



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:35 AM UTC

PDB ID : 1GZ3 / pdb\_00001gz3  
Title : Molecular mechanism for the regulation of human mitochondrial NAD(P)<sup>+</sup>-dependent malic enzyme by ATP and fumarate  
Authors : Yang, Z.; Lanks, C.W.; Tong, L.  
Deposited on : 2002-05-14  
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | <b>NOT EXECUTED</b>                                              |
| EDS                            | : | <b>NOT EXECUTED</b>                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

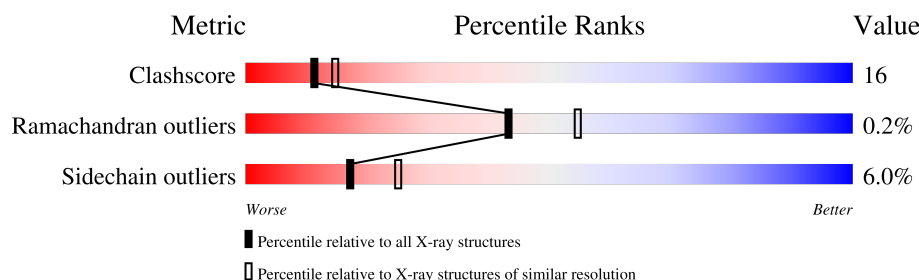
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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            | 190562                      | 6919 (2.30-2.30)                                      |
| Ramachandran outliers | 187476                      | 6854 (2.30-2.30)                                      |
| Sidechain outliers    | 187428                      | 6854 (2.30-2.30)                                      |

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 554    | 68% 28% 5%       |
| 1   | B     | 554    | 66% 30% .        |
| 1   | C     | 554    | 68% 30% .        |
| 1   | D     | 554    | 69% 28% .        |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18818 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.

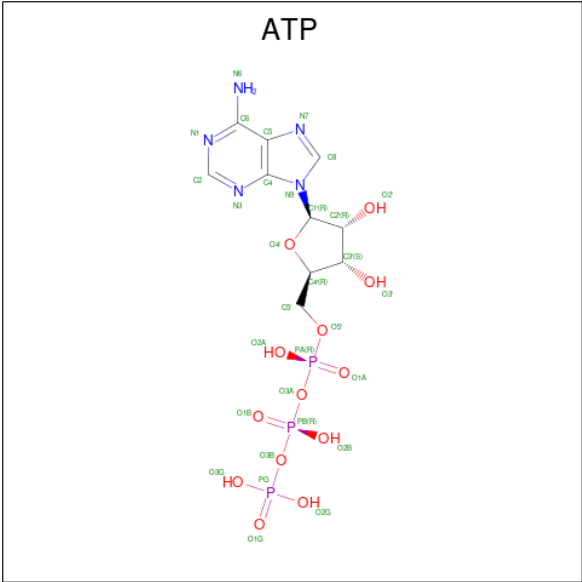
- Molecule 1 is a protein called NAD-dependent malic enzyme, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 554      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4369  | 2799 | 740 | 807 | 23 |         |         |       |
| 1   | B     | 554      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4369  | 2799 | 740 | 807 | 23 |         |         |       |
| 1   | C     | 554      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4369  | 2799 | 740 | 807 | 23 |         |         |       |
| 1   | D     | 554      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4370  | 2799 | 740 | 808 | 23 |         |         |       |

There are 12 discrepancies between the modelled and reference sequences:

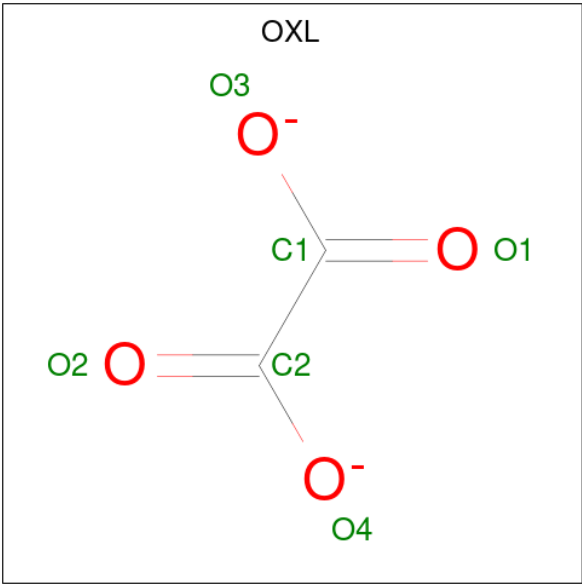
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 197     | GLN      | ARG    | engineered mutation | UNP P23368 |
| A     | 542     | VAL      | ARG    | engineered mutation | UNP P23368 |
| A     | 556     | GLN      | ARG    | conflict            | UNP P23368 |
| B     | 197     | GLN      | ARG    | engineered mutation | UNP P23368 |
| B     | 542     | VAL      | ARG    | engineered mutation | UNP P23368 |
| B     | 556     | GLN      | ARG    | conflict            | UNP P23368 |
| C     | 197     | GLN      | ARG    | engineered mutation | UNP P23368 |
| C     | 542     | VAL      | ARG    | engineered mutation | UNP P23368 |
| C     | 556     | GLN      | ARG    | conflict            | UNP P23368 |
| D     | 197     | GLN      | ARG    | engineered mutation | UNP P23368 |
| D     | 542     | VAL      | ARG    | engineered mutation | UNP P23368 |
| D     | 556     | GLN      | ARG    | conflict            | UNP P23368 |

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |
| 2   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |
| 2   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |
| 2   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |         |

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C<sub>2</sub>O<sub>4</sub>).

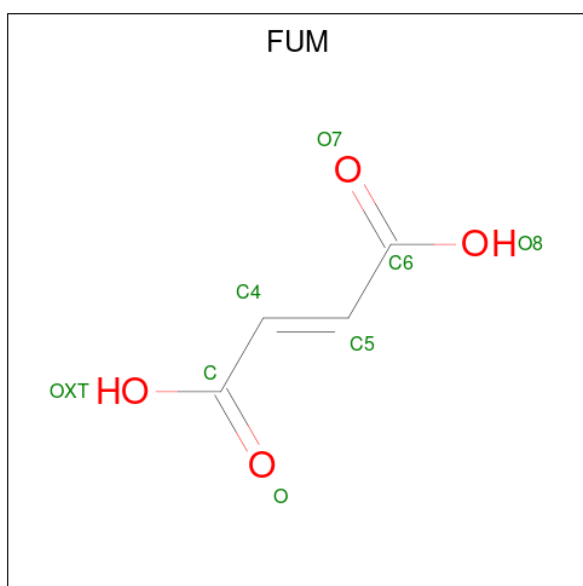


| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 2 | 4 |         |         |
| 3   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 2 | 4 |         |         |
| 3   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 2 | 4 |         |         |
| 3   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 2 | 4 |         |         |

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 1        | Total | Mn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | B     | 1        | Total | Mn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | C     | 1        | Total | Mn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | D     | 1        | Total | Mn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 5 is FUMARIC ACID (CCD ID: FUM) (formula: C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>).



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

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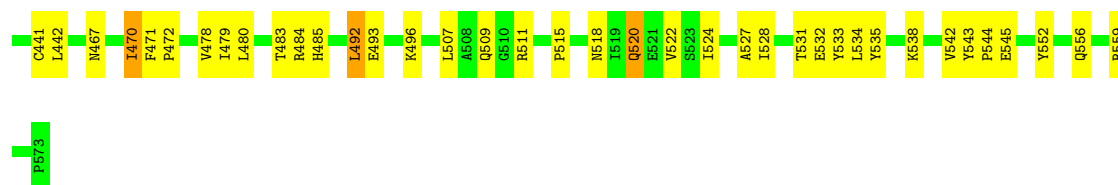
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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 4 | 4 |         |         |
| 5   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 4 | 4 |         |         |

- Molecule 6 is water.

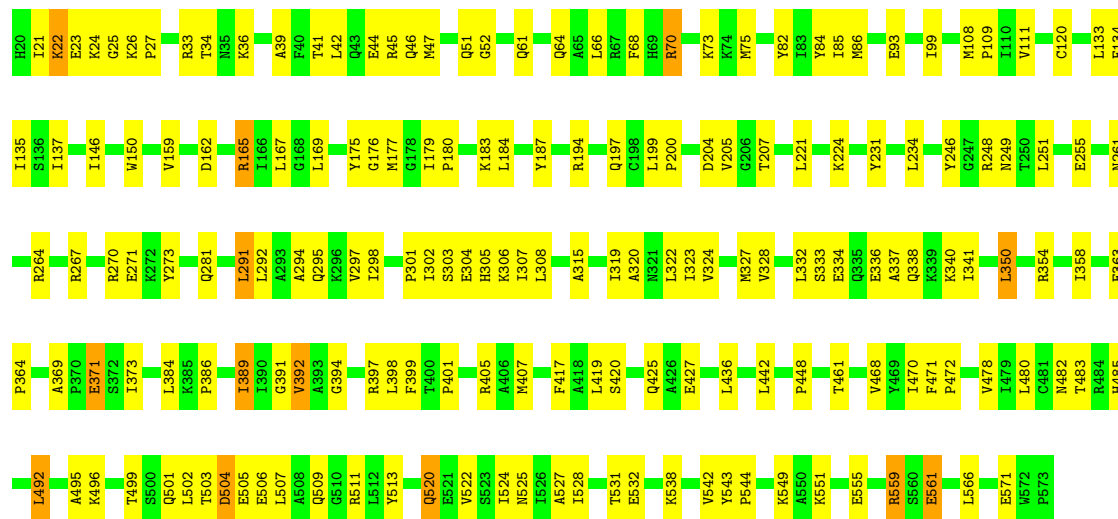
| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 6   | A     | 267      | Total | O   | 0       | 0       |
|     |       |          | 267   | 267 |         |         |
| 6   | B     | 290      | Total | O   | 0       | 0       |
|     |       |          | 290   | 290 |         |         |
| 6   | C     | 300      | Total | O   | 0       | 0       |
|     |       |          | 300   | 300 |         |         |
| 6   | D     | 300      | Total | O   | 0       | 0       |
|     |       |          | 300   | 300 |         |         |





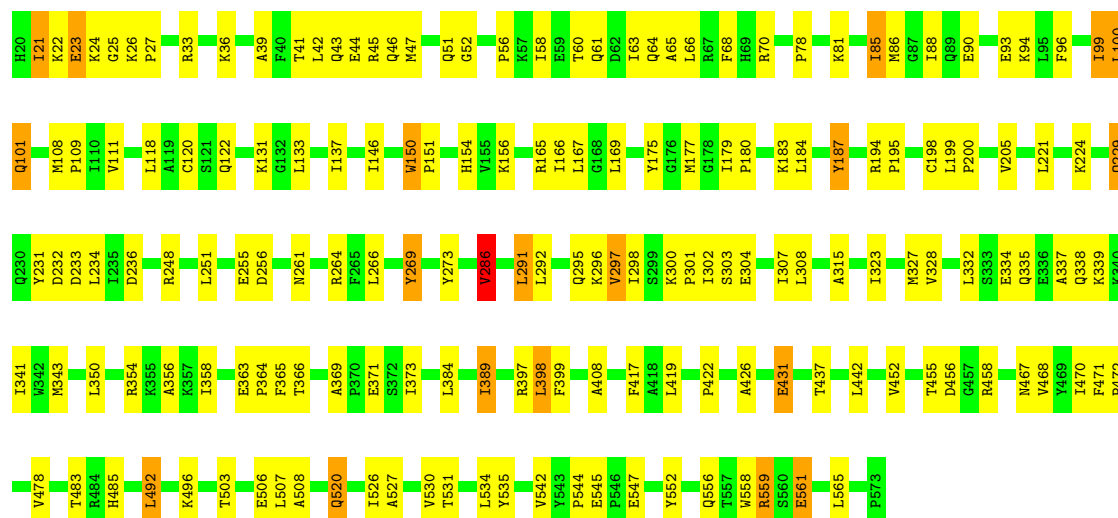
- Molecule 1: NAD-dependent malic enzyme, mitochondrial

Chain C: 68% 30% .



- Molecule 1: NAD-dependent malic enzyme, mitochondrial

Chain D: 69% 28% .





## 4 Data and refinement statistics

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

| Property                                                 | Value                                          | Source    |
|----------------------------------------------------------|------------------------------------------------|-----------|
| Space group                                              | P 1 21 1                                       | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 71.81Å 192.65Å 110.16Å<br>90.00° 89.77° 90.00° | Depositor |
| Resolution (Å)                                           | 20.00 – 2.30                                   | Depositor |
| % Data completeness<br>(in resolution range)             | 91.0 (20.00-2.30)                              | Depositor |
| $R_{merge}$                                              | 0.05                                           | Depositor |
| $R_{sym}$                                                | (Not available)                                | Depositor |
| Refinement program                                       | CNS 1.1                                        | Depositor |
| R, $R_{free}$                                            | 0.194 , 0.233                                  | Depositor |
| Estimated twinning fraction                              | No twinning to report.                         | Xtriage   |
| Total number of atoms                                    | 18818                                          | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 26.0                                           | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MN, OXL, FUM

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     | 0.42         | 0/4464      | 0.89        | 11/6047 (0.2%)  |
| 1   | B     | 0.41         | 0/4464      | 0.89        | 13/6047 (0.2%)  |
| 1   | C     | 0.41         | 0/4464      | 0.90        | 13/6047 (0.2%)  |
| 1   | D     | 0.41         | 0/4465      | 0.89        | 10/6047 (0.2%)  |
| All | All   | 0.41         | 0/17857     | 0.89        | 47/24188 (0.2%) |

There are no bond length outliers.

