



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:32 PM UTC

PDB ID : 6COX / pdb\_00006cox  
Title : CYCLOOXYGENASE-2 (PROSTAGLANDIN SYNTHASE-2) COM-  
PLEXED WITH A SELECTIVE INHIBITOR, SC-558 IN I222 SPACE  
GROUP  
Authors : Kurumbail, R.; Stallings, W.  
Deposited on : 1996-12-18  
Resolution : 2.80 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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

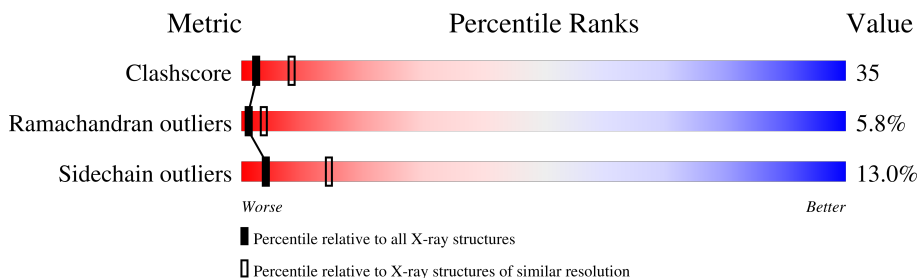
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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                      | 4276 (2.80-2.80)                                      |
| Ramachandran outliers | 187476                      | 4196 (2.80-2.80)                                      |
| Sidechain outliers    | 187428                      | 4198 (2.80-2.80)                                      |

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     | 587    |                  |
| 1   | B     | 587    |                  |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9168 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 CYCLOOXYGENASE-2.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 552      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4473  | 2886 | 748 | 814 | 25 |         |         |       |
| 1   | B     | 552      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4473  | 2886 | 748 | 814 | 25 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

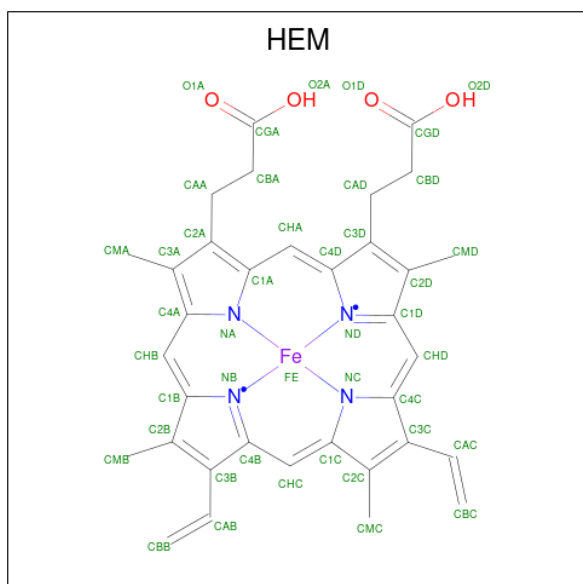
| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 310     | GLN      | ASN    | conflict | UNP Q05769 |
| A     | 333     | LYS      | ARG    | conflict | UNP Q05769 |
| B     | 310     | GLN      | ASN    | conflict | UNP Q05769 |
| B     | 333     | LYS      | ARG    | conflict | UNP Q05769 |

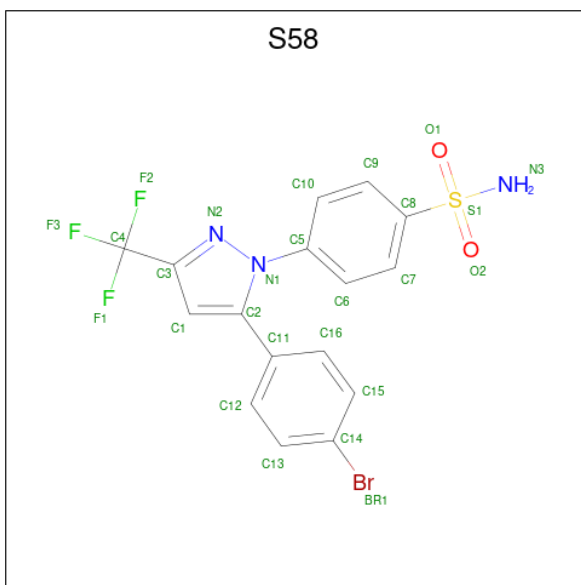
- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





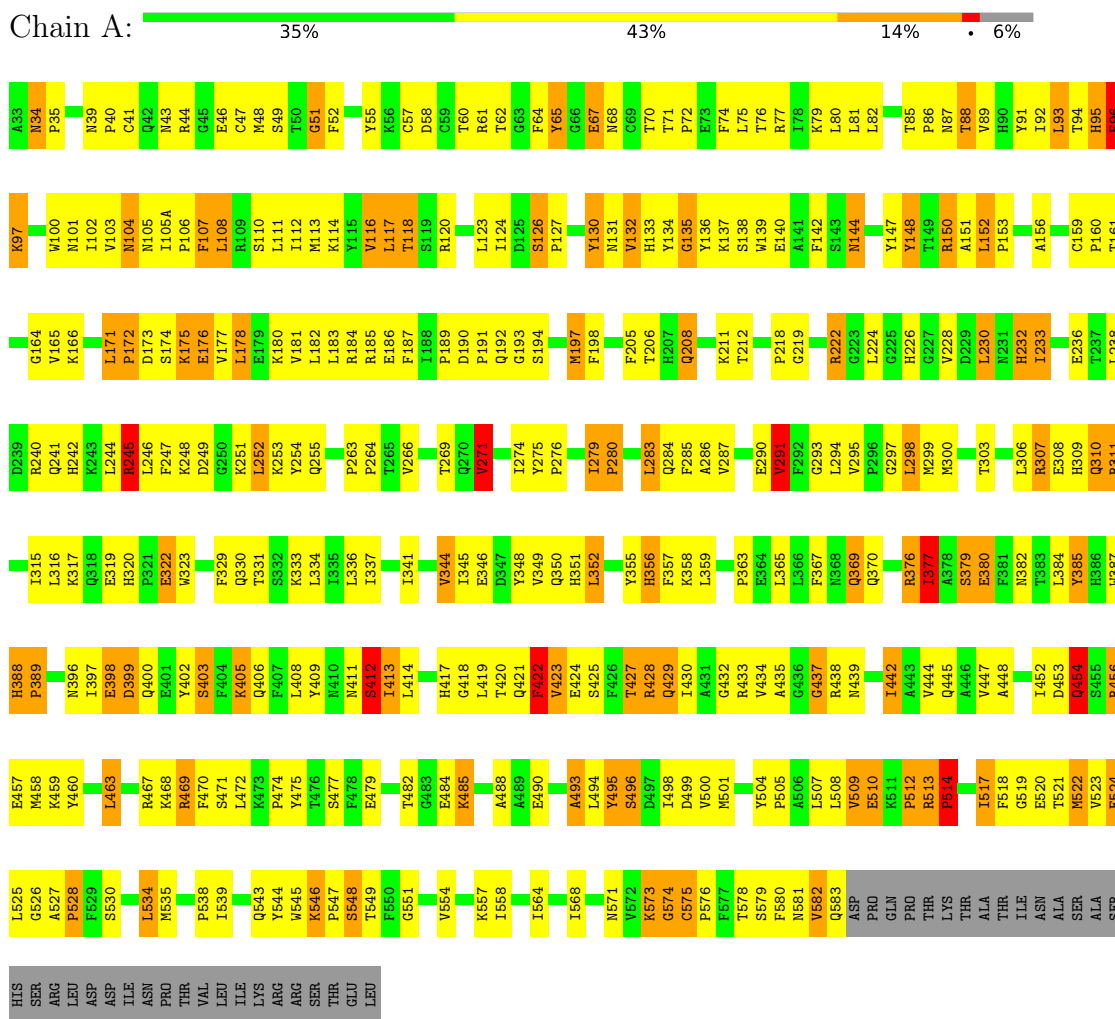
| Mol | Chain | Residues | Atoms |    |    |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---|---|---------|---------|
|     |       |          | Total | Br | C  | F | N | O | S |         |         |
| 4   | A     | 1        | 26    | 1  | 16 | 3 | 3 | 2 | 1 | 0       | 0       |
| 4   | B     | 1        | 26    | 1  | 16 | 3 | 3 | 2 | 1 | 0       | 0       |

