG13 | 1.83                     | 0.60              |
| 1:F:341:ARG:O    | 1:F:345:ILE:HG12 | 2.00                     | 0.60              |
| 1:A:554:ASN:HA   | 1:A:557:VAL:HG12 | 1.82                     | 0.60              |
| 1:D:354:VAL:HG23 | 1:D:372:PRO:HA   | 1.83                     | 0.60              |
| 1:D:497:ILE:HD12 | 1:D:594:VAL:HG22 | 1.83                     | 0.60              |
| 1:C:429:SER:HB2  | 1:C:431:GLU:OE2  | 2.01                     | 0.60              |
| 1:C:700:GLU:O    | 1:C:704:VAL:HG23 | 2.01                     | 0.60              |
| 1:A:658:ILE:HD12 | 1:A:658:ILE:N    | 2.17                     | 0.60              |
| 1:E:329:LYS:HG2  | 1:E:330:SER:N    | 2.14                     | 0.60              |
| 1:F:601:MET:HE1  | 1:F:637:VAL:HG13 | 1.82                     | 0.60              |
| 1:D:429:SER:HB2  | 1:D:431:GLU:OE2  | 2.02                     | 0.60              |
| 1:E:423:PHE:HE1  | 1:E:481:LEU:HB3  | 1.65                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:497:ILE:HD12 | 1:C:594:VAL:HG22 | 1.84                     | 0.59              |
| 1:D:499:PRO:HB3  | 1:D:521:MET:CE   | 2.32                     | 0.59              |
| 1:E:465:ALA:HB3  | 1:E:663:ILE:HG13 | 1.84                     | 0.59              |
| 1:C:713:ALA:HB1  | 1:C:714:PRO:HD2  | 1.84                     | 0.59              |
| 1:F:532:VAL:O    | 1:F:536:GLU:HG2  | 2.02                     | 0.59              |
| 1:A:378:VAL:HG23 | 1:F:387:ASP:OD2  | 2.03                     | 0.59              |
| 1:E:658:ILE:HD12 | 1:E:658:ILE:N    | 2.15                     | 0.59              |
| 1:A:685:THR:HG22 | 1:A:686:GLY:H    | 1.65                     | 0.59              |
| 1:B:423:PHE:HE1  | 1:B:481:LEU:HB3  | 1.68                     | 0.59              |
| 1:B:554:ASN:HA   | 1:B:557:VAL:HG12 | 1.83                     | 0.59              |
| 1:D:341:ARG:O    | 1:D:345:ILE:HG12 | 2.02                     | 0.59              |
| 1:E:370:ILE:HD13 | 1:E:370:ILE:H    | 1.66                     | 0.59              |
| 1:E:370:ILE:HD13 | 1:E:409:VAL:O    | 2.03                     | 0.59              |
| 1:E:462:LEU:HD11 | 1:E:650:ILE:HD13 | 1.83                     | 0.59              |
| 1:A:601:MET:CE   | 1:A:637:VAL:HG13 | 2.33                     | 0.59              |
| 1:D:497:ILE:HG21 | 1:D:600:MET:CE   | 2.32                     | 0.59              |
| 1:C:572:PHE:HZ   | 1:C:579:ASP:HB3  | 1.66                     | 0.59              |
| 1:B:465:ALA:HB1  | 1:B:633:PRO:HG3  | 1.83                     | 0.59              |
| 1:C:500:LYS:HE3  | 1:C:599:ASP:OD2  | 2.02                     | 0.59              |
| 1:A:497:ILE:HD12 | 1:A:594:VAL:HG22 | 1.85                     | 0.58              |
| 1:C:499:PRO:HB3  | 1:C:521:MET:HE1  | 1.83                     | 0.58              |
| 1:D:465:ALA:HB3  | 1:D:663:ILE:HG13 | 1.84                     | 0.58              |
| 1:F:700:GLU:O    | 1:F:704:VAL:HG23 | 2.03                     | 0.58              |
| 1:B:402:VAL:HG13 | 1:B:687:LEU:HD11 | 1.85                     | 0.58              |
| 1:F:658:ILE:HD12 | 1:F:658:ILE:N    | 2.15                     | 0.58              |
| 1:C:329:LYS:CG   | 1:C:330:SER:N    | 2.66                     | 0.58              |
| 1:D:329:LYS:CG   | 1:D:330:SER:N    | 2.66                     | 0.58              |
| 1:B:497:ILE:HD13 | 1:B:600:MET:HE2  | 1.85                     | 0.58              |
| 1:D:329:LYS:H    | 1:D:329:LYS:HD3  | 1.69                     | 0.58              |
| 1:E:601:MET:HE1  | 1:E:637:VAL:HG13 | 1.84                     | 0.58              |
| 1:C:341:ARG:O    | 1:C:345:ILE:HG12 | 2.04                     | 0.58              |
| 1:F:354:VAL:HG23 | 1:F:372:PRO:HA   | 1.85                     | 0.58              |
| 1:F:439:VAL:HG12 | 1:F:483:ILE:HD12 | 1.85                     | 0.58              |
| 1:C:465:ALA:HB1  | 1:C:633:PRO:HG3  | 1.86                     | 0.58              |
| 1:A:500:LYS:HE3  | 1:A:599:ASP:OD2  | 2.03                     | 0.58              |
| 1:C:597:PHE:CE1  | 1:C:601:MET:HE1  | 2.39                     | 0.58              |
| 1:D:599:ASP:OD1  | 1:D:632:ARG:NH1  | 2.37                     | 0.58              |
| 1:D:462:LEU:HD11 | 1:D:650:ILE:CD1  | 2.32                     | 0.57              |
| 1:F:514:LEU:HD11 | 1:F:590:ILE:HD12 | 1.84                     | 0.57              |
| 1:C:550:LEU:HD11 | 1:C:587:LEU:HB2  | 1.86                     | 0.57              |
| 1:C:685:THR:HG22 | 1:C:686:GLY:H    | 1.67                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:402:VAL:HG13 | 1:C:687:LEU:HD11 | 1.86                     | 0.57              |
| 1:F:494:LEU:HD23 | 1:F:591:VAL:HB   | 1.86                     | 0.57              |
| 1:A:661:ARG:HA   | 1:A:666:GLN:H    | 1.68                     | 0.57              |
| 1:E:329:LYS:CG   | 1:E:330:SER:N    | 2.67                     | 0.57              |
| 1:E:685:THR:CG2  | 1:E:686:GLY:N    | 2.67                     | 0.57              |
| 1:B:329:LYS:CG   | 1:B:330:SER:N    | 2.68                     | 0.57              |
| 1:B:370:ILE:HD13 | 1:B:370:ILE:H    | 1.70                     | 0.57              |
| 1:B:550:LEU:HD11 | 1:B:587:LEU:HB2  | 1.85                     | 0.57              |
| 1:B:493:ARG:HD2  | 1:B:512:HIS:O    | 2.05                     | 0.57              |
| 1:A:329:LYS:CG   | 1:A:330:SER:N    | 2.67                     | 0.57              |
| 1:B:601:MET:HE1  | 1:B:637:VAL:HG13 | 1.87                     | 0.57              |
| 1:D:423:PHE:HE1  | 1:D:481:LEU:HB3  | 1.68                     | 0.57              |
| 1:A:462:LEU:HD11 | 1:A:650:ILE:HD13 | 1.87                     | 0.57              |
| 1:D:514:LEU:HD11 | 1:D:590:ILE:HD12 | 1.87                     | 0.57              |
| 1:F:365:ILE:HG12 | 1:F:366:THR:N    | 2.19                     | 0.57              |
| 1:A:465:ALA:HB3  | 1:A:663:ILE:HG13 | 1.87                     | 0.57              |
| 1:A:685:THR:CG2  | 1:A:686:GLY:N    | 2.68                     | 0.57              |
| 1:B:365:ILE:HD11 | 1:B:447:ILE:HB   | 1.86                     | 0.57              |
| 1:F:497:ILE:HG21 | 1:F:600:MET:CE   | 2.35                     | 0.56              |
| 1:C:354:VAL:HG23 | 1:C:372:PRO:HA   | 1.87                     | 0.56              |
| 1:C:658:ILE:N    | 1:C:658:ILE:HD12 | 2.18                     | 0.56              |
| 1:B:521:MET:HE3  | 1:B:600:MET:CG   | 2.30                     | 0.56              |
| 1:E:365:ILE:HD11 | 1:E:447:ILE:HB   | 1.86                     | 0.56              |
| 1:E:470:SER:HB2  | 1:E:652:PHE:HB3  | 1.87                     | 0.56              |
| 1:A:439:VAL:HG12 | 1:A:483:ILE:HD12 | 1.87                     | 0.56              |
| 1:B:465:ALA:HB3  | 1:B:663:ILE:HG13 | 1.87                     | 0.56              |
| 1:B:685:THR:CG2  | 1:B:686:GLY:N    | 2.69                     | 0.56              |
| 1:B:700:GLU:O    | 1:B:704:VAL:HG23 | 2.04                     | 0.56              |
| 1:A:560:ALA:CB   | 1:A:567:LEU:HG   | 2.34                     | 0.56              |
| 1:D:658:ILE:N    | 1:D:658:ILE:HD12 | 2.20                     | 0.56              |
| 1:E:685:THR:HG22 | 1:E:686:GLY:H    | 1.69                     | 0.56              |
| 1:D:370:ILE:H    | 1:D:370:ILE:HD13 | 1.71                     | 0.56              |
| 1:E:550:LEU:HD11 | 1:E:587:LEU:HB2  | 1.86                     | 0.56              |
| 1:E:658:ILE:CD1  | 1:E:658:ILE:H    | 2.18                     | 0.56              |
| 1:F:329:LYS:H    | 1:F:329:LYS:HD3  | 1.70                     | 0.56              |
| 1:F:560:ALA:CB   | 1:F:567:LEU:HG   | 2.35                     | 0.56              |
| 1:D:365:ILE:HD11 | 1:D:447:ILE:HB   | 1.87                     | 0.56              |
| 1:E:329:LYS:HD3  | 1:E:329:LYS:H    | 1.71                     | 0.56              |
| 1:D:387:ASP:OD2  | 1:E:378:VAL:HG23 | 2.05                     | 0.56              |
| 1:E:532:VAL:O    | 1:E:536:GLU:HG2  | 2.05                     | 0.56              |
| 1:A:514:LEU:HD11 | 1:A:590:ILE:HD12 | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:599:ASP:OD1  | 1:C:632:ARG:NH1  | 2.39                     | 0.56              |