All (47) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 470 | ILE  | N-CA-C  | 9.90  | 120.07      | 111.56   |
| 1   | A     | 470 | ILE  | N-CA-C  | 9.19  | 119.47      | 111.56   |
| 1   | B     | 470 | ILE  | N-CA-C  | 9.00  | 119.30      | 111.56   |
| 1   | C     | 470 | ILE  | N-CA-C  | 8.88  | 119.20      | 111.56   |
| 1   | A     | 303 | SER  | N-CA-C  | -7.41 | 103.70      | 112.89   |
| 1   | A     | 419 | LEU  | N-CA-C  | 6.71  | 121.46      | 113.28   |
| 1   | D     | 419 | LEU  | N-CA-C  | 6.69  | 121.44      | 113.28   |
| 1   | D     | 150 | TRP  | CA-C-N  | 6.36  | 126.27      | 119.28   |
| 1   | D     | 150 | TRP  | C-N-CA  | 6.36  | 126.27      | 119.28   |
| 1   | C     | 419 | LEU  | N-CA-C  | 6.26  | 120.91      | 113.28   |
| 1   | C     | 187 | TYR  | N-CA-C  | -5.81 | 104.86      | 111.07   |
| 1   | A     | 269 | TYR  | N-CA-C  | 5.73  | 120.55      | 113.50   |
| 1   | C     | 270 | ARG  | N-CA-C  | 5.73  | 118.30      | 111.71   |
| 1   | A     | 448 | PRO  | N-CA-C  | 5.73  | 120.18      | 111.19   |
| 1   | C     | 307 | ILE  | N-CA-C  | 5.72  | 116.18      | 108.17   |
| 1   | C     | 246 | TYR  | N-CA-C  | 5.71  | 120.40      | 113.38   |
| 1   | D     | 307 | ILE  | N-CA-C  | 5.67  | 116.02      | 107.80   |
| 1   | B     | 167 | LEU  | CB-CA-C | -5.61 | 110.09      | 116.54   |
| 1   | C     | 150 | TRP  | CA-C-N  | 5.60  | 125.44      | 119.28   |
| 1   | C     | 150 | TRP  | C-N-CA  | 5.60  | 125.44      | 119.28   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 341 | ILE  | N-CA-C  | 5.57  | 115.91      | 108.11   |
| 1   | D     | 187 | TYR  | N-CA-C  | -5.57 | 105.11      | 111.07   |
| 1   | D     | 286 | VAL  | CB-CA-C | -5.48 | 104.66      | 112.22   |
| 1   | D     | 269 | TYR  | N-CA-C  | 5.45  | 120.80      | 113.72   |
| 1   | B     | 307 | ILE  | N-CA-C  | 5.44  | 115.69      | 107.80   |
| 1   | A     | 510 | GLY  | N-CA-C  | -5.43 | 107.77      | 115.43   |
| 1   | D     | 341 | ILE  | N-CA-C  | 5.43  | 115.67      | 107.80   |
| 1   | B     | 419 | LEU  | N-CA-C  | 5.32  | 119.77      | 113.28   |
| 1   | A     | 246 | TYR  | N-CA-C  | 5.29  | 119.89      | 113.38   |
| 1   | B     | 256 | ASP  | N-CA-C  | 5.27  | 118.66      | 111.39   |
| 1   | A     | 286 | VAL  | CB-CA-C | -5.19 | 105.33      | 111.97   |
| 1   | B     | 187 | TYR  | N-CA-C  | -5.19 | 105.52      | 111.07   |
| 1   | C     | 162 | ASP  | N-CA-C  | -5.16 | 105.67      | 112.94   |
| 1   | B     | 270 | ARG  | N-CA-C  | 5.15  | 117.63      | 111.71   |
| 1   | C     | 341 | ILE  | N-CA-C  | 5.14  | 115.26      | 107.80   |
| 1   | C     | 442 | LEU  | N-CA-C  | -5.13 | 98.91       | 107.99   |
| 1   | A     | 187 | TYR  | N-CA-C  | -5.13 | 105.58      | 111.07   |
| 1   | D     | 167 | LEU  | CB-CA-C | -5.12 | 110.66      | 116.54   |
| 1   | B     | 150 | TRP  | CA-C-N  | 5.11  | 124.90      | 119.28   |
| 1   | B     | 150 | TRP  | C-N-CA  | 5.11  | 124.90      | 119.28   |
| 1   | C     | 448 | PRO  | N-CA-C  | 5.11  | 118.51      | 110.80   |
| 1   | A     | 256 | ASP  | N-CA-C  | 5.09  | 118.61      | 111.74   |
| 1   | A     | 167 | LEU  | CB-CA-C | -5.09 | 110.69      | 116.54   |
| 1   | C     | 167 | LEU  | CB-CA-C | -5.06 | 110.72      | 116.54   |
| 1   | B     | 300 | LYS  | CA-C-N  | 5.05  | 125.84      | 119.98   |
| 1   | B     | 300 | LYS  | C-N-CA  | 5.05  | 125.84      | 119.98   |
| 1   | B     | 423 | THR  | N-CA-C  | 5.00  | 117.39      | 111.33   |