### 3 Residue-property plots

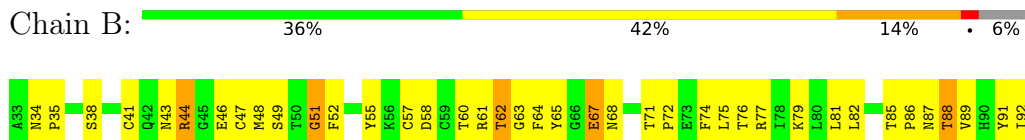
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

#### • Molecule 1: CYCLOOXYGENASE-2



#### • Molecule 1: CYCLOOXYGENASE-2



[illegible]

## 4 Data and refinement statistics

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

| Property                                                 | Value                                           | Source    |
|----------------------------------------------------------|-------------------------------------------------|-----------|
| Space group                                              | I 2 2 2                                         | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 181.17Å 132.81Å 122.74Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 8.00 – 2.80                                     | Depositor |
| % Data completeness<br>(in resolution range)             | 88.5 (8.00-2.80)                                | Depositor |
| $R_{merge}$                                              | 0.09                                            | Depositor |
| $R_{sym}$                                                | 0.09                                            | Depositor |
| Refinement program                                       | X-PLOR 3.1                                      | Depositor |
| R, $R_{free}$                                            | 0.220 , 0.309                                   | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 9168                                            | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 20.0                                            | 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: HEM, NAG, S58

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     | 0.80         | 1/4600 (0.0%) | 1.26        | 55/6237 (0.9%)   |
| 1   | B     | 0.79         | 2/4600 (0.0%) | 1.27        | 46/6237 (0.7%)   |
| All | All   | 0.80         | 3/9200 (0.0%) | 1.27        | 101/12474 (0.8%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 279 | ILE  | CA-CB  | 6.07  | 1.58        | 1.54     |
| 1   | A     | 197 | MET  | SD-CE  | -5.78 | 1.65        | 1.79     |
| 1   | B     | 388 | HIS  | CG-CD2 | 5.49  | 1.41        | 1.35     |