| 1:F:470:SER:HB2  | 1:F:652:PHE:HB3  | 1.88                     | 0.56              |
| 1:E:402:VAL:HG13 | 1:E:687:LEU:HD11 | 1.88                     | 0.56              |
| 1:F:550:LEU:HD11 | 1:F:587:LEU:HB2  | 1.87                     | 0.56              |
| 1:B:462:LEU:HD11 | 1:B:650:ILE:CD1  | 2.36                     | 0.56              |
| 1:A:470:SER:HB2  | 1:A:652:PHE:HB3  | 1.88                     | 0.56              |
| 1:F:685:THR:CG2  | 1:F:686:GLY:N    | 2.69                     | 0.56              |
| 1:C:493:ARG:HD2  | 1:C:512:HIS:O    | 2.06                     | 0.55              |
| 1:C:423:PHE:HE1  | 1:C:481:LEU:HB3  | 1.69                     | 0.55              |
| 1:A:370:ILE:H    | 1:A:370:ILE:HD13 | 1.71                     | 0.55              |
| 1:C:685:THR:CG2  | 1:C:686:GLY:N    | 2.69                     | 0.55              |
| 1:E:499:PRO:HB3  | 1:E:521:MET:HE2  | 1.86                     | 0.55              |
| 1:B:354:VAL:HG23 | 1:B:372:PRO:HA   | 1.88                     | 0.55              |
| 1:B:488:THR:HG23 | 1:B:491:GLU:OE2  | 2.06                     | 0.55              |
| 1:C:560:ALA:CB   | 1:C:567:LEU:HG   | 2.35                     | 0.55              |
| 1:E:465:ALA:HB1  | 1:E:633:PRO:HG3  | 1.88                     | 0.55              |
| 1:A:347:LEU:HB3  | 1:A:352:VAL:HG23 | 1.89                     | 0.55              |
| 1:A:462:LEU:HD11 | 1:A:650:ILE:CD1  | 2.35                     | 0.55              |
| 1:D:532:VAL:O    | 1:D:536:GLU:HG2  | 2.06                     | 0.55              |
| 1:E:560:ALA:CB   | 1:E:567:LEU:HG   | 2.36                     | 0.55              |
| 1:E:494:LEU:HD23 | 1:E:591:VAL:HB   | 1.87                     | 0.55              |
| 1:F:658:ILE:CD1  | 1:F:658:ILE:H    | 2.19                     | 0.55              |
| 1:F:661:ARG:HA   | 1:F:666:GLN:H    | 1.71                     | 0.55              |
| 1:C:494:LEU:HD23 | 1:C:591:VAL:HB   | 1.89                     | 0.55              |
| 1:F:713:ALA:HB1  | 1:F:714:PRO:HD2  | 1.89                     | 0.55              |
| 1:A:713:ALA:HB1  | 1:A:714:PRO:HD2  | 1.89                     | 0.55              |
| 1:E:661:ARG:HA   | 1:E:666:GLN:H    | 1.71                     | 0.54              |
| 1:E:700:GLU:O    | 1:E:704:VAL:HG23 | 2.07                     | 0.54              |
| 1:A:677:ASP:OD1  | 1:A:690:ARG:NH1  | 2.36                     | 0.54              |
| 1:A:658:ILE:CD1  | 1:A:658:ILE:H    | 2.19                     | 0.54              |
| 1:D:465:ALA:HB1  | 1:D:633:PRO:HG3  | 1.89                     | 0.54              |
| 1:F:347:LEU:HB3  | 1:F:352:VAL:HG23 | 1.89                     | 0.54              |
| 1:D:550:LEU:HD11 | 1:D:587:LEU:HB2  | 1.90                     | 0.54              |
| 1:C:329:LYS:HD3  | 1:C:329:LYS:H    | 1.71                     | 0.54              |
| 1:D:685:THR:CG2  | 1:D:686:GLY:N    | 2.70                     | 0.54              |
| 1:F:329:LYS:CG   | 1:F:330:SER:N    | 2.68                     | 0.54              |
| 1:A:329:LYS:H    | 1:A:329:LYS:HD3  | 1.72                     | 0.54              |
| 1:F:649:ARG:HB3  | 1:F:663:ILE:CD1  | 2.37                     | 0.54              |
| 1:A:365:ILE:HD11 | 1:A:447:ILE:HB   | 1.88                     | 0.54              |
| 1:C:462:LEU:HD11 | 1:C:650:ILE:CD1  | 2.38                     | 0.54              |
| 1:D:554:ASN:HA   | 1:D:557:VAL:CG1  | 2.37                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:592:VAL:HB   | 1:B:626:LEU:HD12 | 1.89                     | 0.54              |
| 1:E:599:ASP:OD1  | 1:E:632:ARG:NH1  | 2.40                     | 0.54              |
| 1:A:550:LEU:HD11 | 1:A:587:LEU:HB2  | 1.89                     | 0.54              |
| 1:B:370:ILE:HD13 | 1:B:409:VAL:O    | 2.08                     | 0.53              |
| 1:E:713:ALA:HB1  | 1:E:714:PRO:HD2  | 1.90                     | 0.53              |
| 1:A:465:ALA:HB1  | 1:A:633:PRO:HG3  | 1.88                     | 0.53              |
| 1:B:685:THR:CG2  | 1:B:686:GLY:H    | 2.21                     | 0.53              |
| 1:C:521:MET:HE3  | 1:C:600:MET:CG   | 2.33                     | 0.53              |
| 1:C:717:ILE:HD12 | 1:C:717:ILE:N    | 2.23                     | 0.53              |
| 1:D:560:ALA:CB   | 1:D:567:LEU:HG   | 2.38                     | 0.53              |
| 1:E:516:PRO:HG3  | 1:E:716:TYR:CE1  | 2.44                     | 0.53              |
| 1:D:677:ASP:OD1  | 1:D:690:ARG:NH1  | 2.39                     | 0.53              |
| 1:F:717:ILE:N    | 1:F:717:ILE:HD12 | 2.23                     | 0.53              |
| 1:F:554:ASN:HA   | 1:F:557:VAL:CG1  | 2.39                     | 0.53              |
| 1:C:661:ARG:HA   | 1:C:666:GLN:H    | 1.73                     | 0.53              |
| 1:A:365:ILE:HG12 | 1:A:366:THR:N    | 2.24                     | 0.53              |
| 1:D:494:LEU:HD23 | 1:D:591:VAL:HB   | 1.90                     | 0.53              |
| 1:B:329:LYS:H    | 1:B:329:LYS:HD3  | 1.74                     | 0.53              |
| 1:B:663:ILE:C    | 1:B:663:ILE:HD13 | 2.29                     | 0.53              |
| 1:B:717:ILE:N    | 1:B:717:ILE:HD12 | 2.24                     | 0.53              |
| 1:E:514:LEU:HD11 | 1:E:590:ILE:HD12 | 1.90                     | 0.53              |
| 1:F:685:THR:HG22 | 1:F:686:GLY:H    | 1.73                     | 0.53              |
| 1:A:663:ILE:HD13 | 1:A:663:ILE:C    | 2.29                     | 0.53              |
| 1:B:534:GLU:O    | 1:B:538:ARG:HG3  | 2.09                     | 0.53              |
| 1:B:658:ILE:CD1  | 1:B:658:ILE:H    | 2.17                     | 0.53              |
| 1:C:532:VAL:O    | 1:C:536:GLU:HG2  | 2.09                     | 0.53              |
| 1:A:717:ILE:N    | 1:A:717:ILE:HD12 | 2.24                     | 0.53              |
| 1:C:534:GLU:O    | 1:C:538:ARG:HG3  | 2.09                     | 0.53              |
| 1:F:497:ILE:HD12 | 1:F:594:VAL:HG22 | 1.91                     | 0.53              |
| 1:F:541:LEU:O    | 1:F:545:MET:HG2  | 2.08                     | 0.52              |
| 1:F:497:ILE:HD13 | 1:F:600:MET:HE2  | 1.92                     | 0.52              |
| 1:D:657:LYS:HG2  | 1:D:670:GLU:OE1  | 2.09                     | 0.52              |
| 1:B:560:ALA:CB   | 1:B:567:LEU:HG   | 2.38                     | 0.52              |
| 1:D:601:MET:HE1  | 1:D:637:VAL:HG13 | 1.91                     | 0.52              |
| 1:A:685:THR:CG2  | 1:A:686:GLY:H    | 2.21                     | 0.52              |
| 1:D:470:SER:HB2  | 1:D:652:PHE:HB3  | 1.92                     | 0.52              |
| 1:D:661:ARG:HA   | 1:D:666:GLN:H    | 1.74                     | 0.52              |
| 1:D:672:LEU:HD13 | 1:D:678:MET:HA   | 1.91                     | 0.52              |
| 1:F:465:ALA:HB1  | 1:F:633:PRO:HG3  | 1.92                     | 0.52              |
| 1:D:685:THR:HG22 | 1:D:686:GLY:H    | 1.74                     | 0.52              |
| 1:F:464:VAL:O    | 1:F:629:ALA:HA   | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:329:LYS:CG   | 1:C:330:SER:H    | 2.12                     | 0.52              |
| 1:D:402:VAL:HG13 | 1:D:687:LEU:HD11 | 1.92                     | 0.52              |
| 1:B:657:LYS:HG2  | 1:B:670:GLU:OE1  | 2.10                     | 0.52              |
| 1:B:500:LYS:C    | 1:B:502:LEU:N    | 2.62                     | 0.51              |
| 1:C:354:VAL:HG22 | 1:C:355:SER:N    | 2.25                     | 0.51              |
| 1:C:462:LEU:HD11 | 1:C:650:ILE:HD13 | 1.92                     | 0.51              |
| 1:D:460:PRO:HG2  | 1:D:461:HIS:CD2  | 2.45                     | 0.51              |
| 1:E:685:THR:CG2  | 1:E:686:GLY:H    | 2.24                     | 0.51              |
| 1:A:329:LYS:CG   | 1:A:330:SER:H    | 2.11                     | 0.51              |
| 1:A:699:ASP:HB3  | 1:A:703:ARG:HH11 | 1.75                     | 0.51              |
| 1:F:465:ALA:HB3  | 1:F:663:ILE:HG13 | 1.92                     | 0.51              |
| 1:B:387:ASP:OD2  | 1:C:378:VAL:HG23 | 2.10                     | 0.51              |
| 1:E:677:ASP:OD1  | 1:E:690:ARG:NH1  | 2.36                     | 0.51              |
| 1:D:347:LEU:HB3  | 1:D:352:VAL:HG23 | 1.92                     | 0.51              |