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     | 4369  | 0        | 4400     | 152     | 0            |
| 1   | B     | 4369  | 0        | 4400     | 151     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | C     | 4369  | 0        | 4400     | 152     | 0            |
| 1   | D     | 4370  | 0        | 4400     | 135     | 0            |
| 2   | A     | 31    | 0        | 12       | 1       | 0            |
| 2   | B     | 31    | 0        | 12       | 3       | 0            |
| 2   | C     | 31    | 0        | 12       | 1       | 0            |
| 2   | D     | 31    | 0        | 12       | 1       | 0            |
| 3   | A     | 6     | 0        | 0        | 1       | 0            |
| 3   | B     | 6     | 0        | 0        | 0       | 0            |
| 3   | C     | 6     | 0        | 0        | 0       | 0            |
| 3   | D     | 6     | 0        | 0        | 0       | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | C     | 1     | 0        | 0        | 0       | 0            |
| 4   | D     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 8     | 0        | 1        | 0       | 0            |
| 5   | B     | 8     | 0        | 1        | 1       | 0            |
| 5   | C     | 8     | 0        | 1        | 1       | 0            |
| 5   | D     | 8     | 0        | 1        | 1       | 0            |
| 6   | A     | 267   | 0        | 0        | 6       | 0            |
| 6   | B     | 290   | 0        | 0        | 9       | 0            |
| 6   | C     | 300   | 0        | 0        | 12      | 0            |
| 6   | D     | 300   | 0        | 0        | 9       | 0            |
| All | All   | 18818 | 0        | 17652    | 572     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (572) 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:A:381:VAL:HG13 | 1:A:407:MET:HE3  | 1.37                     | 1.07              |
| 1:C:302:ILE:HD11 | 1:C:327:MET:HG2  | 1.39                     | 1.04              |
| 1:B:332:LEU:HG   | 1:B:336:GLU:HG3  | 1.44                     | 1.00              |
| 1:B:515:PRO:HG2  | 1:B:518:ASN:HD22 | 1.29                     | 0.98              |
| 1:A:123:TYR:CD2  | 1:A:219:MET:HE1  | 2.01                     | 0.95              |
| 1:B:286:VAL:HG21 | 1:B:467:ASN:HA   | 1.46                     | 0.94              |
| 1:A:123:TYR:HD2  | 1:A:219:MET:HE1  | 1.29                     | 0.94              |
| 1:D:323:ILE:HG22 | 1:D:327:MET:HE2  | 1.50                     | 0.92              |
| 1:C:47:MET:HE3   | 1:C:566:LEU:HD22 | 1.51                     | 0.91              |
| 1:B:327:MET:HE3  | 1:B:337:ALA:HB1  | 1.50                     | 0.91              |
| 1:D:343:MET:HE2  | 1:D:365:PHE:HB2  | 1.52                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:323:ILE:HG22 | 1:B:327:MET:HE2  | 1.55                     | 0.89              |
| 1:D:520:GLN:H    | 1:D:520:GLN:HE21 | 1.20                     | 0.89              |
| 1:A:301:PRO:HB2  | 1:A:304:GLU:OE2  | 1.74                     | 0.86              |
| 1:A:527:ALA:O    | 1:A:531:THR:HG23 | 1.75                     | 0.86              |
| 1:D:327:MET:HE3  | 1:D:337:ALA:HB1  | 1.58                     | 0.85              |
| 1:A:301:PRO:HB2  | 1:A:304:GLU:CD   | 2.02                     | 0.85              |
| 1:A:407:MET:HA   | 1:A:407:MET:HE2  | 1.59                     | 0.85              |
| 1:B:527:ALA:O    | 1:B:531:THR:HG23 | 1.76                     | 0.84              |
| 1:C:120:CYS:SG   | 6:C:2093:HOH:O   | 2.34                     | 0.84              |
| 1:A:302:ILE:HB   | 6:A:2133:HOH:O   | 1.76                     | 0.84              |
| 1:B:248:ARG:NH1  | 1:C:544:PRO:HD3  | 1.93                     | 0.83              |
| 1:B:369:ALA:HB1  | 1:B:373:ILE:HD11 | 1.62                     | 0.81              |
| 1:C:120:CYS:HB2  | 6:C:2093:HOH:O   | 1.79                     | 0.81              |
| 1:B:43:GLN:HG2   | 1:B:47:MET:HE3   | 1.59                     | 0.80              |
| 1:D:43:GLN:HG2   | 1:D:47:MET:HE3   | 1.63                     | 0.80              |
| 1:B:295:GLN:HE22 | 1:B:300:LYS:N    | 1.80                     | 0.80              |
| 1:A:211:ALA:HA   | 1:A:214:LYS:HE2  | 1.64                     | 0.79              |
| 1:B:248:ARG:HH11 | 1:C:544:PRO:HD3  | 1.45                     | 0.79              |
| 1:D:371:GLU:CD   | 1:D:371:GLU:H    | 1.88                     | 0.79              |
| 1:C:520:GLN:H    | 1:C:520:GLN:HE21 | 1.31                     | 0.79              |
| 1:A:248:ARG:HD2  | 1:D:544:PRO:HD3  | 1.65                     | 0.78              |
| 1:C:504:ASP:HA   | 1:C:507:LEU:HD12 | 1.65                     | 0.78              |
| 1:D:286:VAL:HG21 | 1:D:467:ASN:HA   | 1.65                     | 0.77              |
| 1:C:315:ALA:CB   | 1:C:392:VAL:HG21 | 2.16                     | 0.76              |
| 1:A:343:MET:HE2  | 1:A:365:PHE:HB2  | 1.65                     | 0.76              |
| 1:C:371:GLU:H    | 1:C:371:GLU:CD   | 1.94                     | 0.76              |
| 1:D:527:ALA:O    | 1:D:531:THR:HG23 | 1.85                     | 0.75              |
| 1:B:371:GLU:CD   | 1:B:371:GLU:H    | 1.94                     | 0.75              |
| 1:A:21:ILE:HG22  | 1:A:23:GLU:H     | 1.51                     | 0.75              |
| 1:A:520:GLN:HE21 | 1:A:520:GLN:H    | 1.32                     | 0.75              |
| 1:B:515:PRO:HG2  | 1:B:518:ASN:ND2  | 2.02                     | 0.75              |
| 1:C:527:ALA:O    | 1:C:531:THR:HG23 | 1.88                     | 0.74              |
| 1:A:381:VAL:CG1  | 1:A:407:MET:HE3  | 2.17                     | 0.74              |
| 1:A:323:ILE:HG22 | 1:A:327:MET:HE2  | 1.67                     | 0.74              |
| 1:B:314:GLU:HB2  | 2:B:601:ATP:O2B  | 1.86                     | 0.74              |
| 1:C:120:CYS:CB   | 6:C:2093:HOH:O   | 2.34                     | 0.74              |
| 1:A:21:ILE:HD11  | 1:A:565:LEU:HD22 | 1.71                     | 0.73              |
| 1:B:249:ASN:ND2  | 1:C:543:TYR:HE2  | 1.86                     | 0.73              |
| 1:D:33:ARG:HD3   | 1:D:93:GLU:OE1   | 1.89                     | 0.73              |
| 1:A:335:GLN:O    | 1:A:339:LYS:HD2  | 1.89                     | 0.73              |
| 1:B:61:GLN:HA    | 1:B:64:GLN:HE21  | 1.54                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:552:TYR:O    | 1:D:556:GLN:HG2  | 1.89                     | 0.72              |
| 1:A:535:TYR:CE2  | 1:A:545:GLU:HG3  | 2.23                     | 0.72              |
| 1:C:327:MET:HE3  | 1:C:337:ALA:HB1  | 1.71                     | 0.72              |
| 1:D:520:GLN:H    | 1:D:520:GLN:NE2  | 1.87                     | 0.72              |
| 1:C:86:MET:HE1   | 1:C:111:VAL:HG23 | 1.71                     | 0.72              |
| 1:C:120:CYS:SG   | 1:C:176:GLY:HA2  | 2.30                     | 0.72              |
| 1:C:47:MET:CE    | 1:C:566:LEU:HD22 | 2.18                     | 0.71              |
| 1:C:165:ARG:NH1  | 2:C:601:ATP:O1G  | 2.24                     | 0.71              |
| 1:A:261:ASN:HD22 | 1:A:264:ARG:HE   | 1.38                     | 0.70              |
| 1:B:520:GLN:H    | 1:B:520:GLN:HE21 | 1.39                     | 0.70              |
| 1:B:260:HIS:O    | 1:B:264:ARG:HG2  | 1.92                     | 0.70              |
| 1:A:315:ALA:CB   | 1:A:392:VAL:HG21 | 2.22                     | 0.70              |
| 1:B:29:MET:HE2   | 1:B:50:LEU:HD22  | 1.73                     | 0.70              |
| 1:D:90:GLU:OE1   | 1:D:131:LYS:HG2  | 1.92                     | 0.70              |
| 1:A:308:LEU:HD23 | 1:A:389:ILE:HD11 | 1.74                     | 0.69              |
| 1:D:296:LYS:HE2  | 1:D:507:LEU:HD11 | 1.74                     | 0.69              |
| 1:A:20:HIS:C     | 1:A:21:ILE:HD12  | 2.18                     | 0.69              |
| 1:C:315:ALA:HB3  | 1:C:392:VAL:HG21 | 1.75                     | 0.69              |
| 1:C:503:THR:OG1  | 1:C:506:GLU:HG3  | 1.93                     | 0.69              |
| 1:B:286:VAL:CG2  | 1:B:467:ASN:HA   | 2.21                     | 0.69              |
| 1:C:179:ILE:HB   | 1:C:180:PRO:HD3  | 1.73                     | 0.68              |
| 1:A:302:ILE:HG22 | 1:A:302:ILE:O    | 1.94                     | 0.68              |
| 1:D:85:ILE:HD11  | 1:D:111:VAL:HG22 | 1.76                     | 0.67              |
| 1:B:249:ASN:HD22 | 1:C:543:TYR:HE2  | 1.40                     | 0.67              |
| 1:C:302:ILE:HA   | 1:C:305:HIS:CE1  | 2.30                     | 0.67              |
| 1:C:261:ASN:ND2  | 1:C:264:ARG:HH21 | 1.93                     | 0.67              |
| 1:B:249:ASN:HB3  | 1:C:543:TYR:OH   | 1.95                     | 0.67              |
| 1:C:492:LEU:HD22 | 1:C:496:LYS:HE3  | 1.76                     | 0.66              |
| 1:B:480:LEU:O    | 1:B:542:VAL:HG21 | 1.97                     | 0.65              |
| 1:C:543:TYR:HA   | 1:C:544:PRO:C    | 2.21                     | 0.65              |
| 1:D:286:VAL:CG2  | 1:D:467:ASN:HA   | 2.26                     | 0.65              |
| 1:A:21:ILE:CD1   | 1:A:565:LEU:HD22 | 2.27                     | 0.65              |
| 1:C:41:THR:OG1   | 1:C:44:GLU:HG3   | 1.97                     | 0.65              |
| 1:D:179:ILE:HB   | 1:D:180:PRO:HD3  | 1.78                     | 0.65              |
| 1:D:334:GLU:O    | 1:D:338:GLN:HG3  | 1.97                     | 0.65              |
| 1:B:179:ILE:HB   | 1:B:180:PRO:HD3  | 1.77                     | 0.64              |
| 1:D:343:MET:HE2  | 1:D:365:PHE:CB   | 2.28                     | 0.64              |
| 1:C:480:LEU:O    | 1:C:542:VAL:HG21 | 1.97                     | 0.64              |
| 1:D:492:LEU:HD22 | 1:D:496:LYS:HE3  | 1.79                     | 0.64              |
| 1:D:369:ALA:HB1  | 1:D:373:ILE:HD11 | 1.78                     | 0.64              |
| 1:A:505:GLU:H    | 1:A:505:GLU:CD   | 2.05                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:332:LEU:HG   | 1:B:336:GLU:CG   | 2.25                     | 0.64              |
| 1:B:391:GLY:HA3  | 1:B:427:GLU:HG2  | 1.80                     | 0.64              |
| 1:D:298:ILE:HD11 | 1:D:442:LEU:HD12 | 1.79                     | 0.64              |
| 1:B:492:LEU:HD22 | 1:B:496:LYS:HE3  | 1.79                     | 0.64              |
| 1:D:363:GLU:HB3  | 1:D:364:PRO:HD3  | 1.79                     | 0.64              |
| 1:C:302:ILE:HA   | 1:C:305:HIS:CG   | 2.33                     | 0.64              |
| 1:B:324:VAL:O    | 1:B:328:VAL:HG23 | 1.98                     | 0.63              |
| 1:C:315:ALA:HB3  | 1:C:392:VAL:CG2  | 2.28                     | 0.63              |
| 1:A:177:MET:HE2  | 1:A:181:VAL:HG23 | 1.80                     | 0.63              |
| 1:A:179:ILE:HB   | 1:A:180:PRO:HD3  | 1.81                     | 0.63              |
| 1:C:495:ALA:O    | 1:C:499:THR:HG22 | 1.99                     | 0.63              |
| 1:C:501:GLN:HE21 | 1:C:522:VAL:HA   | 1.63                     | 0.63              |
| 1:B:177:MET:O    | 1:B:180:PRO:HD2  | 1.98                     | 0.63              |
| 1:A:209:ASN:C    | 1:A:209:ASN:HD22 | 2.06                     | 0.63              |
| 1:C:551:LYS:O    | 1:C:555:GLU:HG3  | 1.99                     | 0.62              |
| 1:A:33:ARG:HD3   | 1:A:93:GLU:OE2   | 1.99                     | 0.62              |
| 1:D:295:GLN:NE2  | 1:D:300:LYS:O    | 2.29                     | 0.62              |
| 1:A:183:LYS:HE3  | 1:A:255:GLU:CD   | 2.24                     | 0.62              |
| 1:B:26:LYS:HA    | 1:B:29:MET:HE3   | 1.82                     | 0.62              |
| 1:C:133:LEU:HD23 | 1:C:134:PHE:N    | 2.14                     | 0.62              |
| 1:C:52:GLY:HA3   | 1:D:146:ILE:HG23 | 1.82                     | 0.62              |
| 1:A:392:VAL:O    | 1:A:392:VAL:HG13 | 1.99                     | 0.62              |
| 1:B:132:GLY:HA2  | 1:B:200:PRO:HG2  | 1.82                     | 0.62              |
| 1:C:301:PRO:HD2  | 6:C:2156:HOH:O   | 1.99                     | 0.62              |
| 1:C:302:ILE:HA   | 1:C:305:HIS:ND1  | 2.14                     | 0.62              |
| 1:C:501:GLN:NE2  | 1:C:522:VAL:HA   | 2.13                     | 0.62              |
| 1:B:335:GLN:HG2  | 1:B:339:LYS:HE2  | 1.82                     | 0.61              |
| 1:D:41:THR:OG1   | 1:D:44:GLU:HG3   | 2.00                     | 0.61              |
| 1:B:286:VAL:HG22 | 1:B:470:ILE:CG1  | 2.31                     | 0.61              |
| 1:A:177:MET:HE1  | 1:A:180:PRO:HB2  | 1.82                     | 0.61              |
| 1:B:286:VAL:HG22 | 1:B:470:ILE:HG12 | 1.82                     | 0.61              |
| 1:D:535:TYR:CE2  | 1:D:545:GLU:HG3  | 2.35                     | 0.61              |
| 1:D:456:ASP:OD1  | 1:D:458:ARG:HD3  | 2.01                     | 0.61              |
| 1:B:543:TYR:HA   | 1:B:544:PRO:C    | 2.26                     | 0.61              |
| 1:C:51:GLN:HE21  | 1:C:51:GLN:HA    | 1.66                     | 0.61              |
| 1:C:33:ARG:HD3   | 1:C:93:GLU:OE2   | 2.01                     | 0.61              |
| 1:A:315:ALA:HB3  | 1:A:392:VAL:HG21 | 1.83                     | 0.60              |
| 1:B:133:LEU:HB2  | 1:B:199:LEU:HD11 | 1.83                     | 0.60              |
| 1:D:535:TYR:OH   | 1:D:542:VAL:CG1  | 2.50                     | 0.60              |
| 1:A:308:LEU:HB3  | 1:A:389:ILE:HD12 | 1.84                     | 0.60              |
| 1:A:292:LEU:O    | 1:A:295:GLN:HG2  | 2.01                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:520:GLN:HG2  | 6:B:2091:HOH:O   | 2.01                     | 0.60              |
| 1:A:177:MET:CE   | 1:A:180:PRO:HB2  | 2.32                     | 0.60              |
| 1:A:493:GLU:HG2  | 6:A:2220:HOH:O   | 2.02                     | 0.60              |
| 1:C:204:ASP:OD2  | 1:C:221:LEU:HD23 | 2.01                     | 0.60              |
| 1:D:68:PHE:CD2   | 1:D:99:ILE:HG13  | 2.37                     | 0.60              |
| 1:D:65:ALA:HA    | 1:D:99:ILE:HD11  | 1.84                     | 0.60              |
| 1:A:506:GLU:O    | 1:A:511:ARG:HB2  | 2.02                     | 0.60              |
| 1:A:544:PRO:HD3  | 1:D:248:ARG:HD2  | 1.83                     | 0.59              |
| 1:B:302:ILE:HD11 | 1:B:327:MET:SD   | 2.42                     | 0.59              |
| 1:A:315:ALA:HB3  | 1:A:392:VAL:CG2  | 2.32                     | 0.59              |
| 1:C:391:GLY:HA3  | 1:C:427:GLU:HG2  | 1.84                     | 0.59              |
| 1:D:300:LYS:HE3  | 1:D:304:GLU:HB3  | 1.85                     | 0.59              |
| 1:B:363:GLU:HB3  | 1:B:364:PRO:HD3  | 1.83                     | 0.58              |
| 1:D:85:ILE:HD12  | 1:D:85:ILE:C     | 2.27                     | 0.58              |
| 1:B:108:MET:HB3  | 1:B:109:PRO:HD3  | 1.84                     | 0.58              |
| 1:A:339:LYS:N    | 1:A:339:LYS:HE3  | 2.18                     | 0.58              |
| 1:C:350:LEU:HD13 | 1:C:358:ILE:CD1  | 2.33                     | 0.58              |
| 1:B:41:THR:OG1   | 1:B:44:GLU:HG3   | 2.03                     | 0.58              |
| 1:B:41:THR:O     | 1:B:45:ARG:HG3   | 2.03                     | 0.58              |
| 1:C:302:ILE:HG13 | 1:C:305:HIS:ND1  | 2.19                     | 0.58              |
| 1:A:68:PHE:CD2   | 1:A:99:ILE:HG13  | 2.39                     | 0.58              |
| 1:B:350:LEU:HD13 | 1:B:358:ILE:CD1  | 2.34                     | 0.58              |
| 1:B:371:GLU:OE1  | 1:B:371:GLU:N    | 2.36                     | 0.58              |
| 1:B:232:ASP:OD1  | 1:B:264:ARG:NH2  | 2.33                     | 0.57              |
| 1:B:232:ASP:CG   | 1:B:264:ARG:HH22 | 2.12                     | 0.57              |
| 1:D:397:ARG:HD3  | 1:D:426:ALA:O    | 2.04                     | 0.57              |
| 1:A:261:ASN:ND2  | 1:A:264:ARG:HE   | 2.00                     | 0.57              |
| 1:C:42:LEU:O     | 1:C:46:GLN:HG3   | 2.03                     | 0.57              |
| 1:A:315:ALA:HB2  | 6:A:2258:HOH:O   | 2.04                     | 0.57              |
| 1:C:324:VAL:O    | 1:C:328:VAL:HG23 | 2.05                     | 0.57              |
| 1:B:295:GLN:NE2  | 1:B:300:LYS:N    | 2.52                     | 0.57              |
| 1:C:315:ALA:HB1  | 1:C:392:VAL:HG21 | 1.87                     | 0.57              |
| 1:C:392:VAL:HG13 | 1:C:392:VAL:O    | 2.03                     | 0.57              |
| 1:C:350:LEU:HD13 | 1:C:358:ILE:HD13 | 1.87                     | 0.57              |
| 1:D:156:LYS:HE2  | 1:D:156:LYS:HA   | 1.85                     | 0.57              |
| 1:A:159:VAL:HG23 | 1:A:184:LEU:HD21 | 1.87                     | 0.57              |
| 1:B:297:VAL:CG1  | 1:B:507:LEU:HD22 | 2.35                     | 0.57              |
| 1:D:229:GLN:HE22 | 1:D:233:ASP:CG   | 2.13                     | 0.57              |
| 1:A:493:GLU:HG3  | 1:A:533:TYR:CD1  | 2.40                     | 0.57              |
| 1:B:334:GLU:O    | 1:B:338:GLN:HG3  | 2.05                     | 0.57              |
| 1:A:177:MET:HE3  | 1:A:177:MET:O    | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:305:HIS:HA   | 6:C:2195:HOH:O   | 2.05                     | 0.56              |
| 1:C:363:GLU:HB3  | 1:C:364:PRO:HD3  | 1.85                     | 0.56              |
| 1:C:528:ILE:O    | 1:C:532:GLU:HG3  | 2.05                     | 0.56              |
| 1:A:480:LEU:HD22 | 1:A:556:GLN:HG2  | 1.87                     | 0.56              |