All (101) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 269 | THR  | N-CA-C | -9.50 | 97.72       | 110.55   |
| 1   | A     | 319 | GLU  | N-CA-C | -9.46 | 102.55      | 114.56   |
| 1   | B     | 137 | LYS  | N-CA-C | 9.29  | 122.36      | 111.02   |
| 1   | A     | 137 | LYS  | N-CA-C | 9.25  | 122.30      | 111.02   |
| 1   | B     | 427 | THR  | N-CA-C | -9.04 | 101.43      | 111.28   |
| 1   | A     | 208 | GLN  | N-CA-C | -9.02 | 101.85      | 113.12   |
| 1   | A     | 269 | THR  | N-CA-C | -8.84 | 98.61       | 110.55   |
| 1   | B     | 208 | GLN  | N-CA-C | -8.77 | 102.16      | 113.12   |
| 1   | A     | 513 | ARG  | N-CA-C | -8.57 | 97.92       | 109.84   |
| 1   | A     | 427 | THR  | N-CA-C | -8.48 | 102.04      | 111.28   |
| 1   | B     | 513 | ARG  | N-CA-C | -8.40 | 98.17       | 109.84   |
| 1   | B     | 319 | GLU  | N-CA-C | -8.21 | 104.13      | 114.56   |
| 1   | A     | 423 | VAL  | N-CA-C | -8.20 | 102.83      | 110.53   |
| 1   | A     | 287 | VAL  | N-CA-C | 7.99  | 125.97      | 109.34   |
| 1   | B     | 148 | TYR  | N-CA-C | -7.91 | 97.74       | 110.32   |
| 1   | B     | 574 | GLY  | N-CA-C | -7.88 | 101.34      | 112.37   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 148 | TYR  | N-CA-C     | -7.73 | 98.03       | 110.32   |
| 1   | B     | 287 | VAL  | N-CA-C     | 7.67  | 125.28      | 109.34   |
| 1   | B     | 423 | VAL  | N-CA-C     | -7.33 | 103.64      | 110.53   |
| 1   | B     | 437 | GLY  | N-CA-C     | -7.32 | 100.17      | 111.00   |
| 1   | B     | 34  | ASN  | CA-C-N     | 7.22  | 127.84      | 119.47   |
| 1   | B     | 34  | ASN  | C-N-CA     | 7.22  | 127.84      | 119.47   |
| 1   | A     | 245 | ARG  | N-CA-C     | 7.13  | 121.67      | 110.32   |
| 1   | A     | 574 | GLY  | N-CA-C     | -7.08 | 103.00      | 112.14   |
| 1   | B     | 454 | GLN  | N-CA-C     | -7.07 | 103.53      | 112.93   |
| 1   | B     | 245 | ARG  | N-CA-C     | 6.95  | 121.36      | 110.17   |
| 1   | A     | 524 | GLU  | N-CA-C     | 6.87  | 119.79      | 111.82   |
| 1   | A     | 34  | ASN  | CA-C-N     | 6.67  | 127.21      | 119.47   |
| 1   | A     | 34  | ASN  | C-N-CA     | 6.67  | 127.21      | 119.47   |
| 1   | A     | 437 | GLY  | N-CA-C     | -6.53 | 101.34      | 111.00   |
| 1   | B     | 526 | GLY  | N-CA-C     | 6.45  | 121.69      | 113.24   |
| 1   | A     | 526 | GLY  | N-CA-C     | 6.43  | 121.66      | 113.24   |
| 1   | B     | 346 | GLU  | N-CA-C     | 6.43  | 121.12      | 113.28   |
| 1   | B     | 524 | GLU  | N-CA-C     | 6.42  | 119.27      | 111.82   |
| 1   | A     | 346 | GLU  | N-CA-C     | 6.39  | 121.16      | 113.23   |
| 1   | A     | 135 | GLY  | N-CA-C     | -6.37 | 105.73      | 115.66   |
| 1   | A     | 454 | GLN  | N-CA-C     | -6.32 | 104.27      | 112.68   |
| 1   | A     | 495 | TYR  | N-CA-C     | 6.32  | 119.11      | 111.40   |
| 1   | B     | 580 | PHE  | N-CA-C     | -6.30 | 105.34      | 113.16   |
| 1   | A     | 62  | THR  | N-CA-C     | -6.27 | 103.01      | 112.04   |
| 1   | A     | 388 | HIS  | ND1-CG-CD2 | 6.23  | 112.33      | 106.10   |
| 1   | B     | 218 | PRO  | N-CA-C     | -6.22 | 100.41      | 110.55   |
| 1   | B     | 62  | THR  | N-CA-C     | -6.20 | 103.12      | 112.04   |
| 1   | A     | 546 | LYS  | CA-C-N     | 6.17  | 127.55      | 119.84   |
| 1   | A     | 546 | LYS  | C-N-CA     | 6.17  | 127.55      | 119.84   |
| 1   | A     | 422 | PHE  | N-CA-C     | -6.12 | 97.78       | 110.80   |
| 1   | A     | 271 | VAL  | N-CA-C     | 6.10  | 116.89      | 108.84   |
| 1   | A     | 218 | PRO  | N-CA-C     | -6.09 | 100.62      | 110.55   |
| 1   | A     | 580 | PHE  | N-CA-C     | -6.04 | 105.67      | 113.16   |
| 1   | B     | 161 | THR  | CA-C-N     | 5.99  | 127.33      | 119.84   |
| 1   | B     | 161 | THR  | C-N-CA     | 5.99  | 127.33      | 119.84   |
| 1   | B     | 546 | LYS  | CA-C-N     | 5.98  | 127.31      | 119.84   |
| 1   | B     | 546 | LYS  | C-N-CA     | 5.98  | 127.31      | 119.84   |
| 1   | B     | 575 | CYS  | CA-C-N     | -5.88 | 113.64      | 119.99   |
| 1   | B     | 575 | CYS  | C-N-CA     | -5.88 | 113.64      | 119.99   |
| 1   | A     | 548 | SER  | N-CA-C     | 5.88  | 117.36      | 111.07   |
| 1   | B     | 233 | ILE  | CB-CA-C    | -5.81 | 104.94      | 111.80   |
| 1   | A     | 403 | SER  | N-CA-C     | -5.80 | 101.11      | 110.32   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | B     | 370 | GLN  | N-CA-C      | -5.79 | 101.71      | 110.28   |
| 1   | B     | 495 | TYR  | N-CA-C      | 5.74  | 118.40      | 111.40   |
| 1   | A     | 370 | GLN  | N-CA-C      | -5.66 | 101.90      | 110.28   |
| 1   | B     | 379 | SER  | N-CA-C      | -5.64 | 104.83      | 110.97   |
| 1   | A     | 130 | TYR  | N-CA-C      | 5.61  | 117.31      | 110.41   |
| 1   | A     | 222 | ARG  | N-CA-C      | -5.59 | 105.81      | 113.30   |
| 1   | B     | 377 | ILE  | N-CA-C      | 5.59  | 116.81      | 108.54   |
| 1   | A     | 377 | ILE  | N-CA-C      | 5.56  | 116.23      | 108.89   |
| 1   | B     | 422 | PHE  | N-CA-C      | -5.53 | 99.01       | 110.80   |
| 1   | B     | 130 | TYR  | N-CA-C      | 5.49  | 117.17      | 110.41   |
| 1   | A     | 494 | LEU  | N-CA-C      | 5.48  | 117.12      | 111.03   |
| 1   | A     | 233 | ILE  | CB-CA-C     | -5.48 | 105.24      | 111.55   |
| 1   | A     | 571 | ASN  | N-CA-C      | 5.44  | 119.90      | 112.88   |
| 1   | B     | 434 | VAL  | N-CA-C      | 5.43  | 115.68      | 110.74   |
| 1   | B     | 107 | PHE  | N-CA-C      | -5.42 | 105.27      | 111.07   |
| 1   | A     | 379 | SER  | N-CA-C      | -5.41 | 105.08      | 110.97   |
| 1   | B     | 403 | SER  | N-CA-C      | -5.36 | 101.80      | 110.32   |
| 1   | B     | 517 | ILE  | N-CA-C      | 5.35  | 118.61      | 111.44   |
| 1   | B     | 176 | GLU  | N-CA-C      | -5.34 | 105.35      | 111.07   |
| 1   | A     | 166 | LYS  | N-CA-C      | 5.33  | 118.17      | 110.28   |
| 1   | A     | 493 | ALA  | N-CA-C      | -5.31 | 105.41      | 111.14   |
| 1   | A     | 575 | CYS  | CA-C-N      | -5.30 | 114.27      | 119.99   |
| 1   | A     | 575 | CYS  | C-N-CA      | -5.30 | 114.27      | 119.99   |
| 1   | A     | 161 | THR  | CA-C-N      | 5.28  | 126.44      | 119.84   |
| 1   | A     | 161 | THR  | C-N-CA      | 5.28  | 126.44      | 119.84   |
| 1   | A     | 388 | HIS  | ND1-CE1-NE2 | 5.27  | 113.67      | 108.40   |
| 1   | A     | 456 | ARG  | N-CA-C      | -5.27 | 105.62      | 111.36   |
| 1   | B     | 166 | LYS  | N-CA-C      | 5.27  | 118.52      | 110.20   |
| 1   | A     | 317 | LYS  | CA-C-N      | -5.24 | 114.12      | 122.66   |
| 1   | A     | 317 | LYS  | C-N-CA      | -5.24 | 114.12      | 122.66   |
| 1   | B     | 251 | LYS  | N-CA-C      | 5.24  | 117.44      | 110.53   |
| 1   | B     | 548 | SER  | N-CA-C      | 5.21  | 116.64      | 111.07   |
| 1   | A     | 118 | THR  | N-CA-C      | 5.17  | 117.71      | 111.40   |
| 1   | A     | 517 | ILE  | N-CA-C      | 5.14  | 118.33      | 111.44   |
| 1   | A     | 95  | HIS  | N-CA-C      | 5.12  | 116.59      | 109.31   |
| 1   | B     | 388 | HIS  | ND1-CG-CD2  | 5.12  | 111.22      | 106.10   |
| 1   | A     | 291 | VAL  | N-CA-C      | 5.08  | 119.36      | 113.42   |
| 1   | B     | 222 | ARG  | N-CA-C      | -5.08 | 106.50      | 113.30   |
| 1   | B     | 118 | THR  | N-CA-C      | 5.04  | 117.75      | 111.24   |
| 1   | B     | 300 | MET  | N-CA-C      | -5.04 | 105.69      | 111.14   |
| 1   | A     | 171 | LEU  | CA-C-N      | 5.02  | 126.11      | 119.84   |
| 1   | A     | 171 | LEU  | C-N-CA      | 5.02  | 126.11      | 119.84   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | A     | 434 | VAL  | N-CA-C | 5.00 | 115.29      | 110.74   |

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     | 4473  | 0        | 4375     | 330     | 0            |
| 1   | B     | 4473  | 0        | 4375     | 322     | 0            |
| 2   | A     | 42    | 0        | 39       | 1       | 0            |
| 2   | B     | 42    | 0        | 39       | 0       | 0            |
| 3   | A     | 43    | 0        | 30       | 2       | 0            |
| 3   | B     | 43    | 0        | 30       | 1       | 0            |
| 4   | A     | 26    | 0        | 11       | 3       | 0            |
| 4   | B     | 26    | 0        | 11       | 2       | 0            |
| All | All   | 9168  | 0        | 8910     | 634     | 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 35.