| 1:D:390:ARG:HE   | 1:E:378:VAL:CG2  | 2.22                     | 0.51              |
| 1:C:516:PRO:HG3  | 1:C:716:TYR:CE1  | 2.44                     | 0.51              |
| 1:C:354:VAL:HG22 | 1:C:355:SER:H    | 1.76                     | 0.51              |
| 1:F:677:ASP:OD1  | 1:F:690:ARG:NH1  | 2.39                     | 0.51              |
| 1:C:685:THR:CG2  | 1:C:686:GLY:H    | 2.23                     | 0.51              |
| 1:A:547:VAL:HG12 | 1:A:549:ASN:H    | 1.76                     | 0.51              |
| 1:F:488:THR:HG23 | 1:F:491:GLU:OE2  | 2.12                     | 0.51              |
| 1:A:354:VAL:HG21 | 1:A:370:ILE:CG1  | 2.41                     | 0.50              |
| 1:C:495:ILE:HG13 | 1:C:514:LEU:HD12 | 1.93                     | 0.50              |
| 1:B:462:LEU:HD11 | 1:B:650:ILE:HD13 | 1.92                     | 0.50              |
| 1:B:494:LEU:HD23 | 1:B:591:VAL:HB   | 1.93                     | 0.50              |
| 1:B:470:SER:HB2  | 1:B:652:PHE:HB3  | 1.93                     | 0.50              |
| 1:F:499:PRO:HB3  | 1:F:521:MET:HE2  | 1.93                     | 0.50              |
| 1:B:713:ALA:HB1  | 1:B:714:PRO:HD2  | 1.92                     | 0.50              |
| 1:A:554:ASN:HA   | 1:A:557:VAL:CG1  | 2.41                     | 0.50              |
| 1:B:599:ASP:OD1  | 1:B:632:ARG:NH1  | 2.44                     | 0.50              |
| 1:D:354:VAL:HG21 | 1:D:370:ILE:CG1  | 2.41                     | 0.50              |
| 1:E:592:VAL:HB   | 1:E:626:LEU:HD12 | 1.94                     | 0.50              |
| 1:E:717:ILE:O    | 1:E:719:ASP:N    | 2.45                     | 0.50              |
| 1:E:373:ALA:O    | 1:E:376:VAL:HG13 | 2.11                     | 0.50              |
| 1:D:501:MET:HE1  | 1:E:618:LYS:HE2  | 1.93                     | 0.50              |
| 1:F:592:VAL:HB   | 1:F:626:LEU:HD12 | 1.94                     | 0.50              |
| 1:B:672:LEU:HD13 | 1:B:678:MET:HA   | 1.94                     | 0.50              |
| 1:E:663:ILE:HG23 | 1:E:664:LEU:HG   | 1.93                     | 0.50              |
| 1:D:717:ILE:HD12 | 1:D:717:ILE:N    | 2.26                     | 0.50              |
| 1:F:599:ASP:OD1  | 1:F:632:ARG:NH1  | 2.45                     | 0.49              |
| 1:C:501:MET:CE   | 1:D:618:LYS:HE2  | 2.41                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:592:VAL:HB   | 1:C:626:LEU:HD12 | 1.94                     | 0.49              |
| 1:E:380:ARG:O    | 1:E:384:LEU:CD2  | 2.59                     | 0.49              |
| 1:E:699:ASP:HB3  | 1:E:703:ARG:HH11 | 1.76                     | 0.49              |
| 1:A:717:ILE:O    | 1:A:719:ASP:N    | 2.46                     | 0.49              |
| 1:D:373:ALA:O    | 1:D:376:VAL:HG13 | 2.12                     | 0.49              |
| 1:D:497:ILE:HD13 | 1:D:600:MET:HE2  | 1.94                     | 0.49              |
| 1:E:462:LEU:HD11 | 1:E:650:ILE:HD12 | 1.94                     | 0.49              |
| 1:E:717:ILE:HD12 | 1:E:717:ILE:N    | 2.27                     | 0.49              |
| 1:A:592:VAL:HB   | 1:A:626:LEU:HD12 | 1.94                     | 0.49              |
| 1:B:563:ALA:O    | 1:B:565:THR:N    | 2.46                     | 0.49              |
| 1:B:717:ILE:O    | 1:B:719:ASP:N    | 2.46                     | 0.49              |
| 1:C:365:ILE:HG12 | 1:C:366:THR:N    | 2.28                     | 0.49              |
| 1:E:460:PRO:HG2  | 1:E:461:HIS:CD2  | 2.48                     | 0.49              |
| 1:B:373:ALA:O    | 1:B:376:VAL:HG13 | 2.12                     | 0.49              |
| 1:D:717:ILE:O    | 1:D:719:ASP:N    | 2.46                     | 0.49              |
| 1:F:364:VAL:HG22 | 1:F:418:ARG:HG3  | 1.95                     | 0.49              |
| 1:D:597:PHE:CD1  | 1:D:601:MET:HE2  | 2.48                     | 0.49              |
| 1:E:390:ARG:HE   | 1:F:378:VAL:CG2  | 2.26                     | 0.49              |
| 1:A:549:ASN:OD1  | 1:A:551:ALA:HB3  | 2.13                     | 0.49              |
| 1:B:393:ALA:HB2  | 1:C:407:THR:CG2  | 2.43                     | 0.49              |
| 1:C:672:LEU:HD13 | 1:C:678:MET:HA   | 1.93                     | 0.49              |
| 1:D:713:ALA:HB1  | 1:D:714:PRO:HD2  | 1.94                     | 0.49              |
| 1:B:452:ILE:C    | 1:B:453:ILE:HD12 | 2.33                     | 0.49              |
| 1:C:364:VAL:HG22 | 1:C:418:ARG:HG3  | 1.95                     | 0.49              |
| 1:B:639:THR:O    | 1:B:643:LYS:HG3  | 2.13                     | 0.48              |
| 1:D:500:LYS:C    | 1:D:502:LEU:N    | 2.62                     | 0.48              |
| 1:F:672:LEU:HD13 | 1:F:678:MET:HA   | 1.95                     | 0.48              |
| 1:F:711:ARG:HG3  | 1:F:711:ARG:NH2  | 2.24                     | 0.48              |
| 1:A:500:LYS:C    | 1:A:502:LEU:N    | 2.63                     | 0.48              |
| 1:B:332:SER:OG   | 1:B:334:GLU:HG3  | 2.13                     | 0.48              |
| 1:F:663:ILE:HD13 | 1:F:663:ILE:C    | 2.33                     | 0.48              |
| 1:B:516:PRO:HG3  | 1:B:716:TYR:CE1  | 2.49                     | 0.48              |
| 1:D:663:ILE:HD13 | 1:D:663:ILE:C    | 2.32                     | 0.48              |
| 1:E:493:ARG:NH2  | 1:E:513:LEU:O    | 2.46                     | 0.48              |
| 1:E:534:GLU:O    | 1:E:538:ARG:HG3  | 2.13                     | 0.48              |
| 1:C:493:ARG:NH2  | 1:C:513:LEU:O    | 2.46                     | 0.48              |
| 1:B:549:ASN:OD1  | 1:B:551:ALA:HB3  | 2.14                     | 0.48              |
| 1:C:500:LYS:C    | 1:C:502:LEU:N    | 2.62                     | 0.48              |
| 1:D:631:GLN:O    | 1:D:633:PRO:HD3  | 2.13                     | 0.48              |
| 1:F:515:CYS:HB3  | 1:F:720:ILE:HG21 | 1.95                     | 0.48              |
| 1:B:365:ILE:HG12 | 1:B:366:THR:N    | 2.28                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:380:ARG:O    | 1:B:384:LEU:CD2  | 2.61                     | 0.48              |
| 1:B:554:ASN:HA   | 1:B:557:VAL:CG1  | 2.43                     | 0.48              |
| 1:E:521:MET:HE3  | 1:E:600:MET:CG   | 2.38                     | 0.48              |
| 1:F:380:ARG:O    | 1:F:384:LEU:CD2  | 2.61                     | 0.48              |
| 1:C:677:ASP:OD1  | 1:C:690:ARG:NH1  | 2.40                     | 0.48              |
| 1:F:597:PHE:CE1  | 1:F:601:MET:HE1  | 2.49                     | 0.48              |
| 1:F:717:ILE:O    | 1:F:719:ASP:N    | 2.47                     | 0.48              |
| 1:B:631:GLN:C    | 1:B:633:PRO:HD3  | 2.33                     | 0.48              |
| 1:C:470:SER:HB2  | 1:C:652:PHE:HB3  | 1.95                     | 0.48              |
| 1:D:463:LEU:HG   | 1:D:646:ILE:HG21 | 1.96                     | 0.48              |
| 1:E:457:ALA:HA   | 1:E:625:HIS:CD2  | 2.48                     | 0.48              |
| 1:A:532:VAL:O    | 1:A:536:GLU:HG2  | 2.14                     | 0.48              |
| 1:C:717:ILE:O    | 1:C:719:ASP:N    | 2.46                     | 0.48              |
| 1:E:347:LEU:HB3  | 1:E:352:VAL:HG23 | 1.96                     | 0.48              |
| 1:B:354:VAL:HG21 | 1:B:370:ILE:CG1  | 2.44                     | 0.48              |
| 1:B:532:VAL:O    | 1:B:536:GLU:HG2  | 2.13                     | 0.48              |
| 1:B:661:ARG:HA   | 1:B:666:GLN:H    | 1.79                     | 0.48              |
| 1:C:601:MET:HE3  | 1:C:637:VAL:HG13 | 1.96                     | 0.48              |
| 1:E:554:ASN:HA   | 1:E:557:VAL:CG1  | 2.43                     | 0.48              |
| 1:F:521:MET:HE3  | 1:F:600:MET:CG   | 2.43                     | 0.47              |
| 1:A:648:THR:OG1  | 1:A:683:PRO:HD3  | 2.13                     | 0.47              |
| 1:B:711:ARG:NH2  | 1:B:711:ARG:HG3  | 2.27                     | 0.47              |
| 1:C:354:VAL:HG21 | 1:C:370:ILE:CG1  | 2.43                     | 0.47              |
| 1:C:649:ARG:HB3  | 1:C:663:ILE:CD1  | 2.44                     | 0.47              |
| 1:E:663:ILE:HD13 | 1:E:663:ILE:C    | 2.34                     | 0.47              |
| 1:C:649:ARG:HB3  | 1:C:663:ILE:HD13 | 1.96                     | 0.47              |