| 1:A:209:ASN:HD21 | 1:A:211:ALA:HB3  | 1.71                     | 0.56              |
| 1:B:528:ILE:O    | 1:B:532:GLU:HG3  | 2.04                     | 0.56              |
| 1:C:333:SER:OG   | 1:C:336:GLU:HG3  | 2.06                     | 0.56              |
| 1:D:41:THR:O     | 1:D:45:ARG:HG3   | 2.06                     | 0.56              |
| 1:D:165:ARG:NH1  | 2:D:601:ATP:O1G  | 2.38                     | 0.56              |
| 1:D:42:LEU:O     | 1:D:46:GLN:HG3   | 2.06                     | 0.56              |
| 1:C:177:MET:O    | 1:C:180:PRO:HD2  | 2.06                     | 0.56              |
| 1:A:495:ALA:O    | 1:A:499:THR:HG22 | 2.06                     | 0.55              |
| 1:C:315:ALA:HB2  | 6:C:2152:HOH:O   | 2.06                     | 0.55              |
| 1:C:559:ARG:HB3  | 1:C:561:GLU:HG2  | 1.87                     | 0.55              |
| 1:C:369:ALA:HB1  | 1:C:373:ILE:HD11 | 1.88                     | 0.55              |
| 1:D:455:THR:HG23 | 6:D:2228:HOH:O   | 2.06                     | 0.55              |
| 1:A:350:LEU:HD13 | 1:A:358:ILE:CD1  | 2.36                     | 0.55              |
| 1:B:133:LEU:HD11 | 1:B:146:ILE:HG22 | 1.88                     | 0.55              |
| 1:A:21:ILE:HD12  | 1:A:21:ILE:N     | 2.21                     | 0.55              |
| 1:A:52:GLY:HA3   | 1:B:146:ILE:HG23 | 1.88                     | 0.55              |
| 1:A:65:ALA:HA    | 1:A:99:ILE:HD11  | 1.89                     | 0.55              |
| 1:B:33:ARG:HD3   | 1:B:93:GLU:OE2   | 2.06                     | 0.55              |
| 1:A:315:ALA:HB1  | 1:A:392:VAL:HG21 | 1.88                     | 0.55              |
| 1:B:518:ASN:O    | 1:B:522:VAL:HG23 | 2.07                     | 0.55              |
| 1:C:82:TYR:CE1   | 1:C:86:MET:HE3   | 2.42                     | 0.55              |
| 1:A:308:LEU:HB3  | 1:A:389:ILE:CD1  | 2.38                     | 0.54              |
| 1:C:538:LYS:N    | 1:C:538:LYS:HD2  | 2.21                     | 0.54              |
| 1:C:86:MET:CE    | 1:C:111:VAL:HG23 | 2.37                     | 0.54              |
| 1:D:520:GLN:HE21 | 1:D:520:GLN:N    | 1.99                     | 0.54              |
| 1:A:294:ALA:O    | 1:A:297:VAL:HG22 | 2.07                     | 0.54              |
| 1:A:520:GLN:H    | 1:A:520:GLN:NE2  | 2.04                     | 0.54              |
| 1:B:308:LEU:HB3  | 1:B:389:ILE:HD12 | 1.89                     | 0.54              |
| 1:B:543:TYR:OH   | 1:C:249:ASN:HB3  | 2.07                     | 0.54              |
| 1:A:165:ARG:NH2  | 3:A:603:OXL:O2   | 2.38                     | 0.54              |
| 1:B:65:ALA:HA    | 1:B:99:ILE:HD11  | 1.90                     | 0.54              |
| 1:C:85:ILE:HG13  | 1:C:86:MET:N     | 2.22                     | 0.54              |
| 1:C:183:LYS:HE2  | 1:C:255:GLU:CD   | 2.33                     | 0.54              |
| 1:A:302:ILE:O    | 1:A:340:LYS:HE3  | 2.08                     | 0.53              |
| 1:B:29:MET:HE1   | 1:B:53:LEU:HD13  | 1.91                     | 0.53              |
| 1:A:297:VAL:HG23 | 1:A:298:ILE:HG23 | 1.89                     | 0.53              |
| 1:A:371:GLU:H    | 1:A:371:GLU:CD   | 2.17                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:503:THR:OG1  | 1:A:506:GLU:HG3  | 2.08                     | 0.53              |
| 1:B:333:SER:OG   | 1:B:336:GLU:HG2  | 2.09                     | 0.53              |
| 1:A:363:GLU:HB3  | 1:A:364:PRO:HD3  | 1.90                     | 0.53              |
| 1:C:133:LEU:HD21 | 1:C:146:ILE:CG2  | 2.38                     | 0.53              |
| 1:B:157:ALA:HB2  | 1:B:479:ILE:HD11 | 1.91                     | 0.53              |
| 1:C:308:LEU:HD23 | 1:C:389:ILE:HD11 | 1.90                     | 0.53              |
| 5:C:605:FUM:H5   | 6:C:2043:HOH:O   | 2.09                     | 0.53              |
| 1:D:184:LEU:HD12 | 1:D:200:PRO:HG3  | 1.90                     | 0.52              |
| 1:B:29:MET:HE1   | 1:B:53:LEU:CD1   | 2.39                     | 0.52              |
| 5:B:605:FUM:H5   | 6:B:2289:HOH:O   | 2.09                     | 0.52              |
| 1:B:86:MET:SD    | 1:B:111:VAL:HG23 | 2.48                     | 0.52              |
| 1:D:308:LEU:HB3  | 1:D:389:ILE:HD12 | 1.91                     | 0.52              |
| 1:A:96:PHE:O     | 1:A:100:LEU:HD13 | 2.10                     | 0.52              |
| 1:D:120:CYS:O    | 1:D:175:TYR:HB3  | 2.09                     | 0.52              |
| 1:A:175:TYR:CD2  | 1:A:219:MET:HE2  | 2.45                     | 0.52              |
| 1:B:159:VAL:HG23 | 1:B:184:LEU:HD21 | 1.92                     | 0.52              |
| 1:D:535:TYR:OH   | 1:D:542:VAL:HG12 | 2.08                     | 0.52              |
| 1:D:154:HIS:HB2  | 6:D:2078:HOH:O   | 2.10                     | 0.52              |
| 1:D:297:VAL:HG12 | 1:D:507:LEU:HD22 | 1.92                     | 0.52              |
| 1:B:302:ILE:HA   | 1:B:305:HIS:ND1  | 2.24                     | 0.52              |
| 1:B:308:LEU:HD23 | 1:B:389:ILE:HD11 | 1.91                     | 0.52              |
| 1:C:41:THR:O     | 1:C:45:ARG:HG3   | 2.09                     | 0.52              |
| 1:A:350:LEU:HD13 | 1:A:358:ILE:HD12 | 1.91                     | 0.51              |
| 1:C:68:PHE:CE2   | 1:C:99:ILE:HG23  | 2.44                     | 0.51              |
| 1:B:483:THR:OG1  | 1:B:534:LEU:HD13 | 2.11                     | 0.51              |
| 1:A:66:LEU:HD22  | 1:B:217:PHE:HZ   | 1.76                     | 0.51              |
| 1:B:298:ILE:HG22 | 1:B:300:LYS:HB2  | 1.91                     | 0.51              |
| 1:B:315:ALA:O    | 1:B:319:ILE:HG13 | 2.11                     | 0.51              |
| 1:D:36:LYS:HB3   | 1:D:39:ALA:HB3   | 1.93                     | 0.51              |
| 1:D:118:LEU:HD11 | 1:D:122:GLN:HE22 | 1.76                     | 0.51              |
| 1:A:205:VAL:HG11 | 1:A:231:TYR:HD1  | 1.76                     | 0.51              |
| 1:D:23:GLU:HG3   | 1:D:27:PRO:HB2   | 1.92                     | 0.51              |
| 1:A:354:ARG:CZ   | 1:A:356:ALA:HB3  | 2.41                     | 0.51              |
| 1:B:61:GLN:HA    | 1:B:64:GLN:NE2   | 2.25                     | 0.51              |
| 1:B:389:ILE:HB   | 1:B:407:MET:HE2  | 1.92                     | 0.50              |
| 1:C:308:LEU:HB3  | 1:C:389:ILE:HD12 | 1.93                     | 0.50              |
| 1:D:169:LEU:CD2  | 1:D:422:PRO:HD3  | 2.41                     | 0.50              |
| 1:D:535:TYR:OH   | 1:D:542:VAL:HG11 | 2.12                     | 0.50              |
| 1:A:559:ARG:HB3  | 1:A:561:GLU:HG2  | 1.94                     | 0.50              |
| 1:B:297:VAL:HG12 | 1:B:507:LEU:HD22 | 1.91                     | 0.50              |
| 1:B:535:TYR:CE2  | 1:B:545:GLU:HG3  | 2.46                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:306:LYS:CG   | 1:C:386:PRO:HA   | 2.41                     | 0.50              |
| 1:D:101:GLN:O    | 1:D:101:GLN:HG2  | 2.10                     | 0.50              |
| 1:D:328:VAL:HA   | 1:D:332:LEU:O    | 2.12                     | 0.50              |
| 1:B:166:ILE:HD12 | 1:B:179:ILE:HG13 | 1.93                     | 0.50              |
| 1:B:297:VAL:CG2  | 1:B:442:LEU:HD11 | 2.42                     | 0.50              |
| 1:B:493:GLU:HG3  | 1:B:533:TYR:CD1  | 2.46                     | 0.50              |
| 1:C:501:GLN:HE22 | 1:C:525:ASN:HD22 | 1.59                     | 0.50              |
| 1:D:81:LYS:O     | 1:D:85:ILE:HG23  | 2.11                     | 0.50              |
| 1:D:23:GLU:CG    | 1:D:27:PRO:HB2   | 2.41                     | 0.50              |
| 1:D:389:ILE:HG23 | 1:D:399:PHE:CE1  | 2.47                     | 0.50              |
| 1:D:478:VAL:HG13 | 1:D:483:THR:HB   | 1.94                     | 0.50              |
| 1:B:552:TYR:O    | 1:B:556:GLN:HG2  | 2.12                     | 0.49              |
| 1:C:520:GLN:H    | 1:C:520:GLN:NE2  | 2.05                     | 0.49              |
| 1:A:503:THR:OG1  | 1:A:505:GLU:HG2  | 2.12                     | 0.49              |
| 1:A:537:ASN:O    | 1:A:539:MET:HG3  | 2.11                     | 0.49              |
| 1:C:303:SER:HA   | 1:C:340:LYS:NZ   | 2.28                     | 0.49              |
| 1:D:315:ALA:HB2  | 6:D:2294:HOH:O   | 2.11                     | 0.49              |
| 1:B:484:ARG:HG2  | 1:C:543:TYR:CZ   | 2.48                     | 0.49              |
| 1:D:108:MET:HB3  | 1:D:109:PRO:HD3  | 1.93                     | 0.49              |
| 1:B:301:PRO:HB2  | 1:B:304:GLU:HG3  | 1.94                     | 0.49              |
| 1:C:328:VAL:HA   | 1:C:332:LEU:O    | 2.12                     | 0.49              |
| 1:D:85:ILE:HD11  | 1:D:86:MET:SD    | 2.52                     | 0.49              |
| 1:D:397:ARG:NH1  | 6:D:2186:HOH:O   | 2.46                     | 0.49              |
| 1:A:273:TYR:O    | 1:A:485:HIS:HD2  | 1.95                     | 0.49              |
| 1:C:524:ILE:O    | 1:C:528:ILE:HG13 | 2.13                     | 0.49              |
| 1:D:468:VAL:HA   | 1:D:471:PHE:CE2  | 2.47                     | 0.49              |
| 1:D:302:ILE:HD11 | 1:D:332:LEU:HD22 | 1.95                     | 0.49              |
| 1:D:389:ILE:HG23 | 1:D:399:PHE:CZ   | 2.48                     | 0.49              |
| 1:A:328:VAL:HA   | 1:A:332:LEU:O    | 2.13                     | 0.49              |
| 1:A:478:VAL:HG13 | 1:A:483:THR:HB   | 1.94                     | 0.48              |
| 1:B:249:ASN:CB   | 1:C:543:TYR:OH   | 2.59                     | 0.48              |
| 1:C:371:GLU:OE1  | 1:C:371:GLU:N    | 2.44                     | 0.48              |
| 1:B:73:LYS:HG2   | 6:B:2025:HOH:O   | 2.13                     | 0.48              |
| 1:C:51:GLN:HA    | 1:C:51:GLN:NE2   | 2.28                     | 0.48              |
| 1:D:232:ASP:CG   | 1:D:264:ARG:HH22 | 2.21                     | 0.48              |
| 1:A:389:ILE:HG23 | 1:A:399:PHE:CE1  | 2.49                     | 0.48              |
| 1:B:22:LYS:O     | 1:B:22:LYS:HD3   | 2.14                     | 0.48              |
| 1:B:183:LYS:HE3  | 1:B:255:GLU:CD   | 2.39                     | 0.48              |
| 1:D:456:ASP:CG   | 1:D:458:ARG:HD3  | 2.39                     | 0.48              |
| 1:B:26:LYS:HB3   | 1:B:27:PRO:HD3   | 1.95                     | 0.48              |
| 1:B:520:GLN:HB3  | 6:B:2092:HOH:O   | 2.12                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:294:ALA:O    | 1:C:297:VAL:HG22 | 2.13                     | 0.48              |
| 1:C:511:ARG:HA   | 6:C:2263:HOH:O   | 2.12                     | 0.48              |
| 1:D:526:ILE:O    | 1:D:530:VAL:HG23 | 2.14                     | 0.48              |
| 1:A:303:SER:HA   | 1:A:340:LYS:CE   | 2.44                     | 0.48              |
| 1:C:133:LEU:HB2  | 1:C:199:LEU:HD11 | 1.95                     | 0.48              |
| 1:A:166:ILE:HA   | 1:A:256:ASP:OD2  | 2.13                     | 0.48              |
| 1:B:165:ARG:NH1  | 1:B:167:LEU:O    | 2.47                     | 0.48              |
| 1:B:389:ILE:HG23 | 1:B:399:PHE:CE1  | 2.49                     | 0.48              |
| 1:C:301:PRO:HG2  | 1:C:304:GLU:HB2  | 1.94                     | 0.48              |
| 1:A:61:GLN:HA    | 1:A:64:GLN:HE21  | 1.78                     | 0.48              |
| 1:A:146:ILE:HG23 | 1:B:52:GLY:HA3   | 1.95                     | 0.48              |
| 1:A:432:GLU:O    | 1:A:436:LEU:HB2  | 2.14                     | 0.48              |
| 1:B:120:CYS:O    | 1:B:175:TYR:HB3  | 2.13                     | 0.48              |
| 1:A:41:THR:OG1   | 1:A:44:GLU:HG3   | 2.14                     | 0.48              |
| 1:B:286:VAL:HG21 | 1:B:467:ASN:CA   | 2.31                     | 0.48              |
| 1:A:137:ILE:HA   | 1:A:234:LEU:HD22 | 1.96                     | 0.47              |
| 1:B:166:ILE:HA   | 1:B:256:ASP:OD2  | 2.14                     | 0.47              |
| 1:A:36:LYS:HB3   | 1:A:39:ALA:HB3   | 1.96                     | 0.47              |
| 1:A:177:MET:O    | 1:A:180:PRO:HD2  | 2.14                     | 0.47              |
| 1:B:165:ARG:NH1  | 2:B:601:ATP:O1G  | 2.47                     | 0.47              |
| 1:C:471:PHE:CG   | 1:C:472:PRO:HD3  | 2.49                     | 0.47              |
| 1:D:408:ALA:HB2  | 1:D:437:THR:HG22 | 1.96                     | 0.47              |
| 1:B:196:ASP:C    | 1:B:196:ASP:OD1  | 2.57                     | 0.47              |
| 1:B:22:LYS:HE2   | 1:D:24:LYS:O     | 2.14                     | 0.47              |
| 1:B:111:VAL:HG22 | 6:B:2052:HOH:O   | 2.15                     | 0.47              |
| 1:D:308:LEU:HB3  | 1:D:389:ILE:CD1  | 2.44                     | 0.47              |
| 1:B:22:LYS:HE3   | 1:D:25:GLY:HA3   | 1.97                     | 0.47              |
| 1:B:284:ALA:HA   | 1:B:319:ILE:HG12 | 1.96                     | 0.47              |
| 1:D:51:GLN:NE2   | 1:D:51:GLN:HA    | 2.29                     | 0.47              |
| 1:A:315:ALA:CB   | 1:A:392:VAL:CG2  | 2.91                     | 0.47              |
| 1:A:503:THR:O    | 1:A:507:LEU:HD13 | 2.15                     | 0.47              |
| 1:B:132:GLY:CA   | 1:B:200:PRO:HG2  | 2.44                     | 0.47              |
| 1:D:286:VAL:HG21 | 1:D:467:ASN:CA   | 2.40                     | 0.47              |
| 1:B:389:ILE:HG23 | 1:B:399:PHE:CZ   | 2.49                     | 0.47              |
| 1:D:335:GLN:O    | 1:D:339:LYS:HG2  | 2.15                     | 0.47              |
| 1:D:559:ARG:HB3  | 1:D:561:GLU:HG2  | 1.97                     | 0.47              |
| 1:B:81:LYS:O     | 1:B:85:ILE:HG23  | 2.15                     | 0.46              |
| 1:B:154:HIS:HB2  | 6:B:2080:HOH:O   | 2.14                     | 0.46              |
| 1:A:302:ILE:O    | 1:A:302:ILE:CG2  | 2.61                     | 0.46              |
| 1:B:524:ILE:O    | 1:B:528:ILE:HG13 | 2.15                     | 0.46              |
| 1:C:146:ILE:HG23 | 1:D:52:GLY:HA3   | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:286:VAL:HG21 | 1:A:467:ASN:HA   | 1.97                     | 0.46              |
| 1:A:315:ALA:O    | 1:A:319:ILE:HG13 | 2.15                     | 0.46              |
| 1:B:282:GLY:O    | 1:B:286:VAL:HG23 | 2.15                     | 0.46              |
| 1:A:85:ILE:HD12  | 1:A:111:VAL:HG13 | 1.97                     | 0.46              |
| 1:C:384:LEU:N    | 1:C:384:LEU:HD12 | 2.30                     | 0.46              |
| 1:D:297:VAL:HG22 | 1:D:298:ILE:HG13 | 1.98                     | 0.46              |
| 1:C:133:LEU:HD23 | 1:C:133:LEU:C    | 2.40                     | 0.46              |
| 1:C:505:GLU:O    | 1:C:509:GLN:NE2  | 2.49                     | 0.46              |
| 1:D:150:TRP:CE2  | 1:D:199:LEU:HD13 | 2.51                     | 0.46              |
| 1:D:298:ILE:CD1  | 1:D:442:LEU:HD12 | 2.43                     | 0.46              |
| 1:C:315:ALA:O    | 1:C:319:ILE:HG13 | 2.16                     | 0.46              |
| 1:A:150:TRP:CE2  | 1:A:199:LEU:HD13 | 2.51                     | 0.46              |
| 1:B:195:PRO:HD2  | 6:B:2094:HOH:O   | 2.15                     | 0.46              |
| 1:D:45:ARG:CZ    | 1:D:58:ILE:HD13  | 2.45                     | 0.46              |
| 1:D:111:VAL:HG13 | 6:D:2047:HOH:O   | 2.16                     | 0.46              |
| 1:A:41:THR:O     | 1:A:45:ARG:HG3   | 2.16                     | 0.46              |
| 1:A:184:LEU:HD12 | 1:A:200:PRO:HG3  | 1.98                     | 0.46              |
| 1:C:506:GLU:O    | 1:C:511:ARG:CG   | 2.64                     | 0.46              |
| 1:A:133:LEU:HB2  | 1:A:199:LEU:HD11 | 1.98                     | 0.45              |
| 1:B:273:TYR:O    | 1:B:485:HIS:HD2  | 1.97                     | 0.45              |
| 1:C:61:GLN:HA    | 1:C:64:GLN:HE21  | 1.80                     | 0.45              |
| 1:D:471:PHE:CG   | 1:D:472:PRO:HD3  | 2.51                     | 0.45              |
| 1:A:334:GLU:O    | 1:A:338:GLN:HG3  | 2.16                     | 0.45              |
| 1:C:461:THR:N    | 6:C:2243:HOH:O   | 2.35                     | 0.45              |
| 1:C:478:VAL:HG13 | 1:C:483:THR:HB   | 1.96                     | 0.45              |
| 1:C:294:ALA:O    | 1:C:298:ILE:HG12 | 2.16                     | 0.45              |
| 1:D:26:LYS:HB3   | 1:D:27:PRO:HD3   | 1.98                     | 0.45              |
| 1:A:323:ILE:CG2  | 1:A:327:MET:HE2  | 2.44                     | 0.45              |
| 1:A:392:VAL:HG13 | 6:A:2262:HOH:O   | 2.16                     | 0.45              |
| 1:A:85:ILE:HD12  | 1:A:111:VAL:CG1  | 2.47                     | 0.45              |
| 1:A:294:ALA:O    | 1:A:298:ILE:HG12 | 2.17                     | 0.45              |
| 1:A:468:VAL:HA   | 1:A:471:PHE:CE2  | 2.51                     | 0.45              |
| 1:B:101:GLN:HB2  | 6:B:2042:HOH:O   | 2.15                     | 0.45              |
| 1:C:207:THR:O    | 1:C:224:LYS:HA   | 2.17                     | 0.45              |
| 1:D:23:GLU:HA    | 1:D:23:GLU:OE1   | 2.17                     | 0.45              |
| 1:D:51:GLN:HA    | 1:D:51:GLN:HE21  | 1.81                     | 0.45              |
| 1:B:249:ASN:ND2  | 1:C:543:TYR:CE2  | 2.74                     | 0.45              |
| 1:B:309:PHE:HB2  | 1:B:343:MET:HG2  | 1.99                     | 0.45              |
| 1:C:468:VAL:HA   | 1:C:471:PHE:CE2  | 2.52                     | 0.45              |
| 1:D:483:THR:OG1  | 1:D:534:LEU:HD13 | 2.16                     | 0.45              |