All (634) 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:283:LEU:HD22 | 1:A:411:ASN:HB2  | 1.32                     | 1.11              |
| 1:B:280:PRO:HD2  | 1:B:283:LEU:HD23 | 1.35                     | 1.09              |
| 1:A:279:ILE:HG23 | 1:A:283:LEU:HG   | 1.32                     | 1.08              |
| 1:B:279:ILE:HG23 | 1:B:283:LEU:HG   | 1.37                     | 1.07              |
| 1:A:458:MET:HE3  | 1:A:460:TYR:HE1  | 1.17                     | 1.05              |
| 1:B:458:MET:HE3  | 1:B:460:TYR:HE1  | 1.20                     | 1.03              |
| 1:A:280:PRO:HD2  | 1:A:283:LEU:HD23 | 1.41                     | 1.02              |
| 1:B:283:LEU:HD22 | 1:B:411:ASN:HB2  | 1.39                     | 1.00              |
| 1:B:156:ALA:HB3  | 1:B:159:CYS:SG   | 2.01                     | 0.99              |
| 1:A:156:ALA:HB3  | 1:A:159:CYS:SG   | 2.03                     | 0.99              |
| 1:B:75:LEU:HD11  | 1:B:79:LYS:HE2   | 1.50                     | 0.94              |

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| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 1:B:458:MET:HE3     | 1:B:460:TYR:CE1  | 2.03                     | 0.93              |
| 1:A:458:MET:HE3     | 1:A:460:TYR:CE1  | 2.04                     | 0.92              |
| 1:A:75:LEU:HD11     | 1:A:79:LYS:HE2   | 1.57                     | 0.86              |
| 1:B:208:GLN:NE2     | 1:B:228:VAL:HA   | 1.90                     | 0.86              |
| 1:A:208:GLN:NE2     | 1:A:228:VAL:HA   | 1.92                     | 0.84              |
| 1:B:283:LEU:HB2     | 1:B:411:ASN:ND2  | 1.93                     | 0.83              |
| 1:A:124:ILE:HD11    | 1:A:528:PRO:HB3  | 1.61                     | 0.82              |
| 1:A:191:PRO:HD2     | 1:A:433:ARG:HG3  | 1.60                     | 0.82              |
| 1:B:341:ILE:HG23    | 1:B:534:LEU:HD12 | 1.62                     | 0.82              |
| 1:A:104:ASN:ND2     | 1:A:358:LYS:HB2  | 1.97                     | 0.80              |
| 1:B:104:ASN:ND2     | 1:B:358:LYS:HB2  | 1.98                     | 0.79              |
| 1:A:341:ILE:HG23    | 1:A:534:LEU:HD12 | 1.64                     | 0.79              |
| 1:A:283:LEU:HB2     | 1:A:411:ASN:ND2  | 1.97                     | 0.79              |
| 1:A:294:LEU:HA      | 1:A:409:TYR:HB3  | 1.63                     | 0.78              |
| 1:B:190:ASP:HB2     | 1:B:432:GLY:O    | 1.84                     | 0.77              |
| 1:B:530:SER:O       | 1:B:534:LEU:HD23 | 1.86                     | 0.76              |
| 1:A:190:ASP:HB2     | 1:A:432:GLY:O    | 1.86                     | 0.75              |
| 1:B:280:PRO:CD      | 1:B:283:LEU:HD23 | 2.13                     | 0.74              |
| 1:B:124:ILE:HD11    | 1:B:528:PRO:HB3  | 1.69                     | 0.74              |
| 1:A:322:GLU:HG2     | 1:B:52:PHE:H     | 1.51                     | 0.74              |
| 1:B:41:CYS:SG       | 1:B:47:CYS:HB2   | 2.28                     | 0.74              |
| 1:A:283:LEU:CD2     | 1:A:411:ASN:HB2  | 2.15                     | 0.74              |
| 1:B:197:MET:HE2     | 1:B:423:VAL:HG13 | 1.68                     | 0.74              |
| 1:B:283:LEU:HB2     | 1:B:411:ASN:CG   | 2.11                     | 0.74              |
| 1:A:322:GLU:HG2     | 1:B:52:PHE:N     | 2.02                     | 0.74              |
| 1:A:197:MET:HE2     | 1:A:423:VAL:HG13 | 1.70                     | 0.73              |
| 1:B:294:LEU:HA      | 1:B:409:TYR:HB3  | 1.69                     | 0.73              |
| 1:A:105(A):ILE:HG22 | 1:A:108:LEU:H    | 1.52                     | 0.73              |
| 1:A:52:PHE:H        | 1:B:322:GLU:HG2  | 1.54                     | 0.72              |
| 1:B:504:TYR:HB3     | 1:B:505:PRO:HD3  | 1.70                     | 0.72              |
| 1:B:279:ILE:HG13    | 1:B:283:LEU:HD21 | 1.71                     | 0.72              |
| 1:A:52:PHE:N        | 1:B:322:GLU:HG2  | 2.05                     | 0.72              |
| 1:A:518:PHE:CD1     | 1:A:522:MET:HG2  | 2.25                     | 0.72              |
| 1:A:470:PHE:CD1     | 1:A:525:LEU:HD22 | 2.24                     | 0.72              |
| 1:B:105(A):ILE:HG22 | 1:B:108:LEU:H    | 1.53                     | 0.72              |
| 1:A:41:CYS:SG       | 1:A:47:CYS:HB2   | 2.29                     | 0.72              |
| 1:B:244:LEU:HD23    | 1:B:271:VAL:HG11 | 1.70                     | 0.72              |
| 1:A:283:LEU:HB2     | 1:A:411:ASN:CG   | 2.15                     | 0.71              |
| 1:B:518:PHE:CD1     | 1:B:522:MET:HG2  | 2.24                     | 0.71              |
| 1:A:303:THR:O       | 1:A:307:ARG:HD3  | 1.91                     | 0.71              |
| 1:A:194:SER:OG      | 1:A:351:HIS:HE1  | 1.73                     | 0.71              |