| 1:E:500:LYS:C    | 1:E:502:LEU:N    | 2.63                     | 0.47              |
| 1:E:639:THR:O    | 1:E:643:LYS:HG3  | 2.14                     | 0.47              |
| 1:F:354:VAL:HG21 | 1:F:370:ILE:CG1  | 2.45                     | 0.47              |
| 1:A:317:PRO:C    | 1:A:319:SER:H    | 2.18                     | 0.47              |
| 1:C:365:ILE:HD11 | 1:C:447:ILE:HB   | 1.96                     | 0.47              |
| 1:D:521:MET:CE   | 1:D:600:MET:HG3  | 2.37                     | 0.47              |
| 1:D:658:ILE:CD1  | 1:D:658:ILE:H    | 2.23                     | 0.47              |
| 1:E:354:VAL:HG23 | 1:E:372:PRO:CA   | 2.45                     | 0.47              |
| 1:F:460:PRO:HG2  | 1:F:461:HIS:CD2  | 2.49                     | 0.47              |
| 1:F:631:GLN:O    | 1:F:633:PRO:HD3  | 2.13                     | 0.47              |
| 1:A:631:GLN:C    | 1:A:633:PRO:HD3  | 2.33                     | 0.47              |
| 1:B:460:PRO:HG2  | 1:B:461:HIS:CD2  | 2.49                     | 0.47              |
| 1:C:658:ILE:H    | 1:C:658:ILE:CD1  | 2.23                     | 0.47              |
| 1:C:631:GLN:C    | 1:C:633:PRO:HD3  | 2.35                     | 0.47              |
| 1:D:354:VAL:HG22 | 1:D:355:SER:N    | 2.30                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:354:VAL:HG22 | 1:B:355:SER:N    | 2.30                     | 0.47              |
| 1:A:515:CYS:HB3  | 1:A:720:ILE:HG21 | 1.96                     | 0.47              |
| 1:A:601:MET:HE1  | 1:A:637:VAL:HG13 | 1.97                     | 0.47              |
| 1:C:663:ILE:HD13 | 1:C:663:ILE:C    | 2.35                     | 0.47              |
| 1:D:516:PRO:HG3  | 1:D:716:TYR:CE1  | 2.50                     | 0.47              |
| 1:F:365:ILE:HD11 | 1:F:447:ILE:HB   | 1.96                     | 0.47              |
| 1:A:663:ILE:HG23 | 1:A:664:LEU:HG   | 1.97                     | 0.47              |
| 1:D:354:VAL:HG22 | 1:D:355:SER:H    | 1.80                     | 0.47              |
| 1:F:685:THR:CG2  | 1:F:686:GLY:H    | 2.26                     | 0.47              |
| 1:F:373:ALA:O    | 1:F:376:VAL:HG13 | 2.14                     | 0.47              |
| 1:A:460:PRO:HG2  | 1:A:461:HIS:CD2  | 2.50                     | 0.46              |
| 1:A:534:GLU:O    | 1:A:538:ARG:HG3  | 2.14                     | 0.46              |
| 1:F:597:PHE:CD1  | 1:F:601:MET:HE2  | 2.50                     | 0.46              |
| 1:B:699:ASP:HB3  | 1:B:703:ARG:HH11 | 1.80                     | 0.46              |
| 1:D:550:LEU:HD22 | 1:D:623:GLY:HA3  | 1.96                     | 0.46              |
| 1:D:601:MET:HE3  | 1:D:637:VAL:HG13 | 1.96                     | 0.46              |
| 1:C:320:LEU:O    | 1:C:703:ARG:NH2  | 2.45                     | 0.46              |
| 1:D:501:MET:CE   | 1:E:618:LYS:HE2  | 2.45                     | 0.46              |
| 1:F:354:VAL:HG22 | 1:F:355:SER:H    | 1.80                     | 0.46              |
| 1:A:516:PRO:HG3  | 1:A:716:TYR:CE1  | 2.51                     | 0.46              |
| 1:B:663:ILE:HG23 | 1:B:664:LEU:HG   | 1.97                     | 0.46              |
| 1:C:317:PRO:C    | 1:C:319:SER:H    | 2.17                     | 0.46              |
| 1:D:663:ILE:HG23 | 1:D:664:LEU:HG   | 1.96                     | 0.46              |
| 1:E:464:VAL:O    | 1:E:629:ALA:HA   | 2.15                     | 0.46              |
| 1:F:495:ILE:HG13 | 1:F:514:LEU:HD12 | 1.97                     | 0.46              |
| 1:F:516:PRO:HG3  | 1:F:716:TYR:CE1  | 2.51                     | 0.46              |
| 1:C:465:ALA:CB   | 1:C:663:ILE:HG13 | 2.45                     | 0.46              |
| 1:B:601:MET:HE3  | 1:B:637:VAL:HG13 | 1.97                     | 0.46              |
| 1:D:685:THR:CG2  | 1:D:686:GLY:H    | 2.27                     | 0.46              |
| 1:C:554:ASN:HA   | 1:C:557:VAL:CG1  | 2.45                     | 0.46              |
| 1:C:601:MET:HE1  | 1:C:637:VAL:HG13 | 1.97                     | 0.46              |
| 1:E:541:LEU:O    | 1:E:545:MET:HG2  | 2.15                     | 0.46              |
| 1:B:648:THR:OG1  | 1:B:683:PRO:HD3  | 2.16                     | 0.46              |
| 1:D:329:LYS:CD   | 1:D:329:LYS:H    | 2.28                     | 0.46              |
| 1:D:521:MET:HE3  | 1:D:600:MET:CG   | 2.35                     | 0.46              |
| 1:D:592:VAL:HB   | 1:D:626:LEU:HD12 | 1.98                     | 0.46              |
| 1:F:547:VAL:HG12 | 1:F:549:ASN:H    | 1.79                     | 0.46              |
| 1:A:597:PHE:CD1  | 1:A:601:MET:HE2  | 2.52                     | 0.46              |
| 1:B:329:LYS:CG   | 1:B:330:SER:H    | 2.13                     | 0.46              |
| 1:B:354:VAL:HG23 | 1:B:371:GLN:C    | 2.36                     | 0.46              |
| 1:F:500:LYS:C    | 1:F:502:LEU:N    | 2.63                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:663:ILE:HG23 | 1:F:664:LEU:HG   | 1.97                     | 0.45              |
| 1:F:657:LYS:HG2  | 1:F:670:GLU:OE1  | 2.15                     | 0.45              |
| 1:B:390:ARG:HE   | 1:C:378:VAL:CG2  | 2.29                     | 0.45              |
| 1:B:631:GLN:O    | 1:B:633:PRO:HD3  | 2.16                     | 0.45              |
| 1:A:494:LEU:CD2  | 1:A:591:VAL:HB   | 2.44                     | 0.45              |
| 1:A:672:LEU:HD13 | 1:A:678:MET:HA   | 1.98                     | 0.45              |
| 1:C:699:ASP:HB3  | 1:C:703:ARG:HH11 | 1.81                     | 0.45              |
| 1:D:597:PHE:CE1  | 1:D:601:MET:HE1  | 2.51                     | 0.45              |
| 1:F:329:LYS:N    | 1:F:329:LYS:HD3  | 2.31                     | 0.45              |
| 1:B:541:LEU:O    | 1:B:545:MET:HG2  | 2.16                     | 0.45              |
| 1:C:560:ALA:HB2  | 1:C:567:LEU:HG   | 1.98                     | 0.45              |
| 1:E:317:PRO:C    | 1:E:319:SER:H    | 2.20                     | 0.45              |
| 1:F:649:ARG:HB3  | 1:F:663:ILE:HD13 | 1.98                     | 0.45              |
| 1:A:364:VAL:HG22 | 1:A:418:ARG:HG3  | 1.98                     | 0.45              |
| 1:C:711:ARG:NH2  | 1:C:711:ARG:HG3  | 2.28                     | 0.45              |
| 1:F:560:ALA:HB2  | 1:F:567:LEU:HG   | 1.98                     | 0.45              |
| 1:B:317:PRO:C    | 1:B:319:SER:H    | 2.19                     | 0.45              |
| 1:B:320:LEU:O    | 1:B:703:ARG:NH2  | 2.42                     | 0.45              |
| 1:C:515:CYS:SG   | 1:C:720:ILE:HD13 | 2.57                     | 0.45              |
| 1:E:329:LYS:CD   | 1:E:329:LYS:H    | 2.30                     | 0.45              |
| 1:F:354:VAL:HG22 | 1:F:355:SER:N    | 2.32                     | 0.45              |
| 1:C:329:LYS:H    | 1:C:329:LYS:CD   | 2.30                     | 0.45              |
| 1:C:432:TYR:HB2  | 1:C:453:ILE:HG12 | 1.99                     | 0.45              |
| 1:D:649:ARG:HB3  | 1:D:663:ILE:CD1  | 2.46                     | 0.45              |
| 1:E:332:SER:OG   | 1:E:334:GLU:HG3  | 2.16                     | 0.45              |
| 1:F:354:VAL:HG23 | 1:F:372:PRO:CA   | 2.46                     | 0.45              |
| 1:F:672:LEU:HD21 | 1:F:679:LEU:HG   | 1.98                     | 0.45              |
| 1:B:347:LEU:HB3  | 1:B:352:VAL:HG23 | 1.98                     | 0.45              |
| 1:B:545:MET:HE1  | 1:B:553:PHE:CE1  | 2.52                     | 0.45              |
| 1:C:663:ILE:HG23 | 1:C:664:LEU:HG   | 1.98                     | 0.45              |
| 1:D:521:MET:HE2  | 1:D:600:MET:HA   | 1.99                     | 0.45              |
| 1:D:639:THR:O    | 1:D:643:LYS:HG3  | 2.17                     | 0.45              |
| 1:A:378:VAL:CG1  | 1:A:401:GLU:HG2  | 2.46                     | 0.45              |
| 1:A:657:LYS:HG2  | 1:A:670:GLU:OE1  | 2.17                     | 0.45              |
| 1:B:409:VAL:HG12 | 1:B:410:GLY:N    | 2.32                     | 0.45              |
| 1:C:332:SER:OG   | 1:C:334:GLU:HG3  | 2.16                     | 0.45              |
| 1:D:465:ALA:CB   | 1:D:663:ILE:HG13 | 2.47                     | 0.45              |
| 1:E:354:VAL:HG21 | 1:E:370:ILE:CG1  | 2.46                     | 0.45              |