| 1:A:471:PHE:CG   | 1:A:472:PRO:HD3  | 2.51                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:302:ILE:HD11 | 1:C:327:MET:CG   | 2.26                     | 0.45              |
| 1:C:22:LYS:HB3   | 1:C:22:LYS:NZ    | 2.31                     | 0.44              |
| 1:C:205:VAL:HG11 | 1:C:231:TYR:HD1  | 1.82                     | 0.44              |
| 1:D:261:ASN:HD22 | 1:D:264:ARG:HE   | 1.65                     | 0.44              |
| 1:A:26:LYS:HB3   | 1:A:27:PRO:HD3   | 1.99                     | 0.44              |
| 1:A:535:TYR:HE2  | 1:A:545:GLU:HG3  | 1.78                     | 0.44              |
| 1:B:509:GLN:HE22 | 1:B:511:ARG:HE   | 1.65                     | 0.44              |
| 1:C:334:GLU:O    | 1:C:338:GLN:HG3  | 2.18                     | 0.44              |
| 1:C:159:VAL:HG23 | 1:C:184:LEU:HD21 | 1.99                     | 0.44              |
| 1:D:85:ILE:HD12  | 1:D:96:PHE:HE1   | 1.81                     | 0.44              |
| 1:D:296:LYS:CE   | 1:D:507:LEU:HD11 | 2.44                     | 0.44              |
| 1:A:152:GLU:HG2  | 1:A:196:ASP:O    | 2.17                     | 0.44              |
| 1:B:177:MET:C    | 1:B:180:PRO:HD2  | 2.42                     | 0.44              |
| 1:B:350:LEU:HD13 | 1:B:358:ILE:HD12 | 1.99                     | 0.44              |
| 1:B:437:THR:HG21 | 1:B:441:CYS:HB3  | 1.99                     | 0.44              |
| 1:C:133:LEU:HD22 | 1:C:135:ILE:HG13 | 1.99                     | 0.44              |
| 1:C:302:ILE:HG21 | 1:C:332:LEU:HD11 | 1.99                     | 0.44              |
| 1:A:99:ILE:HG22  | 1:A:100:LEU:HD12 | 1.99                     | 0.44              |
| 1:B:327:MET:CE   | 1:B:337:ALA:HB1  | 2.34                     | 0.44              |
| 1:B:432:GLU:O    | 1:B:436:LEU:HB2  | 2.18                     | 0.44              |
| 1:B:42:LEU:O     | 1:B:46:GLN:HG3   | 2.17                     | 0.44              |
| 1:B:559:ARG:HH11 | 1:B:559:ARG:HG2  | 1.82                     | 0.44              |
| 1:C:273:TYR:O    | 1:C:485:HIS:HD2  | 2.01                     | 0.44              |
| 1:C:505:GLU:O    | 1:C:509:GLN:HG3  | 2.17                     | 0.44              |
| 1:C:70:ARG:HG2   | 6:C:2029:HOH:O   | 2.17                     | 0.44              |
| 1:D:298:ILE:HG22 | 1:D:300:LYS:HB2  | 1.98                     | 0.44              |
| 1:D:398:LEU:HD12 | 1:D:398:LEU:HA   | 1.83                     | 0.44              |
| 1:A:505:GLU:CD   | 1:A:505:GLU:N    | 2.76                     | 0.44              |
| 1:C:184:LEU:HD12 | 1:C:200:PRO:HG3  | 2.00                     | 0.44              |
| 1:D:85:ILE:HD12  | 1:D:86:MET:N     | 2.32                     | 0.44              |
| 1:D:291:LEU:HD13 | 1:D:417:PHE:CE2  | 2.53                     | 0.44              |
| 1:A:194:ARG:HB2  | 1:A:197:GLN:HG3  | 1.99                     | 0.44              |
| 1:A:286:VAL:CG2  | 1:A:467:ASN:HA   | 2.48                     | 0.44              |
| 1:B:125:HIS:HE1  | 1:B:215:ASP:OD2  | 2.00                     | 0.44              |
| 1:B:286:VAL:HG22 | 1:B:470:ILE:HG13 | 1.99                     | 0.44              |
| 1:A:339:LYS:HE3  | 1:A:339:LYS:CA   | 2.48                     | 0.43              |
| 1:B:66:LEU:HD21  | 1:B:70:ARG:HH11  | 1.83                     | 0.43              |
| 1:C:133:LEU:CD2  | 1:C:135:ILE:HG13 | 2.48                     | 0.43              |
| 1:A:303:SER:HA   | 1:A:340:LYS:HE3  | 1.98                     | 0.43              |
| 1:B:136:SER:HB2  | 1:B:221:LEU:HD22 | 1.99                     | 0.43              |
| 1:C:281:GLN:HG2  | 6:C:2255:HOH:O   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:21:ILE:HG13  | 1:D:565:LEU:HD22 | 2.01                     | 0.43              |
| 1:D:137:ILE:HA   | 1:D:234:LEU:HD22 | 1.99                     | 0.43              |
| 1:D:184:LEU:HD22 | 1:D:198:CYS:HB3  | 2.01                     | 0.43              |
| 1:D:323:ILE:CG2  | 1:D:327:MET:HE2  | 2.35                     | 0.43              |
| 1:B:276:PHE:HB2  | 1:B:281:GLN:OE1  | 2.18                     | 0.43              |
| 1:C:133:LEU:HD21 | 1:C:146:ILE:HG22 | 1.99                     | 0.43              |
| 1:C:291:LEU:HD13 | 1:C:417:PHE:CE2  | 2.53                     | 0.43              |
| 1:C:482:ASN:N    | 1:C:482:ASN:HD22 | 2.16                     | 0.43              |
| 1:D:61:GLN:HA    | 1:D:64:GLN:HE21  | 1.84                     | 0.43              |
| 1:B:394:GLY:HA2  | 1:B:420:SER:HB3  | 1.99                     | 0.43              |
| 1:C:21:ILE:HD11  | 1:C:34:THR:HG21  | 1.99                     | 0.43              |
| 1:C:315:ALA:CB   | 1:C:392:VAL:CG2  | 2.88                     | 0.43              |
| 1:C:319:ILE:O    | 1:C:323:ILE:HG13 | 2.18                     | 0.43              |
| 1:C:509:GLN:HB2  | 1:C:511:ARG:HG2  | 2.01                     | 0.43              |
| 1:C:520:GLN:O    | 1:C:524:ILE:HG12 | 2.18                     | 0.43              |
| 1:A:69:HIS:HE1   | 1:A:102:ASP:OD2  | 2.00                     | 0.43              |
| 1:B:328:VAL:HA   | 1:B:332:LEU:O    | 2.19                     | 0.43              |
| 1:C:75:MET:HE1   | 1:C:84:TYR:CG    | 2.54                     | 0.43              |
| 1:C:194:ARG:HB2  | 1:C:197:GLN:HG3  | 2.00                     | 0.43              |
| 1:C:549:LYS:HD2  | 1:C:549:LYS:H    | 1.84                     | 0.43              |
| 1:A:23:GLU:CG    | 1:A:27:PRO:HB2   | 2.49                     | 0.43              |
| 1:A:319:ILE:O    | 1:A:323:ILE:HG13 | 2.19                     | 0.43              |
| 1:B:45:ARG:CZ    | 1:B:58:ILE:HD13  | 2.48                     | 0.43              |
| 1:C:23:GLU:OE1   | 1:C:23:GLU:HA    | 2.19                     | 0.43              |
| 1:D:183:LYS:HE3  | 1:D:255:GLU:CD   | 2.44                     | 0.43              |
| 1:D:308:LEU:HD23 | 1:D:389:ILE:HD11 | 2.01                     | 0.43              |
| 1:A:120:CYS:O    | 1:A:175:TYR:HB3  | 2.18                     | 0.43              |
| 1:A:401:PRO:O    | 1:A:405:ARG:HG3  | 2.18                     | 0.43              |
| 1:C:389:ILE:HG23 | 1:C:399:PHE:CZ   | 2.54                     | 0.43              |
| 1:A:263:PHE:CZ   | 1:A:314:GLU:HA   | 2.53                     | 0.43              |
| 6:A:2004:HOH:O   | 1:C:22:LYS:HE2   | 2.18                     | 0.43              |
| 1:B:150:TRP:HA   | 1:B:151:PRO:HD3  | 1.86                     | 0.43              |
| 1:A:354:ARG:NE   | 1:A:358:ILE:HD11 | 2.34                     | 0.43              |
| 1:B:36:LYS:HB3   | 1:B:39:ALA:HB3   | 2.01                     | 0.43              |
| 1:C:502:LEU:HD21 | 1:C:513:TYR:C    | 2.44                     | 0.43              |
| 1:A:301:PRO:HD2  | 1:A:304:GLU:OE1  | 2.18                     | 0.42              |
| 1:C:36:LYS:HB3   | 1:C:39:ALA:HB3   | 2.00                     | 0.42              |
| 1:B:194:ARG:HB2  | 1:B:197:GLN:HG3  | 2.01                     | 0.42              |
| 1:A:280:ILE:O    | 1:A:284:ALA:HB2  | 2.19                     | 0.42              |
| 1:B:295:GLN:NE2  | 1:B:300:LYS:O    | 2.52                     | 0.42              |
| 1:B:297:VAL:HG22 | 1:B:442:LEU:HD11 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:442:LEU:HD23 | 1:B:442:LEU:HA   | 1.86                     | 0.42              |
| 1:D:78:PRO:HD2   | 6:D:2024:HOH:O   | 2.18                     | 0.42              |
| 1:D:236:ASP:OD2  | 1:D:269:TYR:OH   | 2.33                     | 0.42              |
| 1:A:545:GLU:HG2  | 1:A:549:LYS:NZ   | 2.34                     | 0.42              |
| 1:D:184:LEU:O    | 1:D:187:TYR:HB2  | 2.19                     | 0.42              |
| 1:A:391:GLY:HA3  | 1:A:427:GLU:HG2  | 2.02                     | 0.42              |
| 1:B:125:HIS:N    | 1:B:125:HIS:ND1  | 2.68                     | 0.42              |
| 1:B:507:LEU:HA   | 1:B:507:LEU:HD23 | 1.66                     | 0.42              |
| 1:D:85:ILE:CD1   | 1:D:96:PHE:HE1   | 2.33                     | 0.42              |
| 1:C:306:LYS:HE2  | 6:C:2167:HOH:O   | 2.19                     | 0.42              |
| 1:B:137:ILE:HA   | 1:B:234:LEU:HD22 | 2.01                     | 0.42              |
| 1:B:544:PRO:HD3  | 1:C:248:ARG:HG2  | 2.02                     | 0.42              |
| 1:C:68:PHE:CZ    | 1:C:85:ILE:HG22  | 2.55                     | 0.42              |
| 1:C:120:CYS:SG   | 1:C:175:TYR:O    | 2.63                     | 0.42              |
| 1:A:108:MET:HB3  | 1:A:109:PRO:HD3  | 2.01                     | 0.42              |
| 1:B:271:GLU:OE2  | 1:B:271:GLU:HA   | 2.20                     | 0.42              |
| 1:B:322:LEU:HD12 | 1:B:322:LEU:HA   | 1.89                     | 0.42              |
| 1:D:99:ILE:HG22  | 1:D:100:LEU:N    | 2.35                     | 0.42              |
| 1:D:273:TYR:O    | 1:D:485:HIS:HD2  | 2.03                     | 0.42              |
| 1:D:431:GLU:OE1  | 1:D:452:VAL:HG13 | 2.20                     | 0.42              |
| 1:A:130:PRO:HG3  | 1:B:54:LEU:HD23  | 2.01                     | 0.42              |
| 1:A:401:PRO:HA   | 1:A:436:LEU:HD23 | 2.02                     | 0.42              |
| 1:B:66:LEU:CD2   | 1:B:70:ARG:HH11  | 2.33                     | 0.42              |
| 1:B:345:ASP:HB2  | 2:B:601:ATP:O2'  | 2.20                     | 0.42              |
| 1:D:195:PRO:HD2  | 6:D:2092:HOH:O   | 2.19                     | 0.42              |
| 1:A:23:GLU:HG3   | 1:A:27:PRO:HB2   | 2.02                     | 0.42              |
| 1:A:324:VAL:O    | 1:A:328:VAL:HG23 | 2.20                     | 0.42              |
| 1:C:320:ALA:O    | 1:C:324:VAL:HG23 | 2.20                     | 0.42              |
| 1:D:85:ILE:HD11  | 1:D:111:VAL:CG2  | 2.49                     | 0.42              |
| 1:A:359:ASP:OD2  | 1:A:362:GLN:HG3  | 2.20                     | 0.41              |
| 1:B:515:PRO:CG   | 1:B:518:ASN:HD22 | 2.14                     | 0.41              |
| 1:D:205:VAL:HG11 | 1:D:231:TYR:HD1  | 1.85                     | 0.41              |
| 1:D:508:ALA:N    | 6:D:2251:HOH:O   | 2.53                     | 0.41              |
| 1:A:276:PHE:HB2  | 1:A:281:GLN:OE1  | 2.20                     | 0.41              |
| 1:A:389:ILE:HG23 | 1:A:399:PHE:CZ   | 2.55                     | 0.41              |
| 1:A:398:LEU:HD12 | 1:A:398:LEU:HA   | 1.92                     | 0.41              |
| 1:A:528:ILE:O    | 1:A:532:GLU:HG3  | 2.20                     | 0.41              |
| 1:B:308:LEU:HB3  | 1:B:389:ILE:CD1  | 2.50                     | 0.41              |
| 1:B:325:MET:HE2  | 1:B:492:LEU:HD12 | 2.02                     | 0.41              |
| 1:C:389:ILE:HG23 | 1:C:399:PHE:CE1  | 2.55                     | 0.41              |
| 1:D:177:MET:O    | 1:D:180:PRO:HD2  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:350:LEU:HD22 | 1:D:354:ARG:CZ   | 2.50                     | 0.41              |
| 1:D:358:ILE:HD13 | 1:D:366:THR:HG21 | 2.00                     | 0.41              |
| 1:A:211:ALA:HA   | 1:A:214:LYS:CE   | 2.44                     | 0.41              |
| 1:A:304:GLU:H    | 1:A:304:GLU:HG3  | 1.69                     | 0.41              |
| 1:A:399:PHE:CG   | 1:A:427:GLU:HB3  | 2.55                     | 0.41              |
| 1:B:97:TYR:CE2   | 1:B:188:THR:HB   | 2.56                     | 0.41              |
| 1:B:297:VAL:HG12 | 1:B:507:LEU:HD13 | 2.03                     | 0.41              |
| 1:C:26:LYS:N     | 1:C:27:PRO:CD    | 2.82                     | 0.41              |
| 1:A:210:ILE:HD13 | 1:A:210:ILE:HA   | 1.93                     | 0.41              |
| 1:B:297:VAL:HG11 | 1:B:507:LEU:HD22 | 2.01                     | 0.41              |
| 1:D:184:LEU:HD23 | 1:D:184:LEU:HA   | 1.89                     | 0.41              |
| 1:A:345:ASP:HB2  | 2:A:601:ATP:O2'  | 2.21                     | 0.41              |
| 1:B:243:THR:HG21 | 1:B:273:TYR:CD2  | 2.56                     | 0.41              |
| 1:B:471:PHE:CG   | 1:B:472:PRO:HD3  | 2.55                     | 0.41              |
| 1:C:25:GLY:C     | 1:C:27:PRO:HD2   | 2.45                     | 0.41              |
| 1:C:369:ALA:HB1  | 1:C:373:ILE:CD1  | 2.49                     | 0.41              |
| 1:D:85:ILE:CD1   | 1:D:111:VAL:HG22 | 2.49                     | 0.41              |
| 1:D:88:ILE:HG22  | 1:D:96:PHE:HB2   | 2.03                     | 0.41              |
| 1:D:503:THR:OG1  | 1:D:506:GLU:HG3  | 2.20                     | 0.41              |
| 1:A:315:ALA:HB3  | 1:A:392:VAL:HG22 | 2.02                     | 0.41              |
| 1:C:177:MET:C    | 1:C:180:PRO:HD2  | 2.45                     | 0.41              |
| 1:C:389:ILE:HB   | 1:C:407:MET:HE2  | 2.03                     | 0.41              |
| 1:C:398:LEU:HD13 | 1:C:398:LEU:HA   | 1.88                     | 0.41              |
| 1:D:60:THR:H     | 1:D:63:ILE:HD12  | 1.86                     | 0.41              |
| 1:D:131:LYS:O    | 1:D:177:MET:HE3  | 2.20                     | 0.41              |
| 1:D:354:ARG:CZ   | 1:D:356:ALA:HB3  | 2.50                     | 0.41              |
| 1:C:24:LYS:O     | 1:C:27:PRO:HD2   | 2.20                     | 0.41              |
| 1:D:229:GLN:NE2  | 1:D:233:ASP:CG   | 2.78                     | 0.41              |
| 1:B:538:LYS:HA   | 6:B:2261:HOH:O   | 2.20                     | 0.41              |
| 1:C:137:ILE:HA   | 1:C:234:LEU:HD22 | 2.01                     | 0.41              |
| 1:C:350:LEU:HD22 | 1:C:354:ARG:NH1  | 2.36                     | 0.41              |
| 1:D:194:ARG:HA   | 1:D:195:PRO:HD3  | 1.96                     | 0.41              |
| 1:A:177:MET:CE   | 1:A:177:MET:O    | 2.69                     | 0.41              |
| 1:A:322:LEU:HD23 | 1:A:322:LEU:HA   | 1.88                     | 0.41              |
| 1:B:478:VAL:HG13 | 1:B:483:THR:HB   | 2.03                     | 0.41              |
| 1:C:73:LYS:HE2   | 1:C:73:LYS:HB2   | 1.96                     | 0.41              |
| 1:C:221:LEU:HD22 | 1:D:56:PRO:CB    | 2.50                     | 0.41              |
| 1:C:384:LEU:N    | 1:C:384:LEU:CD1  | 2.84                     | 0.41              |
| 1:D:150:TRP:HA   | 1:D:151:PRO:HD3  | 1.85                     | 0.41              |
| 1:D:229:GLN:NE2  | 1:D:233:ASP:OD2  | 2.54                     | 0.41              |
| 1:D:442:LEU:HD23 | 1:D:442:LEU:HA   | 1.88                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:359:ASP:OD2  | 1:B:362:GLN:HG3  | 2.21                     | 0.41              |
| 1:C:394:GLY:HA2  | 1:C:420:SER:HB3  | 2.03                     | 0.41              |
| 1:C:401:PRO:O    | 1:C:405:ARG:HG3  | 2.21                     | 0.41              |
| 1:D:94:LYS:HD3   | 1:D:558:TRP:CZ2  | 2.55                     | 0.41              |
| 1:D:302:ILE:CD1  | 1:D:332:LEU:HD22 | 2.51                     | 0.41              |
| 1:A:232:ASP:CG   | 1:A:264:ARG:HH22 | 2.28                     | 0.40              |
| 1:B:300:LYS:HA   | 1:B:301:PRO:HD3  | 1.79                     | 0.40              |
| 1:C:271:GLU:HA   | 1:C:271:GLU:OE2  | 2.20                     | 0.40              |
| 1:C:302:ILE:HA   | 1:C:305:HIS:CD2  | 2.56                     | 0.40              |
| 1:C:322:LEU:HD12 | 1:C:322:LEU:HA   | 1.97                     | 0.40              |
| 1:D:166:ILE:HA   | 1:D:256:ASP:OD2  | 2.21                     | 0.40              |
| 1:D:300:LYS:HA   | 1:D:301:PRO:HD3  | 1.89                     | 0.40              |
| 1:D:384:LEU:HD12 | 1:D:384:LEU:N    | 2.35                     | 0.40              |
| 1:C:51:GLN:HE21  | 1:C:51:GLN:CA    | 2.28                     | 0.40              |
| 1:C:68:PHE:CE1   | 1:C:85:ILE:HG22  | 2.56                     | 0.40              |
| 1:A:46:GLN:HG2   | 1:A:51:GLN:HG3   | 2.02                     | 0.40              |
| 1:A:177:MET:HE3  | 1:A:180:PRO:HD2  | 2.04                     | 0.40              |
| 1:A:355:LYS:HE2  | 1:A:355:LYS:HB2  | 1.90                     | 0.40              |
| 1:A:369:ALA:HA   | 1:A:370:PRO:HD3  | 1.88                     | 0.40              |
| 1:A:493:GLU:HG3  | 1:A:533:TYR:CG   | 2.56                     | 0.40              |
| 1:D:169:LEU:HD21 | 1:D:422:PRO:HD3  | 2.03                     | 0.40              |
| 1:A:209:ASN:C    | 1:A:209:ASN:ND2  | 2.76                     | 0.40              |
| 1:A:538:LYS:NZ   | 6:A:2238:HOH:O   | 2.54                     | 0.40              |
| 1:A:125:HIS:CD2  | 1:A:125:HIS:N    | 2.89                     | 0.40              |
| 1:A:194:ARG:HA   | 1:A:195:PRO:HD3  | 1.96                     | 0.40              |
| 1:A:261:ASN:HD22 | 1:A:264:ARG:NE   | 2.12                     | 0.40              |
| 1:C:108:MET:HB3  | 1:C:109:PRO:HD3  | 2.03                     | 0.40              |
| 5:D:605:FUM:H5   | 6:D:2036:HOH:O   | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed         | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|------------------|------------|---------|----------|-------------|----|
| 1   | A     | 552/554 (100%)   | 536 (97%)  | 15 (3%) | 1 (0%)   | 43          | 55 |
| 1   | B     | 552/554 (100%)   | 536 (97%)  | 15 (3%) | 1 (0%)   | 43          | 55 |
| 1   | C     | 552/554 (100%)   | 538 (98%)  | 12 (2%) | 2 (0%)   | 30          | 38 |
| 1   | D     | 552/554 (100%)   | 540 (98%)  | 11 (2%) | 1 (0%)   | 43          | 55 |
| All | All   | 2208/2216 (100%) | 2150 (97%) | 53 (2%) | 5 (0%)   | 43          | 55 |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 397 | ARG  |
| 1   | B     | 397 | ARG  |
| 1   | A     | 392 | VAL  |
| 1   | D     | 21  | ILE  |
| 1   | C     | 392 | VAL  |