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| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 1:B:295:VAL:HB      | 1:B:298:LEU:CD2  | 2.20                     | 0.71              |
| 1:A:283:LEU:O       | 1:A:283:LEU:HD12 | 1.91                     | 0.70              |
| 1:B:388:HIS:CE1     | 1:B:447:VAL:HG11 | 2.26                     | 0.70              |
| 1:B:276:PRO:HD2     | 1:B:279:ILE:HD13 | 1.73                     | 0.70              |
| 1:A:504:TYR:HB3     | 1:A:505:PRO:HD3  | 1.73                     | 0.70              |
| 1:A:206:THR:HG21    | 1:A:385:TYR:CE1  | 2.27                     | 0.70              |
| 1:A:530:SER:O       | 1:A:534:LEU:HD23 | 1.91                     | 0.69              |
| 1:B:303:THR:O       | 1:B:307:ARG:HD3  | 1.92                     | 0.69              |
| 1:A:244:LEU:HD23    | 1:A:271:VAL:HG11 | 1.73                     | 0.69              |
| 1:A:81:LEU:HD12     | 1:A:81:LEU:O     | 1.93                     | 0.69              |
| 1:B:191:PRO:HD2     | 1:B:433:ARG:HG3  | 1.75                     | 0.69              |
| 1:B:578:THR:HG22    | 1:B:579:SER:N    | 2.07                     | 0.69              |
| 1:B:315:ILE:HG21    | 1:B:558:ILE:HD11 | 1.76                     | 0.69              |
| 1:A:110:SER:HB2     | 1:A:365:LEU:HD21 | 1.75                     | 0.68              |
| 1:B:48:MET:HE3      | 1:B:49:SER:H     | 1.57                     | 0.68              |
| 1:B:470:PHE:CD1     | 1:B:525:LEU:HD22 | 2.29                     | 0.68              |
| 1:A:578:THR:HG22    | 1:A:579:SER:N    | 2.08                     | 0.68              |
| 1:B:283:LEU:CD2     | 1:B:411:ASN:HB2  | 2.21                     | 0.68              |
| 1:A:197:MET:HE3     | 1:A:578:THR:HG21 | 1.76                     | 0.67              |
| 1:A:472:LEU:HD21    | 1:A:524:GLU:HG3  | 1.77                     | 0.67              |
| 1:A:150:ARG:NH2     | 1:A:458:MET:O    | 2.27                     | 0.67              |
| 1:A:105(A):ILE:HD12 | 1:A:108:LEU:HD12 | 1.75                     | 0.67              |
| 1:A:120:ARG:HG3     | 1:A:120:ARG:HH11 | 1.60                     | 0.67              |
| 1:A:244:LEU:CD2     | 1:A:271:VAL:HG11 | 2.25                     | 0.67              |
| 1:A:279:ILE:HG13    | 1:A:283:LEU:HD21 | 1.76                     | 0.67              |
| 1:B:160:PRO:HG2     | 1:B:165:VAL:HA   | 1.77                     | 0.67              |
| 1:A:403:SER:HB2     | 1:A:405:LYS:HZ2  | 1.60                     | 0.67              |
| 1:A:482:THR:HG22    | 1:A:509:VAL:CG1  | 2.25                     | 0.66              |
| 1:B:385:TYR:CE2     | 4:B:701:S58:BR1  | 3.04                     | 0.66              |
| 1:A:185:ARG:HE      | 1:A:438:ARG:HD3  | 1.61                     | 0.66              |
| 1:A:427:THR:HB      | 1:A:428:ARG:NH1  | 2.10                     | 0.66              |
| 1:B:192:GLN:OE1     | 1:B:517:ILE:HG22 | 1.96                     | 0.66              |
| 1:B:205:PHE:CE1     | 1:B:344:VAL:HG21 | 2.31                     | 0.66              |
| 1:A:123:LEU:O       | 1:A:469:ARG:NH2  | 2.29                     | 0.66              |
| 1:A:485:LYS:HA      | 1:A:488:ALA:HB3  | 1.77                     | 0.66              |
| 1:B:105(A):ILE:HD12 | 1:B:108:LEU:HD12 | 1.76                     | 0.66              |
| 1:A:152:LEU:HD23    | 1:A:153:PRO:HD2  | 1.78                     | 0.66              |
| 1:A:192:GLN:OE1     | 1:A:517:ILE:HG22 | 1.95                     | 0.66              |
| 1:B:574:GLY:O       | 1:B:576:PRO:HD3  | 1.94                     | 0.66              |
| 1:A:124:ILE:HD11    | 1:A:528:PRO:CB   | 2.26                     | 0.66              |
| 1:B:274:ILE:HD12    | 1:B:291:VAL:HG23 | 1.78                     | 0.66              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:185:ARG:HE    | 1:B:438:ARG:HD3  | 1.60                     | 0.65              |
| 1:B:400:GLN:OE1   | 1:B:400:GLN:HA   | 1.96                     | 0.65              |
| 1:A:173:ASP:HB3   | 1:A:176:GLU:HB2  | 1.78                     | 0.65              |
| 1:A:322:GLU:HB3   | 1:B:52:PHE:CD1   | 2.31                     | 0.65              |
| 1:A:388:HIS:CE1   | 1:A:447:VAL:HG11 | 2.31                     | 0.65              |
| 1:A:568:ILE:CG2   | 1:A:576:PRO:HD2  | 2.26                     | 0.65              |
| 1:B:175:LYS:HE3   | 1:B:175:LYS:HA   | 1.78                     | 0.65              |
| 1:A:85:THR:O      | 1:A:89:VAL:HG23  | 1.96                     | 0.65              |
| 1:B:81:LEU:HD12   | 1:B:81:LEU:O     | 1.96                     | 0.65              |
| 1:A:279:ILE:HG23  | 1:A:283:LEU:CG   | 2.19                     | 0.65              |
| 1:B:472:LEU:HD21  | 1:B:524:GLU:HG3  | 1.78                     | 0.64              |
| 1:B:182:LEU:O     | 1:B:438:ARG:HA   | 1.97                     | 0.64              |
| 1:B:568:ILE:CG2   | 1:B:576:PRO:HD2  | 2.27                     | 0.64              |
| 1:A:264:PRO:HG2   | 1:A:286:ALA:HB3  | 1.80                     | 0.64              |
| 1:B:283:LEU:HD12  | 1:B:283:LEU:O    | 1.97                     | 0.64              |
| 1:B:295:VAL:HB    | 1:B:298:LEU:HD23 | 1.79                     | 0.64              |
| 1:A:454:GLN:HA    | 1:A:457:GLU:HG3  | 1.80                     | 0.64              |
| 1:A:191:PRO:CD    | 1:A:433:ARG:HG3  | 2.27                     | 0.64              |
| 1:A:48:MET:HE3    | 1:A:49:SER:H     | 1.62                     | 0.64              |
| 1:A:160:PRO:HG2   | 1:A:165:VAL:HA   | 1.78                     | 0.64              |
| 1:A:280:PRO:CD    | 1:A:283:LEU:HD23 | 2.23                     | 0.64              |