| 1:E:450:ARG:HG2  | 1:E:450:ARG:HH21 | 1.82                     | 0.45              |
| 1:E:672:LEU:HD21 | 1:E:679:LEU:HG   | 1.99                     | 0.45              |
| 1:F:459:MET:N    | 1:F:460:PRO:HA   | 2.32                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:472:LYS:O    | 1:F:476:VAL:HG23 | 2.17                     | 0.45              |
| 1:A:464:VAL:O    | 1:A:629:ALA:HA   | 2.16                     | 0.45              |
| 1:B:563:ALA:C    | 1:B:565:THR:H    | 2.19                     | 0.45              |
| 1:E:672:LEU:HD13 | 1:E:678:MET:HA   | 1.99                     | 0.45              |
| 1:A:354:VAL:HG23 | 1:A:372:PRO:CA   | 2.46                     | 0.44              |
| 1:B:465:ALA:CB   | 1:B:663:ILE:HG13 | 2.47                     | 0.44              |
| 1:D:329:LYS:N    | 1:D:329:LYS:HD3  | 2.29                     | 0.44              |
| 1:E:649:ARG:HB3  | 1:E:663:ILE:CD1  | 2.47                     | 0.44              |
| 1:B:495:ILE:HG13 | 1:B:514:LEU:HD12 | 1.98                     | 0.44              |
| 1:B:649:ARG:HB3  | 1:B:663:ILE:CD1  | 2.48                     | 0.44              |
| 1:F:329:LYS:H    | 1:F:329:LYS:CD   | 2.29                     | 0.44              |
| 1:E:393:ALA:HB2  | 1:F:407:THR:CG2  | 2.48                     | 0.44              |
| 1:A:599:ASP:OD1  | 1:A:632:ARG:NH1  | 2.51                     | 0.44              |
| 1:C:373:ALA:O    | 1:C:376:VAL:HG13 | 2.17                     | 0.44              |
| 1:C:459:MET:N    | 1:C:460:PRO:HA   | 2.33                     | 0.44              |
| 1:E:365:ILE:HG12 | 1:E:366:THR:N    | 2.32                     | 0.44              |
| 1:A:329:LYS:CD   | 1:A:329:LYS:H    | 2.31                     | 0.44              |
| 1:A:378:VAL:CG2  | 1:F:390:ARG:HE   | 2.31                     | 0.44              |
| 1:D:354:VAL:HG23 | 1:D:372:PRO:CA   | 2.46                     | 0.44              |
| 1:D:393:ALA:HB2  | 1:E:407:THR:CG2  | 2.48                     | 0.44              |
| 1:B:450:ARG:HG2  | 1:B:450:ARG:HH21 | 1.82                     | 0.44              |
| 1:C:427:LEU:HD22 | 1:C:432:TYR:CZ   | 2.52                     | 0.44              |
| 1:D:332:SER:OG   | 1:D:334:GLU:HG3  | 2.18                     | 0.44              |
| 1:E:593:VAL:HG12 | 1:E:627:ILE:HB   | 1.99                     | 0.44              |
| 1:F:450:ARG:HH21 | 1:F:450:ARG:HG2  | 1.83                     | 0.44              |
| 1:C:380:ARG:O    | 1:C:384:LEU:CD2  | 2.62                     | 0.44              |
| 1:C:550:LEU:HD22 | 1:C:623:GLY:HA3  | 1.99                     | 0.44              |
| 1:C:563:ALA:C    | 1:C:565:THR:H    | 2.21                     | 0.44              |
| 1:C:631:GLN:O    | 1:C:633:PRO:HD3  | 2.18                     | 0.44              |
| 1:D:320:LEU:O    | 1:D:703:ARG:NH2  | 2.43                     | 0.44              |
| 1:F:534:GLU:O    | 1:F:538:ARG:HG3  | 2.18                     | 0.44              |
| 1:A:322:ASP:HA   | 1:A:323:PRO:HD3  | 1.83                     | 0.44              |
| 1:A:612:ILE:HD12 | 1:A:628:LEU:HD11 | 1.99                     | 0.44              |
| 1:C:612:ILE:HD12 | 1:C:628:LEU:HD11 | 1.99                     | 0.44              |
| 1:F:317:PRO:C    | 1:F:319:SER:H    | 2.21                     | 0.44              |
| 1:F:432:TYR:HB2  | 1:F:453:ILE:HG12 | 1.99                     | 0.44              |
| 1:A:563:ALA:O    | 1:A:565:THR:N    | 2.51                     | 0.44              |
| 1:B:354:VAL:HG23 | 1:B:372:PRO:CA   | 2.48                     | 0.44              |
| 1:B:597:PHE:CD1  | 1:B:601:MET:HE2  | 2.53                     | 0.44              |
| 1:C:518:VAL:HG22 | 1:C:721:LEU:HD21 | 2.00                     | 0.44              |
| 1:A:329:LYS:HD3  | 1:A:329:LYS:N    | 2.32                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:716:TYR:C    | 1:C:717:ILE:HD12 | 2.39                     | 0.43              |
| 1:F:494:LEU:CD2  | 1:F:591:VAL:HB   | 2.48                     | 0.43              |
| 1:E:521:MET:HB3  | 1:E:604:VAL:HG23 | 2.00                     | 0.43              |
| 1:E:578:ASP:O    | 1:E:579:ASP:C    | 2.56                     | 0.43              |
| 1:E:631:GLN:O    | 1:E:633:PRO:HD3  | 2.18                     | 0.43              |
| 1:A:332:SER:OG   | 1:A:334:GLU:HG3  | 2.18                     | 0.43              |
| 1:C:563:ALA:O    | 1:C:565:THR:N    | 2.51                     | 0.43              |
| 1:E:329:LYS:N    | 1:E:329:LYS:HD3  | 2.32                     | 0.43              |
| 1:E:409:VAL:HG12 | 1:E:410:GLY:N    | 2.33                     | 0.43              |
| 1:C:547:VAL:HG12 | 1:C:549:ASN:H    | 1.82                     | 0.43              |
| 1:B:446:ASP:OD2  | 1:B:450:ARG:HB2  | 2.19                     | 0.43              |
| 1:D:364:VAL:HB   | 1:D:692:HIS:CE1  | 2.54                     | 0.43              |
| 1:E:432:TYR:HB2  | 1:E:453:ILE:HG12 | 2.01                     | 0.43              |
| 1:C:450:ARG:HH21 | 1:C:450:ARG:HG2  | 1.82                     | 0.43              |
| 1:E:547:VAL:HG12 | 1:E:549:ASN:H    | 1.81                     | 0.43              |
| 1:E:494:LEU:CD2  | 1:E:591:VAL:HB   | 2.49                     | 0.43              |
| 1:E:597:PHE:CE1  | 1:E:601:MET:HE1  | 2.53                     | 0.43              |
| 1:A:427:LEU:HD22 | 1:A:432:TYR:CE2  | 2.54                     | 0.43              |
| 1:B:678:MET:HG2  | 1:B:691:VAL:O    | 2.19                     | 0.43              |
| 1:C:347:LEU:HB3  | 1:C:352:VAL:HG23 | 2.01                     | 0.43              |
| 1:D:341:ARG:N    | 1:D:341:ARG:HD2  | 2.34                     | 0.43              |
| 1:D:515:CYS:HB3  | 1:D:720:ILE:HG21 | 2.01                     | 0.43              |
| 1:F:320:LEU:O    | 1:F:703:ARG:NH2  | 2.44                     | 0.43              |
| 1:E:515:CYS:HB3  | 1:E:720:ILE:HG21 | 2.00                     | 0.43              |
| 1:A:452:ILE:C    | 1:A:453:ILE:HD12 | 2.38                     | 0.43              |
| 1:A:597:PHE:CE1  | 1:A:601:MET:HE1  | 2.54                     | 0.43              |
| 1:B:497:ILE:HD13 | 1:B:600:MET:CE   | 2.49                     | 0.43              |
| 1:B:515:CYS:HB3  | 1:B:720:ILE:HG21 | 2.00                     | 0.43              |
| 1:E:560:ALA:HB2  | 1:E:567:LEU:HG   | 2.00                     | 0.43              |
| 1:E:648:THR:OG1  | 1:E:683:PRO:HD3  | 2.19                     | 0.43              |
| 1:A:563:ALA:C    | 1:A:565:THR:H    | 2.22                     | 0.43              |
| 1:A:566:PRO:HB2  | 1:A:583:GLN:OE1  | 2.19                     | 0.43              |
| 1:A:678:MET:HG2  | 1:A:691:VAL:O    | 2.19                     | 0.43              |
| 1:B:541:LEU:HD22 | 1:B:553:PHE:CE1  | 2.54                     | 0.43              |
| 1:C:322:ASP:HA   | 1:C:323:PRO:HD3  | 1.84                     | 0.43              |
| 1:D:563:ALA:O    | 1:D:565:THR:N    | 2.52                     | 0.43              |
| 1:D:578:ASP:O    | 1:D:579:ASP:C    | 2.57                     | 0.43              |
| 1:D:711:ARG:NH2  | 1:D:711:ARG:HG3  | 2.31                     | 0.43              |
| 1:F:518:VAL:HG22 | 1:F:721:LEU:HD21 | 2.01                     | 0.43              |
| 1:B:329:LYS:H    | 1:B:329:LYS:CD   | 2.32                     | 0.42              |
| 1:F:373:ALA:O    | 1:F:376:VAL:CG1  | 2.66                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:563:ALA:O    | 1:F:565:THR:N    | 2.52                     | 0.42              |
| 1:A:446:ASP:OD2  | 1:A:450:ARG:HB2  | 2.20                     | 0.42              |
| 1:A:711:ARG:NH2  | 1:A:711:ARG:HG3  | 2.31                     | 0.42              |
| 1:B:547:VAL:HG12 | 1:B:549:ASN:H    | 1.84                     | 0.42              |
| 1:B:521:MET:HE2  | 1:B:600:MET:HA   | 2.01                     | 0.42              |
| 1:C:329:LYS:HD3  | 1:C:329:LYS:N    | 2.32                     | 0.42              |
| 1:F:361:PRO:HA   | 1:F:366:THR:HG23 | 2.00                     | 0.42              |
| 1:B:566:PRO:CB   | 1:B:583:GLN:OE1  | 2.67                     | 0.42              |
| 1:A:618:LYS:HE2  | 1:F:501:MET:CE   | 2.49                     | 0.42              |
| 1:B:493:ARG:NH2  | 1:B:513:LEU:O    | 2.53                     | 0.42              |