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

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     | 470/470 (100%)   | 433 (92%)  | 37 (8%)  | 11          | 15 |
| 1   | B     | 470/470 (100%)   | 442 (94%)  | 28 (6%)  | 17          | 25 |
| 1   | C     | 470/470 (100%)   | 449 (96%)  | 21 (4%)  | 24          | 37 |
| 1   | D     | 470/470 (100%)   | 443 (94%)  | 27 (6%)  | 18          | 27 |
| All | All   | 1880/1880 (100%) | 1767 (94%) | 113 (6%) | 17          | 25 |

All (113) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 66  | LEU  |
| 1   | A     | 70  | ARG  |
| 1   | A     | 85  | ILE  |
| 1   | A     | 99  | ILE  |
| 1   | A     | 101 | GLN  |
| 1   | A     | 114 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 133 | LEU  |
| 1   | A     | 152 | GLU  |
| 1   | A     | 165 | ARG  |
| 1   | A     | 169 | LEU  |
| 1   | A     | 209 | ASN  |
| 1   | A     | 210 | ILE  |
| 1   | A     | 221 | LEU  |
| 1   | A     | 229 | GLN  |
| 1   | A     | 240 | LYS  |
| 1   | A     | 251 | LEU  |
| 1   | A     | 286 | VAL  |
| 1   | A     | 291 | LEU  |
| 1   | A     | 292 | LEU  |
| 1   | A     | 301 | PRO  |
| 1   | A     | 302 | ILE  |
| 1   | A     | 304 | GLU  |
| 1   | A     | 305 | HIS  |
| 1   | A     | 339 | LYS  |
| 1   | A     | 350 | LEU  |
| 1   | A     | 363 | GLU  |
| 1   | A     | 384 | LEU  |
| 1   | A     | 389 | ILE  |
| 1   | A     | 398 | LEU  |
| 1   | A     | 401 | PRO  |
| 1   | A     | 436 | LEU  |
| 1   | A     | 492 | LEU  |
| 1   | A     | 505 | GLU  |
| 1   | A     | 520 | GLN  |
| 1   | A     | 559 | ARG  |
| 1   | A     | 561 | GLU  |
| 1   | A     | 571 | GLU  |
| 1   | B     | 22  | LYS  |
| 1   | B     | 66  | LEU  |
| 1   | B     | 100 | LEU  |
| 1   | B     | 122 | GLN  |
| 1   | B     | 125 | HIS  |
| 1   | B     | 153 | ASN  |
| 1   | B     | 169 | LEU  |
| 1   | B     | 221 | LEU  |
| 1   | B     | 236 | ASP  |
| 1   | B     | 248 | ARG  |
| 1   | B     | 249 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 251 | LEU  |
| 1   | B     | 267 | ARG  |
| 1   | B     | 286 | VAL  |
| 1   | B     | 291 | LEU  |
| 1   | B     | 297 | VAL  |
| 1   | B     | 300 | LYS  |
| 1   | B     | 302 | ILE  |
| 1   | B     | 303 | SER  |
| 1   | B     | 350 | LEU  |
| 1   | B     | 363 | GLU  |
| 1   | B     | 371 | GLU  |
| 1   | B     | 384 | LEU  |
| 1   | B     | 389 | ILE  |
| 1   | B     | 425 | GLN  |
| 1   | B     | 436 | LEU  |
| 1   | B     | 492 | LEU  |
| 1   | B     | 520 | GLN  |
| 1   | C     | 22  | LYS  |
| 1   | C     | 66  | LEU  |
| 1   | C     | 70  | ARG  |
| 1   | C     | 165 | ARG  |
| 1   | C     | 169 | LEU  |
| 1   | C     | 251 | LEU  |
| 1   | C     | 267 | ARG  |
| 1   | C     | 291 | LEU  |
| 1   | C     | 292 | LEU  |
| 1   | C     | 295 | GLN  |
| 1   | C     | 350 | LEU  |
| 1   | C     | 371 | GLU  |
| 1   | C     | 389 | ILE  |
| 1   | C     | 425 | GLN  |
| 1   | C     | 436 | LEU  |
| 1   | C     | 492 | LEU  |
| 1   | C     | 504 | ASP  |
| 1   | C     | 520 | GLN  |
| 1   | C     | 559 | ARG  |
| 1   | C     | 561 | GLU  |
| 1   | C     | 571 | GLU  |
| 1   | D     | 22  | LYS  |
| 1   | D     | 23  | GLU  |
| 1   | D     | 66  | LEU  |
| 1   | D     | 70  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 85  | ILE  |
| 1   | D     | 99  | ILE  |
| 1   | D     | 100 | LEU  |
| 1   | D     | 101 | GLN  |
| 1   | D     | 133 | LEU  |
| 1   | D     | 221 | LEU  |
| 1   | D     | 224 | LYS  |
| 1   | D     | 229 | GLN  |
| 1   | D     | 251 | LEU  |
| 1   | D     | 266 | LEU  |
| 1   | D     | 286 | VAL  |
| 1   | D     | 291 | LEU  |
| 1   | D     | 292 | LEU  |
| 1   | D     | 297 | VAL  |
| 1   | D     | 303 | SER  |
| 1   | D     | 389 | ILE  |
| 1   | D     | 398 | LEU  |
| 1   | D     | 431 | GLU  |
| 1   | D     | 492 | LEU  |
| 1   | D     | 520 | GLN  |
| 1   | D     | 547 | GLU  |
| 1   | D     | 559 | ARG  |
| 1   | D     | 561 | GLU  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 64  | GLN  |
| 1   | A     | 69  | HIS  |
| 1   | A     | 71  | ASN  |
| 1   | A     | 101 | GLN  |
| 1   | A     | 154 | HIS  |
| 1   | A     | 209 | ASN  |
| 1   | A     | 229 | GLN  |
| 1   | A     | 261 | ASN  |
| 1   | A     | 295 | GLN  |
| 1   | A     | 330 | ASN  |
| 1   | A     | 425 | GLN  |
| 1   | A     | 482 | ASN  |
| 1   | A     | 485 | HIS  |
| 1   | A     | 520 | GLN  |
| 1   | A     | 556 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 43  | GLN  |
| 1   | B     | 51  | GLN  |
| 1   | B     | 64  | GLN  |
| 1   | B     | 153 | ASN  |
| 1   | B     | 154 | HIS  |
| 1   | B     | 229 | GLN  |
| 1   | B     | 230 | GLN  |
| 1   | B     | 261 | ASN  |
| 1   | B     | 295 | GLN  |
| 1   | B     | 335 | GLN  |
| 1   | B     | 425 | GLN  |
| 1   | B     | 482 | ASN  |
| 1   | B     | 509 | GLN  |
| 1   | B     | 518 | ASN  |
| 1   | B     | 520 | GLN  |
| 1   | C     | 51  | GLN  |
| 1   | C     | 64  | GLN  |
| 1   | C     | 101 | GLN  |
| 1   | C     | 197 | GLN  |
| 1   | C     | 229 | GLN  |
| 1   | C     | 261 | ASN  |
| 1   | C     | 295 | GLN  |
| 1   | C     | 330 | ASN  |
| 1   | C     | 425 | GLN  |
| 1   | C     | 482 | ASN  |
| 1   | C     | 501 | GLN  |
| 1   | C     | 518 | ASN  |
| 1   | C     | 520 | GLN  |
| 1   | D     | 51  | GLN  |
| 1   | D     | 64  | GLN  |
| 1   | D     | 69  | HIS  |
| 1   | D     | 122 | GLN  |
| 1   | D     | 229 | GLN  |
| 1   | D     | 261 | ASN  |
| 1   | D     | 338 | GLN  |
| 1   | D     | 425 | GLN  |
| 1   | D     | 482 | ASN  |
| 1   | D     | 485 | HIS  |
| 1   | D     | 518 | ASN  |
| 1   | D     | 520 | 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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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$ |
| 3   | OXL  | A     | 603 | 4    | 5,5,5        | 1.69 | 2 (40%)     | 6,6,6       | 2.46 | 2 (33%)     |
| 5   | FUM  | A     | 605 | -    | 7,7,7        | 1.51 | 1 (14%)     | 8,8,8       | 0.65 | 0           |
| 3   | OXL  | D     | 603 | 4    | 5,5,5        | 1.81 | 2 (40%)     | 6,6,6       | 2.48 | 2 (33%)     |
| 2   | ATP  | B     | 601 | -    | 32,33,33     | 1.75 | 5 (15%)     | 48,52,52    | 2.06 | 9 (18%)     |
| 5   | FUM  | B     | 605 | -    | 7,7,7        | 1.64 | 2 (28%)     | 8,8,8       | 0.68 | 0           |
| 3   | OXL  | B     | 603 | 4    | 5,5,5        | 1.88 | 2 (40%)     | 6,6,6       | 2.43 | 2 (33%)     |
| 2   | ATP  | C     | 601 | -    | 32,33,33     | 1.62 | 8 (25%)     | 48,52,52    | 2.03 | 9 (18%)     |
| 2   | ATP  | D     | 601 | -    | 32,33,33     | 1.56 | 5 (15%)     | 48,52,52    | 2.04 | 9 (18%)     |
| 5   | FUM  | C     | 605 | -    | 7,7,7        | 1.64 | 2 (28%)     | 8,8,8       | 0.67 | 0           |
| 5   | FUM  | D     | 605 | -    | 7,7,7        | 1.65 | 2 (28%)     | 8,8,8       | 0.66 | 0           |
| 2   | ATP  | A     | 601 | -    | 32,33,33     | 1.68 | 8 (25%)     | 48,52,52    | 2.02 | 9 (18%)     |
| 3   | OXL  | C     | 603 | 4    | 5,5,5        | 1.78 | 2 (40%)     | 6,6,6       | 2.44 | 2 (33%)     |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | OXL  | A     | 603 | 4    | -       | 0/4/4/4    | -       |
| 5   | FUM  | A     | 605 | -    | -       | 2/5/5/5    | -       |
| 3   | OXL  | D     | 603 | 4    | -       | 0/4/4/4    | -       |
| 2   | ATP  | B     | 601 | -    | -       | 3/22/38/38 | 0/3/3/3 |
| 5   | FUM  | B     | 605 | -    | -       | 2/5/5/5    | -       |
| 3   | OXL  | B     | 603 | 4    | -       | 0/4/4/4    | -       |
| 2   | ATP  | C     | 601 | -    | -       | 2/22/38/38 | 0/3/3/3 |
| 2   | ATP  | D     | 601 | -    | -       | 1/22/38/38 | 0/3/3/3 |
| 5   | FUM  | C     | 605 | -    | -       | 2/5/5/5    | -       |
| 5   | FUM  | D     | 605 | -    | -       | 0/5/5/5    | -       |
| 2   | ATP  | A     | 601 | -    | -       | 3/22/38/38 | 0/3/3/3 |
| 3   | OXL  | C     | 603 | 4    | -       | 0/4/4/4    | -       |