| 1:A:463:LEU:O     | 1:A:467:ARG:HG3  | 1.98                     | 0.64              |
| 1:A:574:GLY:O     | 1:A:576:PRO:HD3  | 1.97                     | 0.64              |
| 1:B:244:LEU:CD2   | 1:B:271:VAL:HG11 | 2.27                     | 0.64              |
| 1:A:105(A):ILE:HB | 1:A:108:LEU:HB2  | 1.80                     | 0.63              |
| 1:A:548:SER:OG    | 1:B:58:ASP:HB2   | 1.99                     | 0.63              |
| 1:B:173:ASP:HB3   | 1:B:176:GLU:HB2  | 1.80                     | 0.63              |
| 1:B:477:SER:HB2   | 1:B:479:GLU:OE1  | 1.98                     | 0.63              |
| 1:B:500:VAL:HG12  | 1:B:500:VAL:O    | 1.99                     | 0.63              |
| 1:A:107:PHE:CD1   | 1:A:107:PHE:N    | 2.67                     | 0.63              |
| 1:B:482:THR:HG22  | 1:B:509:VAL:CG1  | 2.29                     | 0.63              |
| 1:A:198:PHE:CZ    | 1:A:352:LEU:HD13 | 2.34                     | 0.62              |
| 1:B:479:GLU:HG3   | 1:B:488:ALA:HB1  | 1.80                     | 0.62              |
| 1:A:52:PHE:CD1    | 1:B:322:GLU:HB3  | 2.35                     | 0.62              |
| 1:A:306:LEU:HD23  | 1:A:306:LEU:O    | 2.00                     | 0.62              |
| 1:A:359:LEU:HD11  | 4:A:701:S58:F1   | 1.90                     | 0.62              |
| 1:A:205:PHE:CE1   | 1:A:344:VAL:HG21 | 2.34                     | 0.62              |
| 1:A:295:VAL:HB    | 1:A:298:LEU:CD2  | 2.30                     | 0.61              |
| 1:A:573:LYS:HG3   | 1:A:574:GLY:N    | 2.14                     | 0.61              |
| 1:B:107:PHE:CD1   | 1:B:107:PHE:N    | 2.66                     | 0.61              |
| 1:B:420:THR:OG1   | 1:B:573:LYS:HB3  | 1.99                     | 0.61              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:A:96:PHE:N       | 1:A:96:PHE:CD1   | 2.67                     | 0.61              |
| 1:A:315:ILE:HG21   | 1:A:558:ILE:HD11 | 1.80                     | 0.61              |
| 1:B:124:ILE:HD11   | 1:B:528:PRO:CB   | 2.31                     | 0.61              |
| 1:A:87:ASN:C       | 1:A:89:VAL:H     | 2.08                     | 0.61              |
| 1:A:105:ASN:O      | 1:A:106:PRO:HD3  | 1.99                     | 0.61              |
| 1:A:320:HIS:HB3    | 1:A:323:TRP:CD1  | 2.36                     | 0.61              |
| 1:B:110:SER:HB2    | 1:B:365:LEU:HD21 | 1.82                     | 0.61              |
| 1:B:105(A):ILE:CG2 | 1:B:108:LEU:HB2  | 2.30                     | 0.61              |
| 1:B:397:ILE:HA     | 1:B:425:SER:HB3  | 1.83                     | 0.61              |
| 1:A:279:ILE:CG2    | 1:A:284:GLN:HG2  | 2.31                     | 0.61              |
| 1:B:51:GLY:O       | 1:B:52:PHE:HB2   | 2.01                     | 0.61              |
| 1:A:58:ASP:HB2     | 1:B:548:SER:OG   | 2.00                     | 0.61              |
| 1:B:485:LYS:HA     | 1:B:488:ALA:HB3  | 1.83                     | 0.61              |
| 1:A:208:GLN:HE21   | 1:A:228:VAL:HA   | 1.66                     | 0.61              |
| 1:B:96:PHE:CD1     | 1:B:96:PHE:N     | 2.69                     | 0.61              |
| 1:B:150:ARG:NH2    | 1:B:458:MET:O    | 2.33                     | 0.61              |
| 1:A:60:THR:HG22    | 1:A:61:ARG:HG3   | 1.83                     | 0.60              |
| 1:B:171:LEU:HD23   | 1:B:456:ARG:HE   | 1.65                     | 0.60              |
| 1:B:293:GLY:HA2    | 1:B:299:MET:HE3  | 1.84                     | 0.60              |
| 1:A:420:THR:OG1    | 1:A:573:LYS:HB3  | 2.02                     | 0.60              |
| 1:B:113:MET:HE3    | 1:B:117:LEU:HD13 | 1.83                     | 0.60              |
| 1:A:64:PHE:CE2     | 1:A:72:PRO:HB3   | 2.36                     | 0.60              |
| 1:B:573:LYS:HG3    | 1:B:574:GLY:N    | 2.17                     | 0.60              |
| 1:A:527:ALA:HB3    | 1:A:528:PRO:HD3  | 1.83                     | 0.60              |
| 1:B:194:SER:OG     | 1:B:351:HIS:HE1  | 1.84                     | 0.60              |
| 1:B:527:ALA:HB3    | 1:B:528:PRO:HD3  | 1.83                     | 0.60              |
| 1:B:120:ARG:HG3    | 1:B:120:ARG:HH11 | 1.67                     | 0.59              |
| 1:A:388:HIS:HB3    | 1:A:444:VAL:HG11 | 1.84                     | 0.59              |
| 1:A:477:SER:HB2    | 1:A:479:GLU:OE1  | 2.01                     | 0.59              |
| 1:A:414:LEU:HA     | 1:A:422:PHE:CE2  | 2.38                     | 0.59              |
| 1:A:113:MET:HE3    | 1:A:117:LEU:HD13 | 1.84                     | 0.59              |
| 1:A:333:LYS:O      | 1:A:337:ILE:HG13 | 2.03                     | 0.59              |
| 1:B:333:LYS:O      | 1:B:337:ILE:HG13 | 2.03                     | 0.59              |
| 1:B:482:THR:HG22   | 1:B:509:VAL:HG13 | 1.85                     | 0.59              |
| 1:A:104:ASN:HD21   | 1:A:358:LYS:HB2  | 1.67                     | 0.58              |
| 1:A:182:LEU:O      | 1:A:438:ARG:HA   | 2.02                     | 0.58              |
| 1:A:197:MET:CE     | 1:A:423:VAL:HG13 | 2.32                     | 0.58              |
| 1:B:388:HIS:HB3    | 1:B:444:VAL:HG11 | 1.85                     | 0.58              |
| 1:A:419:LEU:O      | 1:A:423:VAL:HG23 | 2.02                     | 0.58              |
| 1:B:427:THR:HB     | 1:B:428:ARG:NH1  | 2.18                     | 0.58              |
| 1:A:51:GLY:O       | 1:A:52:PHE:HB2   | 2.01                     | 0.58              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:B:60:THR:HG22    | 1:B:61:ARG:HG3   | 1.86                     | 0.58              |
| 1:B:64:PHE:CE2     | 1:B:72:PRO:HB3   | 2.38                     | 0.58              |