| 1:C:539:TYR:OH   | 1:C:621:ALA:HB3  | 2.19                     | 0.42              |
| 1:C:657:LYS:HG2  | 1:C:670:GLU:OE1  | 2.20                     | 0.42              |
| 1:D:380:ARG:O    | 1:D:384:LEU:CD2  | 2.61                     | 0.42              |
| 1:D:518:VAL:HG22 | 1:D:721:LEU:HD21 | 2.01                     | 0.42              |
| 1:E:364:VAL:HG22 | 1:E:418:ARG:HG3  | 2.00                     | 0.42              |
| 1:E:465:ALA:CB   | 1:E:663:ILE:HG13 | 2.49                     | 0.42              |
| 1:A:450:ARG:HH21 | 1:A:450:ARG:HG2  | 1.84                     | 0.42              |
| 1:A:465:ALA:CB   | 1:A:663:ILE:HG13 | 2.49                     | 0.42              |
| 1:C:597:PHE:CD1  | 1:C:601:MET:HE2  | 2.54                     | 0.42              |
| 1:E:702:HIS:O    | 1:E:706:GLU:HG2  | 2.20                     | 0.42              |
| 1:A:495:ILE:HG13 | 1:A:514:LEU:HD12 | 2.02                     | 0.42              |
| 1:A:649:ARG:HB3  | 1:A:663:ILE:CD1  | 2.49                     | 0.42              |
| 1:B:464:VAL:O    | 1:B:629:ALA:HA   | 2.20                     | 0.42              |
| 1:B:566:PRO:HB2  | 1:B:583:GLN:OE1  | 2.18                     | 0.42              |
| 1:C:317:PRO:C    | 1:C:319:SER:N    | 2.73                     | 0.42              |
| 1:C:578:ASP:O    | 1:C:579:ASP:C    | 2.57                     | 0.42              |
| 1:D:720:ILE:HG23 | 1:D:721:LEU:N    | 2.35                     | 0.42              |
| 1:E:495:ILE:HG13 | 1:E:514:LEU:HD12 | 2.02                     | 0.42              |
| 1:E:711:ARG:HG3  | 1:E:711:ARG:NH2  | 2.30                     | 0.42              |
| 1:F:563:ALA:C    | 1:F:565:THR:H    | 2.23                     | 0.42              |
| 1:A:427:LEU:HD22 | 1:A:432:TYR:CZ   | 2.54                     | 0.42              |
| 1:A:501:MET:CE   | 1:B:618:LYS:HE2  | 2.50                     | 0.42              |
| 1:D:365:ILE:HG12 | 1:D:366:THR:N    | 2.34                     | 0.42              |
| 1:D:427:LEU:HD22 | 1:D:432:TYR:CE2  | 2.55                     | 0.42              |
| 1:E:563:ALA:C    | 1:E:565:THR:H    | 2.23                     | 0.42              |
| 1:E:390:ARG:HH11 | 1:F:378:VAL:CG2  | 2.33                     | 0.42              |
| 1:E:550:LEU:HD22 | 1:E:623:GLY:HA3  | 2.02                     | 0.42              |
| 1:F:578:ASP:O    | 1:F:579:ASP:C    | 2.58                     | 0.42              |
| 1:D:354:VAL:HG23 | 1:D:371:GLN:C    | 2.40                     | 0.42              |
| 1:E:370:ILE:HD12 | 1:E:411:ILE:HG13 | 2.01                     | 0.42              |
| 1:E:413:ILE:HA   | 1:E:414:PRO:HD3  | 1.94                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:329:LYS:N    | 1:B:329:LYS:HD3  | 2.34                     | 0.41              |
| 1:B:370:ILE:HD12 | 1:B:411:ILE:HG13 | 2.02                     | 0.41              |
| 1:E:328:GLN:HE21 | 1:E:328:GLN:HB2  | 1.66                     | 0.41              |
| 1:E:612:ILE:HD12 | 1:E:628:LEU:HD11 | 2.01                     | 0.41              |
| 1:E:638:ILE:HG22 | 1:E:643:LYS:CG   | 2.50                     | 0.41              |
| 1:A:560:ALA:HB2  | 1:A:567:LEU:HG   | 2.00                     | 0.41              |
| 1:B:638:ILE:HG22 | 1:B:643:LYS:CG   | 2.51                     | 0.41              |
| 1:C:390:ARG:HH11 | 1:D:378:VAL:CG2  | 2.33                     | 0.41              |
| 1:A:459:MET:N    | 1:A:460:PRO:HA   | 2.36                     | 0.41              |
| 1:B:462:LEU:HD11 | 1:B:650:ILE:HD12 | 2.02                     | 0.41              |
| 1:A:566:PRO:CB   | 1:A:583:GLN:OE1  | 2.69                     | 0.41              |
| 1:A:515:CYS:SG   | 1:A:720:ILE:HD13 | 2.60                     | 0.41              |
| 1:B:672:LEU:HD21 | 1:B:679:LEU:HG   | 2.02                     | 0.41              |
| 1:D:560:ALA:HB2  | 1:D:567:LEU:HG   | 2.01                     | 0.41              |
| 1:D:390:ARG:NE   | 1:E:378:VAL:HG22 | 2.36                     | 0.41              |
| 1:A:317:PRO:C    | 1:A:319:SER:N    | 2.74                     | 0.41              |
| 1:C:373:ALA:O    | 1:C:376:VAL:CG1  | 2.68                     | 0.41              |
| 1:E:580:GLU:HA   | 1:E:581:PRO:HD3  | 1.93                     | 0.41              |
| 1:A:407:THR:CG2  | 1:F:393:ALA:HB2  | 2.51                     | 0.41              |
| 1:C:497:ILE:HD13 | 1:C:600:MET:CE   | 2.47                     | 0.41              |
| 1:E:354:VAL:HG22 | 1:E:355:SER:N    | 2.35                     | 0.41              |
| 1:A:578:ASP:O    | 1:A:579:ASP:C    | 2.58                     | 0.41              |
| 1:A:315:LEU:N    | 1:A:711:ARG:HE   | 2.19                     | 0.41              |
| 1:B:317:PRO:C    | 1:B:319:SER:N    | 2.74                     | 0.41              |
| 1:B:354:VAL:HG21 | 1:B:370:ILE:HG13 | 2.03                     | 0.41              |
| 1:B:459:MET:N    | 1:B:460:PRO:HA   | 2.35                     | 0.41              |
| 1:B:716:TYR:C    | 1:B:717:ILE:HD12 | 2.41                     | 0.41              |
| 1:E:563:ALA:O    | 1:E:565:THR:N    | 2.53                     | 0.41              |
| 1:E:631:GLN:C    | 1:E:633:PRO:HD3  | 2.40                     | 0.41              |
| 1:A:354:VAL:HG21 | 1:A:370:ILE:HG13 | 2.03                     | 0.41              |
| 1:B:463:LEU:HG   | 1:B:646:ILE:HG21 | 2.02                     | 0.41              |
| 1:C:580:GLU:HA   | 1:C:581:PRO:HD3  | 1.95                     | 0.41              |
| 1:E:320:LEU:O    | 1:E:703:ARG:NH2  | 2.47                     | 0.41              |
| 1:F:341:ARG:HD2  | 1:F:341:ARG:N    | 2.35                     | 0.41              |
| 1:B:373:ALA:O    | 1:B:376:VAL:CG1  | 2.68                     | 0.41              |
| 1:C:512:HIS:HE1  | 1:C:708:TRP:CD2  | 2.39                     | 0.41              |
| 1:B:578:ASP:O    | 1:B:579:ASP:C    | 2.58                     | 0.41              |
| 1:C:549:ASN:OD1  | 1:C:551:ALA:HB3  | 2.21                     | 0.41              |
| 1:E:341:ARG:HD2  | 1:E:341:ARG:N    | 2.35                     | 0.41              |
| 1:E:347:LEU:HA   | 1:E:347:LEU:HD23 | 1.92                     | 0.41              |
| 1:F:665:ASP:O    | 1:F:666:GLN:HB2  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:354:VAL:HG22 | 1:A:355:SER:H    | 1.86                     | 0.41              |
| 1:A:457:ALA:HA   | 1:A:625:HIS:CD2  | 2.56                     | 0.41              |
| 1:B:677:ASP:OD1  | 1:B:690:ARG:NH1  | 2.43                     | 0.41              |
| 1:C:672:LEU:HD21 | 1:C:679:LEU:HG   | 2.02                     | 0.41              |
| 1:D:347:LEU:HA   | 1:D:347:LEU:HD23 | 1.95                     | 0.41              |
| 1:E:501:MET:CE   | 1:F:618:LYS:HE2  | 2.51                     | 0.41              |
| 1:E:641:LEU:HD23 | 1:E:641:LEU:HA   | 1.86                     | 0.41              |
| 1:A:521:MET:HE3  | 1:A:600:MET:CG   | 2.46                     | 0.40              |
| 1:A:716:TYR:C    | 1:A:717:ILE:HD12 | 2.41                     | 0.40              |
| 1:C:413:ILE:HA   | 1:C:414:PRO:HD3  | 1.91                     | 0.40              |
| 1:D:354:VAL:HG21 | 1:D:370:ILE:HG13 | 2.02                     | 0.40              |
| 1:E:427:LEU:HD22 | 1:E:432:TYR:CE2  | 2.56                     | 0.40              |
| 1:F:593:VAL:HG12 | 1:F:627:ILE:HB   | 2.03                     | 0.40              |
| 1:A:453:ILE:N    | 1:A:453:ILE:HD12 | 2.36                     | 0.40              |
| 1:B:472:LYS:HE2  | 1:B:472:LYS:HB3  | 1.99                     | 0.40              |
| 1:B:539:TYR:OH   | 1:B:621:ALA:HB3  | 2.21                     | 0.40              |
| 1:C:648:THR:OG1  | 1:C:683:PRO:HD3  | 2.21                     | 0.40              |
| 1:D:450:ARG:HG2  | 1:D:450:ARG:HH21 | 1.86                     | 0.40              |
| 1:D:563:ALA:C    | 1:D:565:THR:H    | 2.25                     | 0.40              |
| 1:E:518:VAL:HG22 | 1:E:721:LEU:HD21 | 2.03                     | 0.40              |
| 1:F:322:ASP:HA   | 1:F:323:PRO:HD3  | 1.79                     | 0.40              |
| 1:A:440:PRO:O    | 1:A:482:SER:HB3  | 2.22                     | 0.40              |