All (41) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B     | 601 | ATP  | PB-O3B | -5.36 | 1.53        | 1.59     |
| 2   | C     | 601 | ATP  | C5-N7  | -4.23 | 1.31        | 1.39     |
| 2   | D     | 601 | ATP  | C5-N7  | -3.95 | 1.31        | 1.39     |
| 2   | A     | 601 | ATP  | C5-N7  | -3.91 | 1.31        | 1.39     |
| 2   | B     | 601 | ATP  | C5-N7  | -3.88 | 1.32        | 1.39     |
| 3   | B     | 603 | OXL  | O2-C2  | 3.25  | 1.30        | 1.22     |
| 2   | B     | 601 | ATP  | C5-C4  | -3.21 | 1.33        | 1.39     |
| 2   | D     | 601 | ATP  | C5-C4  | -3.19 | 1.33        | 1.39     |
| 3   | D     | 603 | OXL  | O2-C2  | 2.94  | 1.29        | 1.22     |
| 2   | C     | 601 | ATP  | C5-C4  | -2.90 | 1.33        | 1.39     |
| 2   | A     | 601 | ATP  | C5-C4  | -2.86 | 1.34        | 1.39     |
| 3   | C     | 603 | OXL  | O2-C2  | 2.82  | 1.29        | 1.22     |
| 5   | B     | 605 | FUM  | C4-C   | 2.76  | 1.55        | 1.48     |
| 5   | D     | 605 | FUM  | C4-C   | 2.73  | 1.55        | 1.48     |
| 2   | A     | 601 | ATP  | PA-O3A | 2.72  | 1.62        | 1.59     |
| 3   | D     | 603 | OXL  | O3-C1  | -2.69 | 1.23        | 1.30     |
| 3   | A     | 603 | OXL  | O2-C2  | 2.65  | 1.29        | 1.22     |
| 5   | B     | 605 | FUM  | C5-C4  | 2.61  | 1.40        | 1.33     |
| 2   | A     | 601 | ATP  | C4-N9  | -2.60 | 1.32        | 1.37     |
| 5   | C     | 605 | FUM  | C5-C4  | 2.59  | 1.40        | 1.33     |
| 2   | C     | 601 | ATP  | C8-N7  | 2.59  | 1.36        | 1.31     |
| 3   | A     | 603 | OXL  | O3-C1  | -2.55 | 1.23        | 1.30     |
| 5   | C     | 605 | FUM  | C4-C   | 2.52  | 1.54        | 1.48     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | C     | 603 | OXL  | O3-C1   | -2.51 | 1.23        | 1.30     |
| 3   | B     | 603 | OXL  | O3-C1   | -2.46 | 1.23        | 1.30     |
| 2   | D     | 601 | ATP  | PA-O3A  | 2.46  | 1.62        | 1.59     |
| 2   | A     | 601 | ATP  | PB-O3B  | -2.44 | 1.56        | 1.59     |
| 2   | B     | 601 | ATP  | C8-N7   | 2.43  | 1.36        | 1.31     |
| 2   | A     | 601 | ATP  | C2-N1   | 2.41  | 1.38        | 1.33     |
| 2   | C     | 601 | ATP  | PA-O3A  | 2.37  | 1.62        | 1.59     |
| 5   | A     | 605 | FUM  | C4-C    | 2.33  | 1.54        | 1.48     |
| 2   | D     | 601 | ATP  | C8-N7   | 2.27  | 1.36        | 1.31     |
| 2   | C     | 601 | ATP  | C2-N1   | 2.23  | 1.37        | 1.33     |
| 2   | D     | 601 | ATP  | C4-N9   | -2.17 | 1.33        | 1.37     |
| 5   | D     | 605 | FUM  | C5-C4   | 2.16  | 1.39        | 1.33     |
| 2   | B     | 601 | ATP  | C4-N9   | -2.13 | 1.33        | 1.37     |
| 2   | A     | 601 | ATP  | C2-N3   | 2.13  | 1.37        | 1.33     |
| 2   | A     | 601 | ATP  | C8-N7   | 2.12  | 1.35        | 1.31     |
| 2   | C     | 601 | ATP  | O4'-C1' | 2.05  | 1.46        | 1.42     |
| 2   | C     | 601 | ATP  | C4-N9   | -2.03 | 1.33        | 1.37     |
| 2   | C     | 601 | ATP  | C2-N3   | 2.00  | 1.37        | 1.33     |

All (44) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | D     | 601 | ATP  | C5-C4-N3 | -5.97 | 118.49      | 126.72   |
| 2   | C     | 601 | ATP  | C5-C4-N3 | -5.94 | 118.53      | 126.72   |
| 2   | B     | 601 | ATP  | C5-C4-N3 | -5.89 | 118.61      | 126.72   |
| 2   | A     | 601 | ATP  | C5-C4-N3 | -5.76 | 118.78      | 126.72   |
| 2   | B     | 601 | ATP  | N3-C2-N1 | -5.41 | 120.39      | 128.58   |
| 2   | D     | 601 | ATP  | N3-C2-N1 | -5.27 | 120.61      | 128.58   |
| 2   | A     | 601 | ATP  | N3-C2-N1 | -5.25 | 120.64      | 128.58   |
| 2   | C     | 601 | ATP  | N3-C2-N1 | -5.16 | 120.77      | 128.58   |
| 2   | B     | 601 | ATP  | C6-C5-N7 | -5.01 | 122.43      | 132.09   |
| 2   | A     | 601 | ATP  | C6-C5-N7 | -4.99 | 122.46      | 132.09   |
| 2   | C     | 601 | ATP  | C6-C5-N7 | -4.99 | 122.47      | 132.09   |
| 2   | D     | 601 | ATP  | C6-C5-N7 | -4.98 | 122.49      | 132.09   |
| 2   | A     | 601 | ATP  | C6-C5-C4 | 4.98  | 123.97      | 117.18   |
| 2   | C     | 601 | ATP  | C6-C5-C4 | 4.93  | 123.91      | 117.18   |
| 2   | D     | 601 | ATP  | N3-C4-N9 | 4.90  | 135.49      | 127.17   |
| 2   | D     | 601 | ATP  | C6-C5-C4 | 4.90  | 123.86      | 117.18   |
| 2   | C     | 601 | ATP  | N3-C4-N9 | 4.87  | 135.45      | 127.17   |
| 2   | B     | 601 | ATP  | N3-C4-N9 | 4.83  | 135.38      | 127.17   |
| 2   | A     | 601 | ATP  | N3-C4-N9 | 4.77  | 135.29      | 127.17   |
| 2   | B     | 601 | ATP  | C6-C5-C4 | 4.77  | 123.69      | 117.18   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | B     | 603 | OXL  | O3-C1-C2   | 4.13  | 120.85      | 112.83   |
| 3   | C     | 603 | OXL  | O3-C1-C2   | 4.08  | 120.74      | 112.83   |
| 3   | D     | 603 | OXL  | O3-C1-C2   | 3.94  | 120.47      | 112.83   |
| 2   | C     | 601 | ATP  | N9-C8-N7   | -3.92 | 108.38      | 113.94   |
| 3   | A     | 603 | OXL  | O3-C1-C2   | 3.91  | 120.42      | 112.83   |
| 2   | B     | 601 | ATP  | N9-C8-N7   | -3.88 | 108.43      | 113.94   |
| 2   | D     | 601 | ATP  | N9-C8-N7   | -3.85 | 108.47      | 113.94   |
| 2   | A     | 601 | ATP  | N9-C8-N7   | -3.83 | 108.51      | 113.94   |
| 3   | A     | 603 | OXL  | O4-C2-C1   | 3.81  | 120.22      | 112.83   |
| 3   | D     | 603 | OXL  | O4-C2-C1   | 3.78  | 120.17      | 112.83   |
| 3   | C     | 603 | OXL  | O4-C2-C1   | 3.57  | 119.76      | 112.83   |
| 3   | B     | 603 | OXL  | O4-C2-C1   | 3.49  | 119.59      | 112.83   |
| 2   | D     | 601 | ATP  | C2-N3-C4   | 3.31  | 119.92      | 111.83   |
| 2   | B     | 601 | ATP  | C2-N3-C4   | 3.27  | 119.81      | 111.83   |
| 2   | C     | 601 | ATP  | C2-N3-C4   | 3.23  | 119.71      | 111.83   |
| 2   | A     | 601 | ATP  | C2-N3-C4   | 3.14  | 119.50      | 111.83   |
| 2   | B     | 601 | ATP  | C4-C5-N7   | 2.83  | 113.82      | 110.58   |
| 2   | D     | 601 | ATP  | C4-C5-N7   | 2.65  | 113.62      | 110.58   |
| 2   | C     | 601 | ATP  | C4-C5-N7   | 2.65  | 113.61      | 110.58   |
| 2   | A     | 601 | ATP  | C4-C5-N7   | 2.60  | 113.56      | 110.58   |
| 2   | B     | 601 | ATP  | O4'-C1'-N9 | 2.60  | 113.08      | 108.09   |
| 2   | A     | 601 | ATP  | O4'-C1'-N9 | 2.51  | 112.92      | 108.09   |
| 2   | D     | 601 | ATP  | O4'-C1'-N9 | 2.45  | 112.80      | 108.09   |
| 2   | C     | 601 | ATP  | O4'-C1'-N9 | 2.33  | 112.56      | 108.09   |

There are no chirality outliers.