| 1:B:91:TYR:O       | 1:B:95:HIS:HD2   | 1.87                     | 0.58              |
| 1:A:175:LYS:HE3    | 1:A:175:LYS:HA   | 1.86                     | 0.58              |
| 1:B:206:THR:HG21   | 1:B:385:TYR:CE1  | 2.38                     | 0.58              |
| 1:A:418:GLY:O      | 1:A:422:PHE:HB2  | 2.03                     | 0.58              |
| 1:A:352:LEU:HD11   | 1:A:518:PHE:CE2  | 2.39                     | 0.57              |
| 1:B:85:THR:O       | 1:B:89:VAL:HG23  | 2.04                     | 0.57              |
| 1:B:123:LEU:O      | 1:B:469:ARG:NH2  | 2.36                     | 0.57              |
| 1:B:280:PRO:HD2    | 1:B:283:LEU:CD2  | 2.24                     | 0.57              |
| 1:A:424:GLU:O      | 1:A:428:ARG:HD2  | 2.05                     | 0.57              |
| 1:A:500:VAL:HG12   | 1:A:500:VAL:O    | 2.04                     | 0.57              |
| 1:A:398:GLU:O      | 1:A:399:ASP:HB3  | 2.04                     | 0.57              |
| 1:A:525:LEU:O      | 1:A:528:PRO:HD2  | 2.04                     | 0.57              |
| 1:B:198:PHE:CZ     | 1:B:352:LEU:HD13 | 2.39                     | 0.57              |
| 1:B:264:PRO:HG2    | 1:B:286:ALA:HB3  | 1.86                     | 0.57              |
| 1:A:320:HIS:HB3    | 1:A:323:TRP:CG   | 2.40                     | 0.57              |
| 1:A:509:VAL:HG12   | 1:A:510:GLU:N    | 2.20                     | 0.57              |
| 1:B:87:ASN:C       | 1:B:89:VAL:H     | 2.11                     | 0.57              |
| 1:B:112:ILE:HB     | 1:B:357:PHE:CZ   | 2.39                     | 0.57              |
| 1:B:389:PRO:HG2    | 1:B:508:LEU:HD22 | 1.87                     | 0.57              |
| 1:B:463:LEU:O      | 1:B:467:ARG:HG3  | 2.05                     | 0.57              |
| 1:B:513:ARG:HH21   | 1:B:520:GLU:HG3  | 1.69                     | 0.57              |
| 1:B:525:LEU:O      | 1:B:528:PRO:HD2  | 2.04                     | 0.57              |
| 1:A:105(A):ILE:CG2 | 1:A:108:LEU:HB2  | 2.35                     | 0.57              |
| 1:A:397:ILE:HA     | 1:A:425:SER:HB3  | 1.86                     | 0.57              |
| 1:A:171:LEU:HD23   | 1:A:456:ARG:HE   | 1.70                     | 0.56              |
| 1:A:197:MET:HG3    | 1:A:578:THR:CG2  | 2.35                     | 0.56              |
| 1:B:124:ILE:HD12   | 1:B:124:ILE:N    | 2.20                     | 0.56              |
| 1:B:43:ASN:O       | 1:B:44:ARG:HB2   | 2.04                     | 0.56              |
| 1:B:105(A):ILE:HB  | 1:B:108:LEU:HB2  | 1.87                     | 0.56              |
| 1:B:226:HIS:ND1    | 1:B:376:ARG:HD2  | 2.21                     | 0.56              |
| 1:B:403:SER:HB2    | 1:B:405:LYS:HD2  | 1.87                     | 0.56              |
| 1:B:279:ILE:CG2    | 1:B:284:GLN:HG2  | 2.34                     | 0.56              |
| 1:A:97:LYS:HG3     | 1:A:356:HIS:CD2  | 2.40                     | 0.56              |
| 1:A:127:PRO:HD2    | 1:B:543:GLN:HE22 | 1.71                     | 0.56              |
| 1:A:194:SER:OG     | 1:A:351:HIS:CE1  | 2.58                     | 0.56              |
| 1:A:295:VAL:HB     | 1:A:298:LEU:HD23 | 1.88                     | 0.56              |
| 1:B:104:ASN:HD21   | 1:B:358:LYS:HB2  | 1.71                     | 0.56              |
| 1:A:198:PHE:HZ     | 1:A:352:LEU:HD13 | 1.71                     | 0.56              |
| 1:A:295:VAL:HG12   | 1:A:297:GLY:H    | 1.71                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:208:GLN:HE21 | 1:B:228:VAL:HA   | 1.67                     | 0.56              |
| 1:B:578:THR:CG2  | 1:B:579:SER:N    | 2.69                     | 0.56              |
| 1:B:185:ARG:HH21 | 1:B:438:ARG:HD3  | 1.70                     | 0.55              |
| 1:B:306:LEU:O    | 1:B:306:LEU:HD23 | 2.07                     | 0.55              |
| 1:A:46:GLU:OE2   | 1:B:546:LYS:HD2  | 2.06                     | 0.55              |
| 1:A:568:ILE:HG22 | 1:A:576:PRO:HD2  | 1.88                     | 0.55              |
| 1:B:74:PHE:O     | 1:B:77:ARG:HB2   | 2.06                     | 0.55              |
| 1:B:103:VAL:HG11 | 1:B:112:ILE:HG13 | 1.89                     | 0.55              |
| 1:B:352:LEU:HD11 | 1:B:518:PHE:CE2  | 2.42                     | 0.55              |
| 1:A:124:ILE:N    | 1:A:124:ILE:HD12 | 2.21                     | 0.55              |
| 1:A:112:ILE:HB   | 1:A:357:PHE:CZ   | 2.42                     | 0.55              |
| 1:B:105:ASN:O    | 1:B:106:PRO:HD3  | 2.06                     | 0.55              |
| 1:A:184:ARG:HB2  | 1:A:439:ASN:C    | 2.32                     | 0.54              |
| 1:A:482:THR:HG22 | 1:A:509:VAL:HG13 | 1.87                     | 0.54              |
| 1:A:578:THR:CG2  | 1:A:579:SER:N    | 2.69                     | 0.54              |
| 1:A:148:TYR:HD1  | 1:A:377:ILE:HG13 | 1.72                     | 0.54              |
| 1:A:344:VAL:O    | 1:A:349:VAL:HG23 | 2.07                     | 0.54              |
| 1:A:58:ASP:OD2   | 1:B:546:LYS:HD3  | 2.08                     | 0.54              |
| 1:A:94:THR:O     | 1:A:356:HIS:ND1  | 2.40                     | 0.54              |
| 1:B:509:VAL:HG12 | 1:B:510:GLU:N    | 2.23                     | 0.54              |
| 1:A:120:ARG:HG3  | 1:A:120:ARG:NH1  | 2.23                     | 0.54              |
| 1:B:178:LEU:HD22 | 1:B:183:LEU:HG   | 1.88                     | 0.54              |
| 1:B:295:VAL:HB   | 1:B:298:LEU:HD22 | 1.87                     | 0.54              |
| 1:B:419:LEU:O    | 1:B:423:VAL:HG23 | 2.07                     | 0.54              |
| 1:A:178:LEU:HD22 | 1:A:183:LEU:HG   | 1.90                     | 0.54              |
| 1:B:252:LEU:O    | 1:B:310:GLN:NE2  | 2.41                     | 0.54              |