| 1:B:560:ALA:HB2  | 1:B:567:LEU:HG   | 2.03                     | 0.40              |
| 1:C:488:THR:HG23 | 1:C:491:GLU:OE2  | 2.20                     | 0.40              |
| 1:D:612:ILE:HD12 | 1:D:628:LEU:HD11 | 2.04                     | 0.40              |
| 1:E:452:ILE:C    | 1:E:453:ILE:HD12 | 2.41                     | 0.40              |
| 1:E:566:PRO:HB2  | 1:E:583:GLN:OE1  | 2.22                     | 0.40              |
| 1:E:566:PRO:CB   | 1:E:583:GLN:OE1  | 2.70                     | 0.40              |
| 1:E:457:ALA:HA   | 1:E:625:HIS:NE2  | 2.36                     | 0.40              |
| 1:E:657:LYS:HG2  | 1:E:670:GLU:OE1  | 2.21                     | 0.40              |
| 1:F:639:THR:O    | 1:F:643:LYS:HG3  | 2.22                     | 0.40              |
| 1:D:427:LEU:HD22 | 1:D:432:TYR:CZ   | 2.57                     | 0.40              |
| 1:F:383:ASN:HA   | 1:F:383:ASN:HD22 | 1.63                     | 0.40              |
| 1:A:320:LEU:O    | 1:A:703:ARG:NH2  | 2.44                     | 0.40              |
| 1:E:418:ARG:NH2  | 1:E:675:HIS:HB2  | 2.36                     | 0.40              |
| 1:F:354:VAL:HG23 | 1:F:371:GLN:C    | 2.41                     | 0.40              |
| 1:F:593:VAL:HG23 | 1:F:593:VAL:O    | 2.20                     | 0.40              |
| 1:F:711:ARG:HH21 | 1:F:711:ARG:CG   | 2.29                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|------------------------|--------------------------|-------------------|
| 1:B:338:ALA:O | 1:D:434:GLU:OE2[4_554] | 2.00                     | 0.20              |

## 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     | 406/491 (83%)   | 373 (92%)  | 27 (7%)  | 6 (2%)   | 12          | 39 |
| 1   | B     | 406/491 (83%)   | 376 (93%)  | 25 (6%)  | 5 (1%)   | 15          | 46 |
| 1   | C     | 406/491 (83%)   | 377 (93%)  | 24 (6%)  | 5 (1%)   | 15          | 46 |
| 1   | D     | 406/491 (83%)   | 380 (94%)  | 21 (5%)  | 5 (1%)   | 15          | 46 |
| 1   | E     | 406/491 (83%)   | 375 (92%)  | 26 (6%)  | 5 (1%)   | 15          | 46 |
| 1   | F     | 406/491 (83%)   | 375 (92%)  | 26 (6%)  | 5 (1%)   | 15          | 46 |
| All | All   | 2436/2946 (83%) | 2256 (93%) | 149 (6%) | 31 (1%)  | 14          | 43 |

All (31) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 501 | MET  |
| 1   | B     | 501 | MET  |
| 1   | C     | 501 | MET  |
| 1   | D     | 501 | MET  |
| 1   | E     | 501 | MET  |
| 1   | F     | 501 | MET  |
| 1   | A     | 330 | SER  |
| 1   | A     | 564 | GLY  |
| 1   | A     | 718 | GLU  |
| 1   | B     | 330 | SER  |
| 1   | B     | 564 | GLY  |
| 1   | B     | 718 | GLU  |
| 1   | C     | 330 | SER  |
| 1   | C     | 564 | GLY  |
| 1   | C     | 718 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 330 | SER  |
| 1   | D     | 564 | GLY  |
| 1   | D     | 718 | GLU  |
| 1   | E     | 330 | SER  |
| 1   | E     | 718 | GLU  |
| 1   | F     | 330 | SER  |
| 1   | F     | 564 | GLY  |
| 1   | F     | 718 | GLU  |
| 1   | E     | 564 | GLY  |
| 1   | A     | 620 | ARG  |
| 1   | E     | 326 | VAL  |
| 1   | F     | 326 | VAL  |
| 1   | C     | 326 | VAL  |
| 1   | A     | 326 | VAL  |
| 1   | B     | 326 | VAL  |
| 1   | D     | 326 | VAL  |

### 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     | 346/419 (83%)   | 328 (95%)  | 18 (5%)  | 27          | 61 |
| 1   | B     | 346/419 (83%)   | 325 (94%)  | 21 (6%)  | 22          | 53 |
| 1   | C     | 346/419 (83%)   | 326 (94%)  | 20 (6%)  | 23          | 56 |
| 1   | D     | 346/419 (83%)   | 326 (94%)  | 20 (6%)  | 23          | 56 |
| 1   | E     | 346/419 (83%)   | 326 (94%)  | 20 (6%)  | 23          | 56 |
| 1   | F     | 346/419 (83%)   | 326 (94%)  | 20 (6%)  | 23          | 56 |
| All | All   | 2076/2514 (83%) | 1957 (94%) | 119 (6%) | 24          | 56 |

All (119) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 329 | LYS  |
| 1   | A     | 337 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 342 | LEU  |
| 1   | A     | 343 | LEU  |
| 1   | A     | 365 | ILE  |
| 1   | A     | 370 | ILE  |
| 1   | A     | 376 | VAL  |
| 1   | A     | 384 | LEU  |
| 1   | A     | 456 | LEU  |
| 1   | A     | 501 | MET  |
| 1   | A     | 502 | LEU  |
| 1   | A     | 506 | ILE  |
| 1   | A     | 519 | THR  |
| 1   | A     | 541 | LEU  |
| 1   | A     | 626 | LEU  |
| 1   | A     | 650 | ILE  |
| 1   | A     | 663 | ILE  |
| 1   | A     | 696 | VAL  |
| 1   | B     | 329 | LYS  |
| 1   | B     | 337 | GLU  |
| 1   | B     | 342 | LEU  |
| 1   | B     | 343 | LEU  |
| 1   | B     | 365 | ILE  |
| 1   | B     | 370 | ILE  |
| 1   | B     | 376 | VAL  |
| 1   | B     | 384 | LEU  |
| 1   | B     | 397 | VAL  |
| 1   | B     | 456 | LEU  |
| 1   | B     | 488 | THR  |
| 1   | B     | 501 | MET  |
| 1   | B     | 502 | LEU  |
| 1   | B     | 506 | ILE  |
| 1   | B     | 519 | THR  |
| 1   | B     | 521 | MET  |
| 1   | B     | 541 | LEU  |
| 1   | B     | 626 | LEU  |
| 1   | B     | 650 | ILE  |
| 1   | B     | 663 | ILE  |
| 1   | B     | 696 | VAL  |
| 1   | C     | 329 | LYS  |
| 1   | C     | 337 | GLU  |
| 1   | C     | 342 | LEU  |
| 1   | C     | 343 | LEU  |
| 1   | C     | 365 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 370 | ILE  |
| 1   | C     | 376 | VAL  |
| 1   | C     | 384 | LEU  |
| 1   | C     | 397 | VAL  |
| 1   | C     | 456 | LEU  |
| 1   | C     | 488 | THR  |
| 1   | C     | 501 | MET  |
| 1   | C     | 502 | LEU  |
| 1   | C     | 506 | ILE  |
| 1   | C     | 519 | THR  |
| 1   | C     | 541 | LEU  |
| 1   | C     | 626 | LEU  |
| 1   | C     | 650 | ILE  |
| 1   | C     | 663 | ILE  |
| 1   | C     | 696 | VAL  |
| 1   | D     | 329 | LYS  |
| 1   | D     | 337 | GLU  |
| 1   | D     | 342 | LEU  |
| 1   | D     | 343 | LEU  |
| 1   | D     | 365 | ILE  |
| 1   | D     | 370 | ILE  |
| 1   | D     | 376 | VAL  |
| 1   | D     | 384 | LEU  |
| 1   | D     | 456 | LEU  |
| 1   | D     | 488 | THR  |
| 1   | D     | 501 | MET  |
| 1   | D     | 502 | LEU  |
| 1   | D     | 506 | ILE  |
| 1   | D     | 519 | THR  |
| 1   | D     | 521 | MET  |
| 1   | D     | 541 | LEU  |
| 1   | D     | 626 | LEU  |
| 1   | D     | 650 | ILE  |
| 1   | D     | 663 | ILE  |
| 1   | D     | 696 | VAL  |
| 1   | E     | 329 | LYS  |
| 1   | E     | 337 | GLU  |
| 1   | E     | 342 | LEU  |
| 1   | E     | 343 | LEU  |
| 1   | E     | 365 | ILE  |
| 1   | E     | 370 | ILE  |
| 1   | E     | 376 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 384 | LEU  |
| 1   | E     | 456 | LEU  |
| 1   | E     | 488 | THR  |
| 1   | E     | 501 | MET  |
| 1   | E     | 502 | LEU  |
| 1   | E     | 506 | ILE  |
| 1   | E     | 519 | THR  |
| 1   | E     | 521 | MET  |
| 1   | E     | 541 | LEU  |
| 1   | E     | 626 | LEU  |
| 1   | E     | 650 | ILE  |
| 1   | E     | 663 | ILE  |
| 1   | E     | 696 | VAL  |
| 1   | F     | 329 | LYS  |
| 1   | F     | 337 | GLU  |
| 1   | F     | 342 | LEU  |
| 1   | F     | 343 | LEU  |
| 1   | F     | 365 | ILE  |
| 1   | F     | 370 | ILE  |
| 1   | F     | 376 | VAL  |
| 1   | F     | 384 | LEU  |
| 1   | F     | 456 | LEU  |
| 1   | F     | 488 | THR  |
| 1   | F     | 501 | MET  |
| 1   | F     | 502 | LEU  |
| 1   | F     | 506 | ILE  |
| 1   | F     | 519 | THR  |
| 1   | F     | 521 | MET  |
| 1   | F     | 541 | LEU  |
| 1   | F     | 626 | LEU  |
| 1   | F     | 650 | ILE  |
| 1   | F     | 663 | ILE  |
| 1   | F     | 696 | VAL  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 328 | GLN  |
| 1   | A     | 383 | ASN  |
| 1   | A     | 415 | ASN  |
| 1   | A     | 554 | ASN  |
| 1   | A     | 631 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 666 | GLN  |
| 1   | B     | 328 | GLN  |
| 1   | B     | 383 | ASN  |
| 1   | B     | 415 | ASN  |
| 1   | B     | 554 | ASN  |
| 1   | B     | 631 | GLN  |
| 1   | C     | 328 | GLN  |
| 1   | C     | 383 | ASN  |
| 1   | C     | 415 | ASN  |
| 1   | C     | 554 | ASN  |
| 1   | C     | 625 | HIS  |
| 1   | C     | 631 | GLN  |
| 1   | D     | 328 | GLN  |
| 1   | D     | 383 | ASN  |
| 1   | D     | 415 | ASN  |
| 1   | D     | 554 | ASN  |
| 1   | D     | 631 | GLN  |
| 1   | D     | 666 | GLN  |
| 1   | E     | 328 | GLN  |
| 1   | E     | 383 | ASN  |
| 1   | E     | 415 | ASN  |
| 1   | E     | 554 | ASN  |
| 1   | E     | 631 | GLN  |
| 1   | E     | 666 | GLN  |