All (15) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 2   | B     | 601 | ATP  | PB-O3B-PG-O3G |
| 2   | A     | 601 | ATP  | PB-O3A-PA-O5' |
| 5   | A     | 605 | FUM  | C4-C5-C6-O7   |
| 5   | B     | 605 | FUM  | C4-C5-C6-O7   |
| 2   | B     | 601 | ATP  | PB-O3B-PG-O2G |
| 5   | A     | 605 | FUM  | C4-C5-C6-O8   |
| 2   | A     | 601 | ATP  | PG-O3B-PB-O1B |
| 5   | C     | 605 | FUM  | C4-C5-C6-O7   |
| 5   | B     | 605 | FUM  | C4-C5-C6-O8   |
| 2   | D     | 601 | ATP  | PG-O3B-PB-O2B |
| 5   | C     | 605 | FUM  | C4-C5-C6-O8   |
| 2   | C     | 601 | ATP  | PG-O3B-PB-O2B |
| 2   | B     | 601 | ATP  | PB-O3B-PG-O1G |

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| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 2   | A     | 601 | ATP  | PG-O3B-PB-O2B |
| 2   | C     | 601 | ATP  | PG-O3B-PB-O1B |

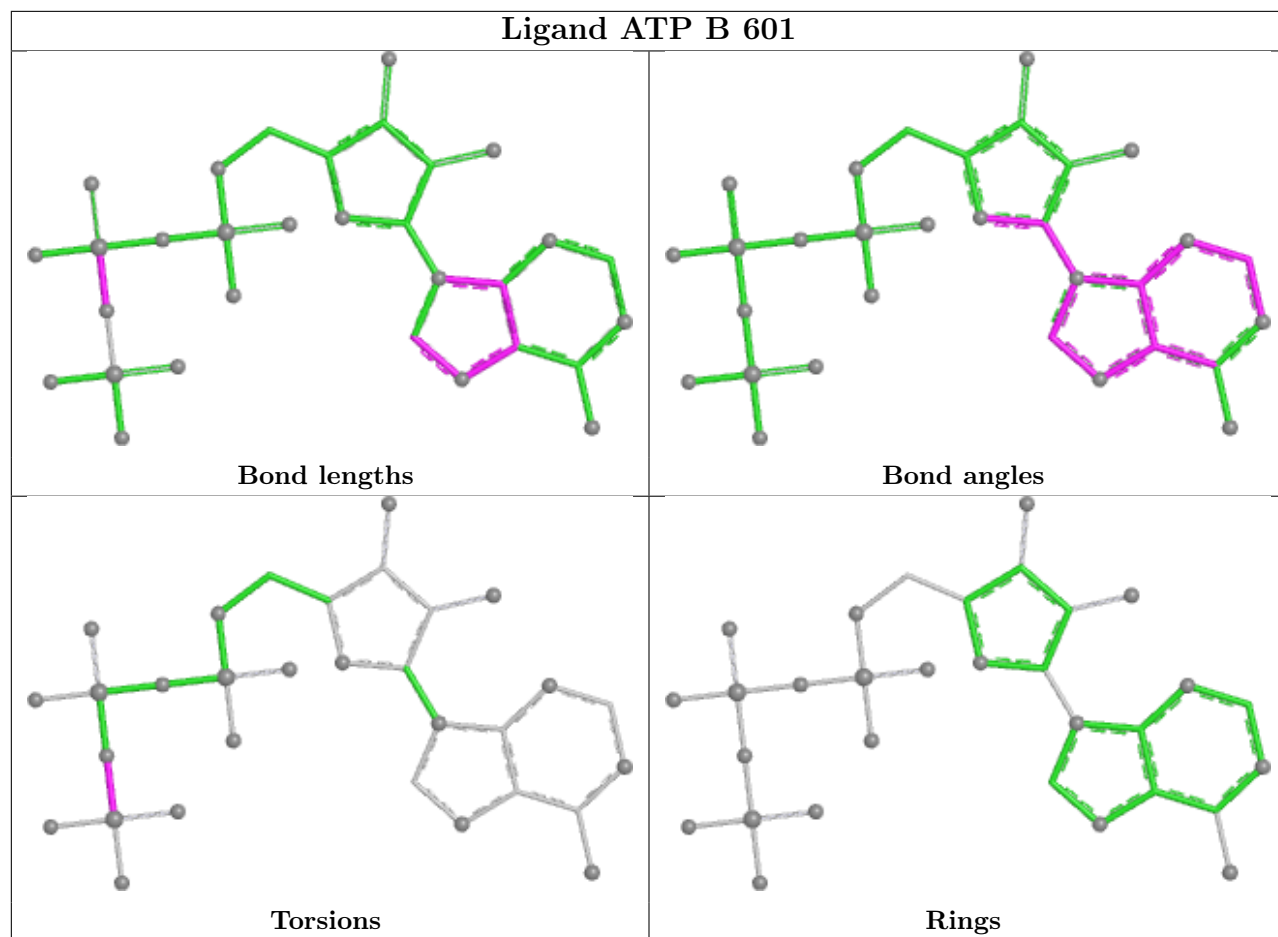
There are no ring outliers.

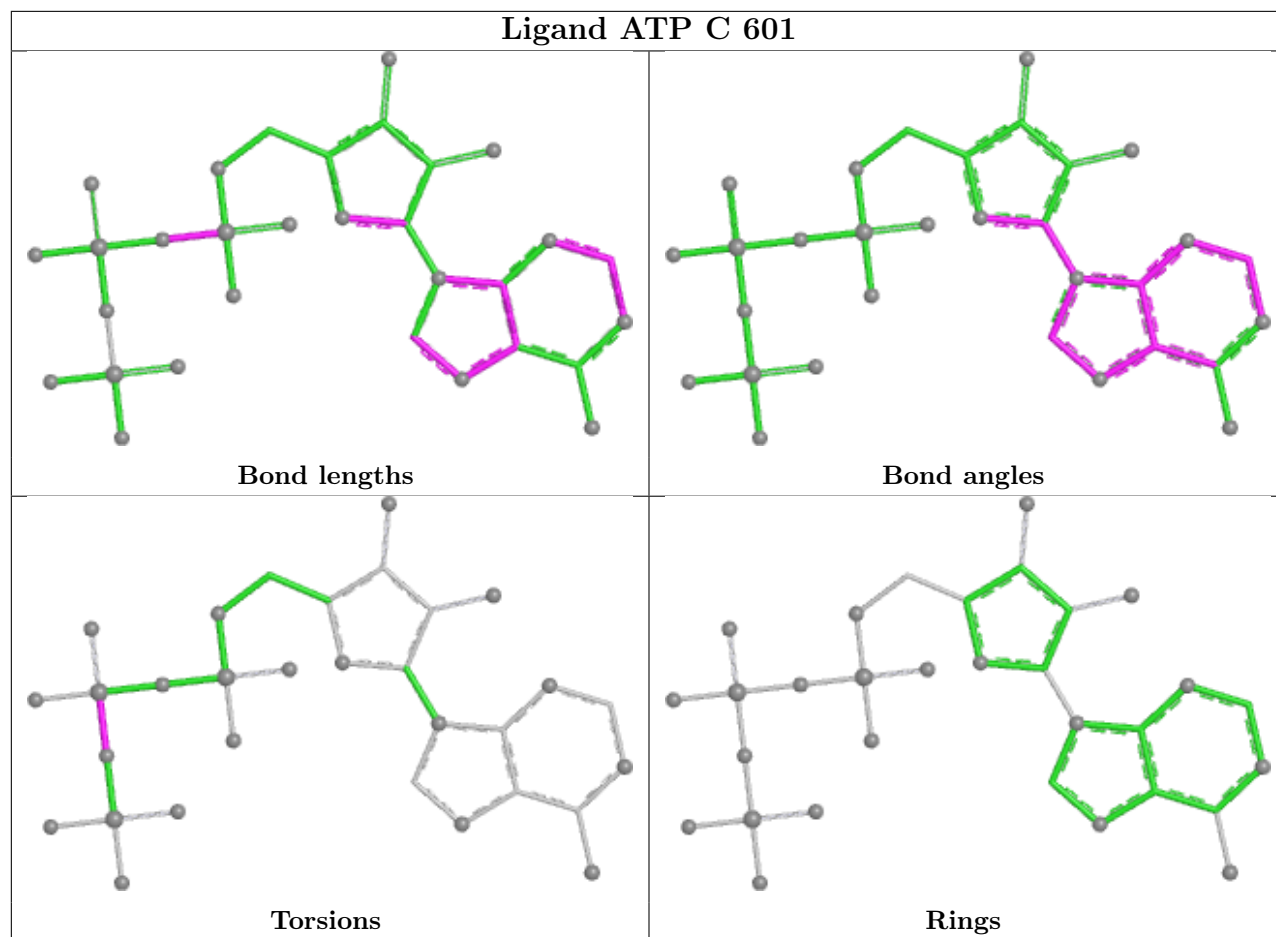
8 monomers are involved in 10 short contacts:

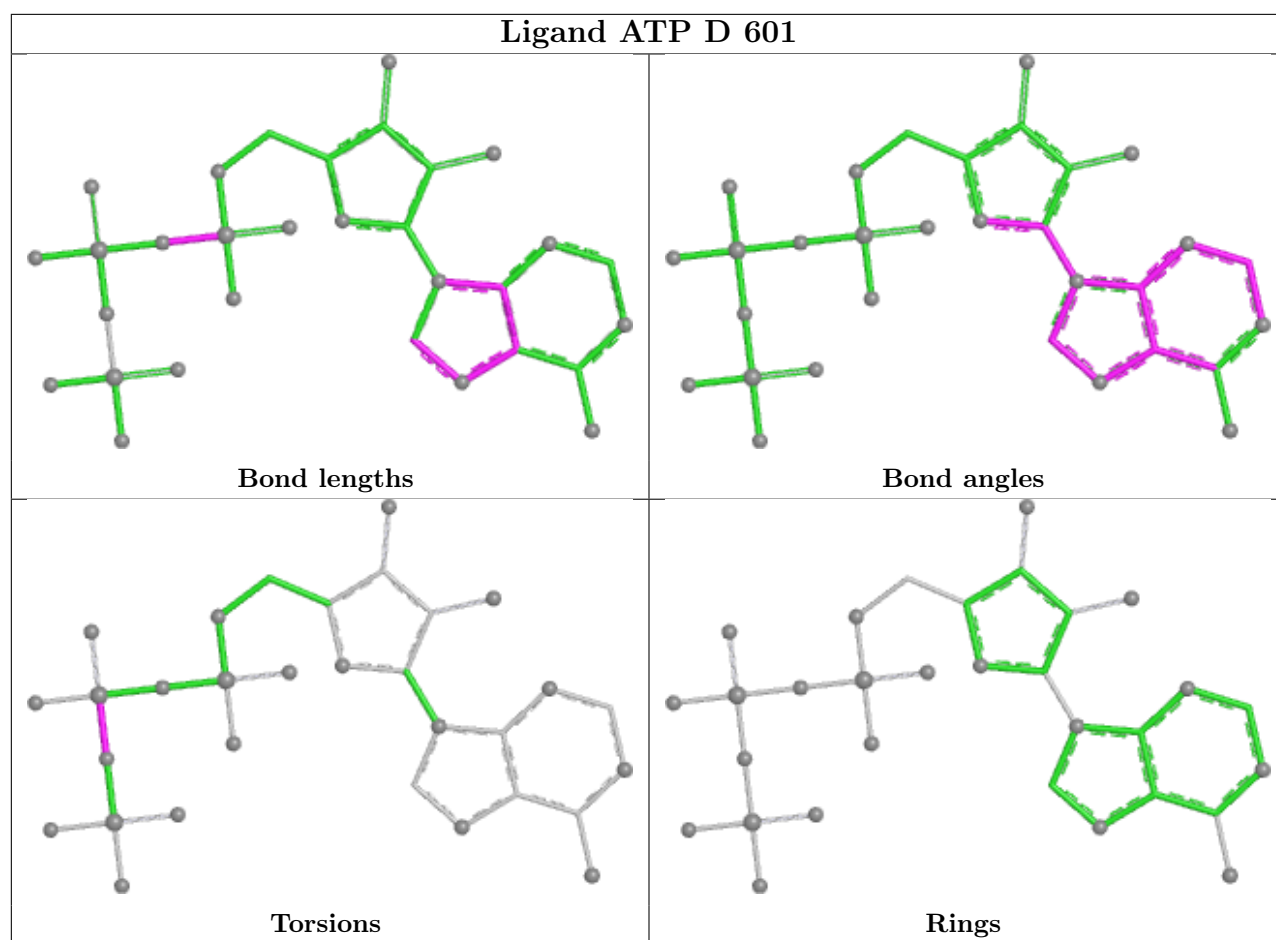
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 603 | OXL  | 1       | 0            |
| 2   | B     | 601 | ATP  | 3       | 0            |
| 5   | B     | 605 | FUM  | 1       | 0            |
| 2   | C     | 601 | ATP  | 1       | 0            |
| 2   | D     | 601 | ATP  | 1       | 0            |
| 5   | C     | 605 | FUM  | 1       | 0            |
| 5   | D     | 605 | FUM  | 1       | 0            |
| 2   | A     | 601 | ATP  | 1       | 0            |

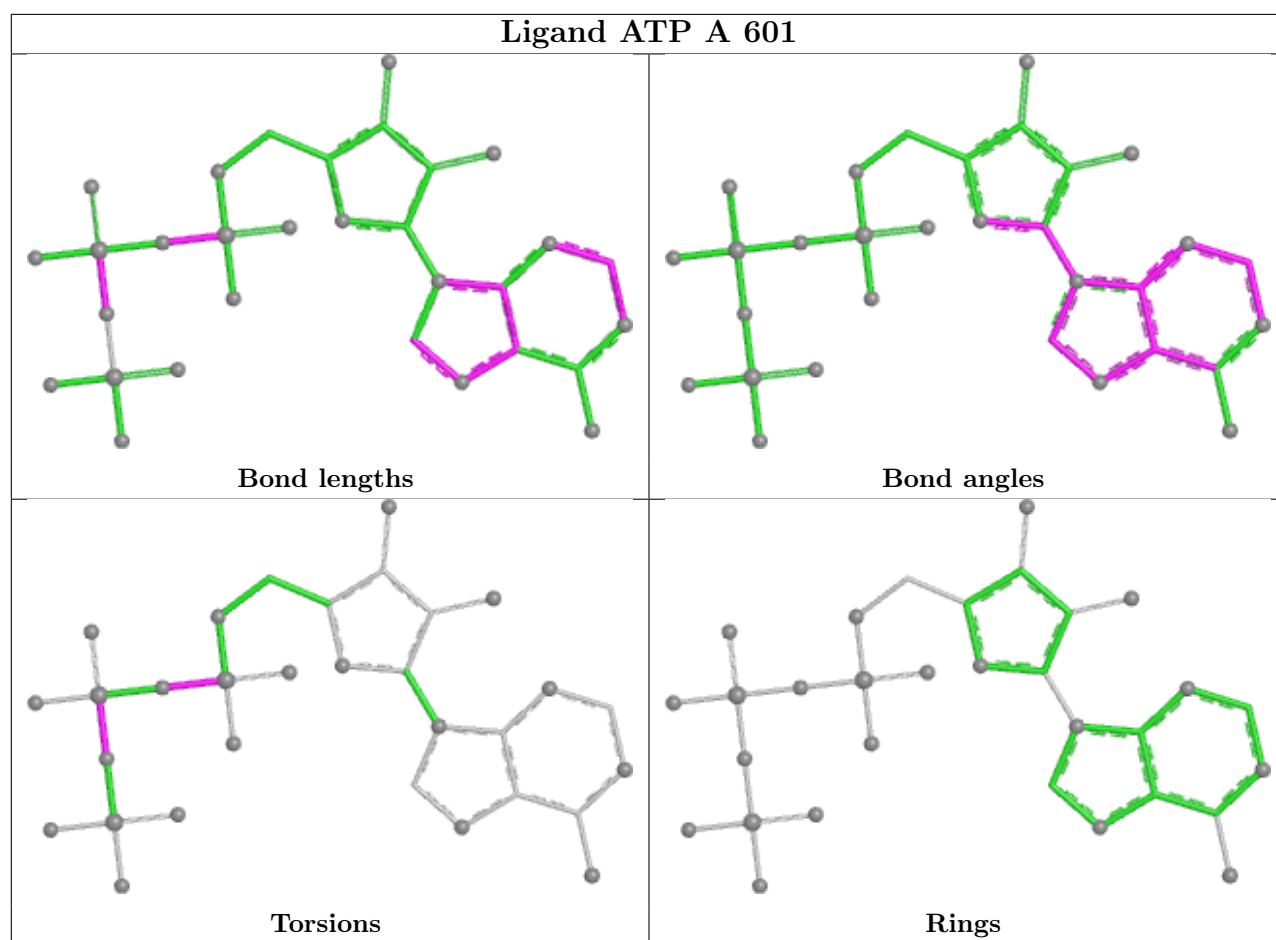
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand ATP B 601









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.