| 1   | F     | 328 | GLN  |
| 1   | F     | 383 | ASN  |
| 1   | F     | 415 | ASN  |
| 1   | F     | 554 | ASN  |
| 1   | F     | 631 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 2   | ADP  | A     | 1723 | -    | 25,29,29     | 0.99 | 1 (4%)      | 24,45,45    | 1.93 | 4 (16%)     |
| 2   | ADP  | B     | 1723 | -    | 25,29,29     | 0.93 | 1 (4%)      | 24,45,45    | 1.94 | 4 (16%)     |
| 2   | ADP  | C     | 1723 | -    | 25,29,29     | 0.94 | 1 (4%)      | 24,45,45    | 1.88 | 4 (16%)     |
| 2   | ADP  | D     | 1723 | -    | 25,29,29     | 0.94 | 1 (4%)      | 24,45,45    | 1.97 | 4 (16%)     |
| 2   | ADP  | E     | 1723 | -    | 25,29,29     | 0.98 | 1 (4%)      | 24,45,45    | 1.96 | 4 (16%)     |
| 2   | ADP  | F     | 1723 | -    | 25,29,29     | 1.02 | 1 (4%)      | 24,45,45    | 1.92 | 4 (16%)     |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | ADP  | A     | 1723 | -    | -       | 0/12/32/32 | 0/3/3/3 |
| 2   | ADP  | B     | 1723 | -    | -       | 0/12/32/32 | 0/3/3/3 |
| 2   | ADP  | C     | 1723 | -    | -       | 0/12/32/32 | 0/3/3/3 |
| 2   | ADP  | D     | 1723 | -    | -       | 0/12/32/32 | 0/3/3/3 |
| 2   | ADP  | E     | 1723 | -    | -       | 0/12/32/32 | 0/3/3/3 |
| 2   | ADP  | F     | 1723 | -    | -       | 0/12/32/32 | 0/3/3/3 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2   | B     | 1723 | ADP  | C2-N1 | 3.22 | 1.39        | 1.33     |
| 2   | D     | 1723 | ADP  | C2-N1 | 3.29 | 1.40        | 1.33     |
| 2   | C     | 1723 | ADP  | C2-N1 | 3.34 | 1.40        | 1.33     |
| 2   | E     | 1723 | ADP  | C2-N1 | 3.44 | 1.40        | 1.33     |
| 2   | A     | 1723 | ADP  | C2-N1 | 3.45 | 1.40        | 1.33     |
| 2   | F     | 1723 | ADP  | C2-N1 | 3.55 | 1.40        | 1.33     |

All (24) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | D     | 1723 | ADP  | N3-C2-N1    | -6.51 | 123.19      | 128.86   |
| 2   | A     | 1723 | ADP  | N3-C2-N1    | -6.42 | 123.26      | 128.86   |
| 2   | E     | 1723 | ADP  | N3-C2-N1    | -6.37 | 123.31      | 128.86   |
| 2   | C     | 1723 | ADP  | N3-C2-N1    | -6.26 | 123.41      | 128.86   |
| 2   | B     | 1723 | ADP  | N3-C2-N1    | -6.14 | 123.51      | 128.86   |
| 2   | F     | 1723 | ADP  | N3-C2-N1    | -6.08 | 123.56      | 128.86   |
| 2   | A     | 1723 | ADP  | C2-N1-C6    | 2.59  | 123.30      | 118.77   |
| 2   | C     | 1723 | ADP  | C5-C6-N6    | 2.60  | 125.77      | 120.47   |
| 2   | F     | 1723 | ADP  | C5-C6-N6    | 2.61  | 125.79      | 120.47   |
| 2   | D     | 1723 | ADP  | C5-C6-N6    | 2.62  | 125.81      | 120.47   |
| 2   | A     | 1723 | ADP  | C5-C6-N6    | 2.65  | 125.87      | 120.47   |
| 2   | C     | 1723 | ADP  | C2-N1-C6    | 2.67  | 123.45      | 118.77   |
| 2   | E     | 1723 | ADP  | C2-N1-C6    | 2.68  | 123.47      | 118.77   |
| 2   | B     | 1723 | ADP  | C2-N1-C6    | 2.71  | 123.51      | 118.77   |
| 2   | E     | 1723 | ADP  | C5-C6-N6    | 2.71  | 126.00      | 120.47   |
| 2   | F     | 1723 | ADP  | C2-N1-C6    | 2.73  | 123.54      | 118.77   |
| 2   | B     | 1723 | ADP  | C5-C6-N6    | 2.78  | 126.14      | 120.47   |
| 2   | D     | 1723 | ADP  | C2-N1-C6    | 2.81  | 123.68      | 118.77   |
| 2   | C     | 1723 | ADP  | C4'-O4'-C1' | 3.29  | 113.27      | 109.77   |
| 2   | F     | 1723 | ADP  | C4'-O4'-C1' | 3.51  | 113.50      | 109.77   |
| 2   | A     | 1723 | ADP  | C4'-O4'-C1' | 3.52  | 113.52      | 109.77   |
| 2   | D     | 1723 | ADP  | C4'-O4'-C1' | 3.57  | 113.57      | 109.77   |
| 2   | E     | 1723 | ADP  | C4'-O4'-C1' | 3.67  | 113.67      | 109.77   |
| 2   | B     | 1723 | ADP  | C4'-O4'-C1' | 3.81  | 113.83      | 109.77   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2 |       | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|-----------------|--------|-----------|-------|-----------------------|---------|
| 1   | A     | 408/491 (83%)   | 0.40   | 23 (5%)   | 25 20 | 48, 72, 110, 136      | 0       |
| 1   | B     | 408/491 (83%)   | 0.16   | 8 (1%)    | 65 62 | 37, 57, 97, 127       | 0       |
| 1   | C     | 408/491 (83%)   | 0.11   | 9 (2%)    | 62 59 | 31, 51, 93, 140       | 0       |
| 1   | D     | 408/491 (83%)   | 0.09   | 4 (0%)    | 82 81 | 32, 49, 85, 131       | 0       |
| 1   | E     | 408/491 (83%)   | 0.27   | 16 (3%)   | 40 35 | 42, 65, 102, 142      | 0       |
| 1   | F     | 408/491 (83%)   | 0.33   | 20 (4%)   | 30 26 | 47, 73, 108, 140      | 0       |
| All | All   | 2448/2946 (83%) | 0.23   | 80 (3%)   | 47 40 | 31, 62, 103, 142      | 0       |

All (80) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 328 | GLN  | 8.3  |
| 1   | E     | 329 | LYS  | 6.1  |
| 1   | C     | 328 | GLN  | 4.4  |
| 1   | F     | 326 | VAL  | 4.2  |
| 1   | C     | 329 | LYS  | 4.0  |
| 1   | A     | 326 | VAL  | 3.8  |
| 1   | C     | 326 | VAL  | 3.8  |
| 1   | A     | 336 | LEU  | 3.6  |
| 1   | E     | 567 | LEU  | 3.5  |
| 1   | A     | 328 | GLN  | 3.5  |
| 1   | B     | 328 | GLN  | 3.4  |
| 1   | F     | 328 | GLN  | 3.4  |
| 1   | F     | 565 | THR  | 3.4  |
| 1   | E     | 331 | TYR  | 3.3  |
| 1   | F     | 316 | PRO  | 3.3  |
| 1   | B     | 326 | VAL  | 3.3  |
| 1   | E     | 326 | VAL  | 3.3  |
| 1   | C     | 327 | LYS  | 3.2  |
| 1   | F     | 584 | LEU  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 331 | TYR  | 3.2  |
| 1   | A     | 581 | PRO  | 3.2  |
| 1   | F     | 329 | LYS  | 3.2  |
| 1   | A     | 318 | LEU  | 3.2  |
| 1   | A     | 584 | LEU  | 3.1  |
| 1   | F     | 427 | LEU  | 3.1  |
| 1   | A     | 562 | GLU  | 3.0  |
| 1   | A     | 325 | GLU  | 3.0  |
| 1   | F     | 419 | GLN  | 2.9  |
| 1   | C     | 330 | SER  | 2.9  |
| 1   | B     | 565 | THR  | 2.8  |
| 1   | A     | 567 | LEU  | 2.8  |
| 1   | A     | 580 | GLU  | 2.8  |
| 1   | E     | 352 | VAL  | 2.8  |
| 1   | A     | 572 | PHE  | 2.7  |
| 1   | A     | 566 | PRO  | 2.7  |
| 1   | F     | 330 | SER  | 2.7  |
| 1   | A     | 565 | THR  | 2.7  |
| 1   | D     | 328 | GLN  | 2.7  |
| 1   | A     | 327 | LYS  | 2.7  |
| 1   | E     | 560 | ALA  | 2.7  |
| 1   | A     | 381 | ILE  | 2.6  |
| 1   | A     | 719 | ASP  | 2.6  |
| 1   | F     | 566 | PRO  | 2.6  |
| 1   | C     | 584 | LEU  | 2.6  |
| 1   | D     | 584 | LEU  | 2.6  |
| 1   | B     | 562 | GLU  | 2.6  |
| 1   | E     | 710 | LEU  | 2.6  |
| 1   | E     | 357 | ASP  | 2.5  |
| 1   | F     | 580 | GLU  | 2.5  |
| 1   | A     | 563 | ALA  | 2.4  |
| 1   | E     | 343 | LEU  | 2.4  |
| 1   | B     | 707 | ALA  | 2.4  |
| 1   | F     | 702 | HIS  | 2.4  |
| 1   | C     | 565 | THR  | 2.4  |
| 1   | C     | 325 | GLU  | 2.4  |
| 1   | A     | 560 | ALA  | 2.4  |
| 1   | F     | 557 | VAL  | 2.4  |
| 1   | D     | 352 | VAL  | 2.3  |
| 1   | F     | 583 | GLN  | 2.3  |
| 1   | E     | 368 | PHE  | 2.3  |
| 1   | E     | 573 | ARG  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 329 | LYS  | 2.3  |
| 1   | F     | 710 | LEU  | 2.3  |
| 1   | F     | 323 | PRO  | 2.2  |
| 1   | E     | 330 | SER  | 2.2  |
| 1   | E     | 718 | GLU  | 2.2  |
| 1   | B     | 567 | LEU  | 2.2  |
| 1   | A     | 330 | SER  | 2.2  |
| 1   | F     | 317 | PRO  | 2.2  |
| 1   | A     | 331 | TYR  | 2.1  |
| 1   | A     | 370 | ILE  | 2.1  |
| 1   | F     | 325 | GLU  | 2.1  |
| 1   | F     | 336 | LEU  | 2.1  |
| 1   | E     | 339 | MET  | 2.1  |
| 1   | E     | 565 | THR  | 2.1  |
| 1   | D     | 560 | ALA  | 2.1  |
| 1   | F     | 582 | PRO  | 2.0  |
| 1   | B     | 578 | ASP  | 2.0  |
| 1   | A     | 582 | PRO  | 2.0  |
| 1   | C     | 580 | GLU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 2   | ADP  | D     | 1723 | 27/27 | 0.92 | 0.22 | 1.15 | 62,72,76,81                | 0     |
| 2   | ADP  | C     | 1723 | 27/27 | 0.92 | 0.22 | 0.70 | 67,82,87,88                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 2   | ADP  | A     | 1723 | 27/27 | 0.86 | 0.23 | 0.67 | 93,96,103,104               | 0     |
| 2   | ADP  | E     | 1723 | 27/27 | 0.90 | 0.22 | 0.32 | 87,90,91,91                 | 0     |
| 2   | ADP  | B     | 1723 | 27/27 | 0.92 | 0.21 | 0.25 | 75,82,85,88                 | 0     |
| 2   | ADP  | F     | 1723 | 27/27 | 0.86 | 0.22 | 0.11 | 87,100,105,105              | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.