| 1:A:578:THR:HG22 | 1:A:579:SER:H    | 1.72                     | 0.54              |
| 1:B:176:GLU:OE1  | 1:B:180:LYS:HE3  | 2.08                     | 0.54              |
| 1:A:134:TYR:HB3  | 1:A:136:TYR:O    | 2.08                     | 0.54              |
| 1:A:279:ILE:CG2  | 1:A:283:LEU:HG   | 2.23                     | 0.54              |
| 1:A:385:TYR:CE2  | 4:A:701:S58:BR1  | 3.16                     | 0.54              |
| 1:B:197:MET:HG3  | 1:B:578:THR:CG2  | 2.38                     | 0.54              |
| 1:A:108:LEU:O    | 1:A:112:ILE:HG12 | 2.08                     | 0.53              |
| 1:B:320:HIS:HB3  | 1:B:323:TRP:CG   | 2.43                     | 0.53              |
| 1:A:400:GLN:HA   | 1:A:400:GLN:OE1  | 2.08                     | 0.53              |
| 1:B:230:LEU:HG   | 1:B:337:ILE:HG12 | 1.91                     | 0.53              |
| 1:B:417:HIS:HB3  | 1:B:421:GLN:O    | 2.09                     | 0.53              |
| 1:A:582:VAL:O    | 1:A:582:VAL:HG13 | 2.09                     | 0.53              |
| 1:A:424:GLU:HA   | 1:A:428:ARG:NH1  | 2.24                     | 0.53              |
| 1:A:463:LEU:HD21 | 1:A:475:TYR:HD2  | 1.73                     | 0.53              |
| 1:B:418:GLY:O    | 1:B:422:PHE:HB2  | 2.08                     | 0.53              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:A:142:PHE:CD1    | 1:A:142:PHE:C    | 2.87                     | 0.53              |
| 1:B:424:GLU:HA     | 1:B:428:ARG:NH1  | 2.23                     | 0.53              |
| 1:B:95:HIS:HB2     | 1:B:96:PHE:CE1   | 2.44                     | 0.53              |
| 1:A:103:VAL:HG11   | 1:A:112:ILE:HG13 | 1.90                     | 0.53              |
| 1:B:133:HIS:ND1    | 1:B:147:TYR:HE2  | 2.07                     | 0.53              |
| 1:B:148:TYR:HD1    | 1:B:377:ILE:HG13 | 1.74                     | 0.53              |
| 1:B:184:ARG:HB2    | 1:B:439:ASN:C    | 2.34                     | 0.53              |
| 1:B:295:VAL:HG12   | 1:B:297:GLY:H    | 1.73                     | 0.53              |
| 1:B:320:HIS:HB3    | 1:B:323:TRP:CD1  | 2.43                     | 0.52              |
| 1:B:279:ILE:HG23   | 1:B:283:LEU:CG   | 2.25                     | 0.52              |
| 1:A:46:GLU:O       | 1:A:57:CYS:HA    | 2.10                     | 0.52              |
| 1:B:173:ASP:OD1    | 1:B:175:LYS:HB3  | 2.10                     | 0.52              |
| 1:B:276:PRO:O      | 1:B:279:ILE:HB   | 2.09                     | 0.52              |
| 1:A:293:GLY:HA2    | 1:A:299:MET:HE3  | 1.90                     | 0.52              |
| 1:A:513:ARG:HH21   | 1:A:520:GLU:HG3  | 1.73                     | 0.52              |
| 1:A:274:ILE:HD12   | 1:A:291:VAL:HG23 | 1.92                     | 0.52              |
| 1:A:574:GLY:O      | 1:A:576:PRO:CD   | 2.58                     | 0.52              |
| 1:B:114:LYS:O      | 1:B:118:THR:HG23 | 2.09                     | 0.52              |
| 1:B:194:SER:OG     | 1:B:351:HIS:CE1  | 2.63                     | 0.52              |
| 1:B:479:GLU:HG2    | 1:B:485:LYS:HD3  | 1.92                     | 0.52              |
| 1:A:185:ARG:HH21   | 1:A:438:ARG:HD3  | 1.74                     | 0.52              |
| 1:B:117:LEU:HD21   | 1:B:535:MET:HE2  | 1.91                     | 0.52              |
| 1:B:197:MET:CE     | 1:B:423:VAL:HG13 | 2.38                     | 0.52              |
| 1:A:113:MET:O      | 1:A:117:LEU:HB2  | 2.10                     | 0.52              |
| 1:A:254:TYR:CD1    | 1:A:254:TYR:C    | 2.88                     | 0.52              |
| 1:A:294:LEU:HD22   | 1:A:409:TYR:CD2  | 2.45                     | 0.52              |
| 1:B:105(A):ILE:CD1 | 1:B:108:LEU:HD12 | 2.40                     | 0.52              |
| 1:A:142:PHE:O      | 1:A:376:ARG:NH2  | 2.37                     | 0.51              |
| 1:A:276:PRO:O      | 1:A:279:ILE:HB   | 2.10                     | 0.51              |
| 1:A:403:SER:HB2    | 1:A:405:LYS:HD2  | 1.92                     | 0.51              |
| 1:B:85:THR:HB      | 1:B:86:PRO:HD2   | 1.90                     | 0.51              |
| 1:A:151:ALA:HB3    | 1:A:380:GLU:HG3  | 1.92                     | 0.51              |
| 1:B:197:MET:HE3    | 1:B:578:THR:HG21 | 1.92                     | 0.51              |
| 1:A:150:ARG:HD2    | 1:A:380:GLU:OE1  | 2.10                     | 0.51              |
| 1:A:230:LEU:HD13   | 1:A:233:ILE:HD12 | 1.92                     | 0.51              |
| 1:A:283:LEU:HD13   | 1:A:411:ASN:CA   | 2.41                     | 0.51              |
| 1:B:254:TYR:CD1    | 1:B:254:TYR:C    | 2.88                     | 0.51              |
| 1:A:246:LEU:O      | 1:A:247:PHE:HB2  | 2.11                     | 0.51              |
| 1:A:266:VAL:HG12   | 1:A:266:VAL:O    | 2.09                     | 0.51              |
| 1:A:403:SER:HB2    | 1:A:405:LYS:NZ   | 2.25                     | 0.51              |
| 1:B:276:PRO:HD2    | 1:B:279:ILE:CD1  | 2.40                     | 0.51              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:B:152:LEU:HD23   | 1:B:153:PRO:HD2  | 1.92                     | 0.51              |
| 1:B:279:ILE:HG22   | 1:B:284:GLN:HG2  | 1.92                     | 0.51              |
| 4:B:701:S58:C11    | 4:B:701:S58:H10  | 2.41                     | 0.51              |
| 1:A:43:ASN:O       | 1:A:44:ARG:HB2   | 2.09                     | 0.51              |
| 1:B:252:LEU:HD22   | 1:B:309:HIS:CG   | 2.46                     | 0.51              |
| 1:B:280:PRO:O      | 1:B:283:LEU:HB3  | 2.11                     | 0.51              |
| 1:A:148:TYR:CD1    | 1:A:377:ILE:HG13 | 2.45                     | 0.51              |
| 1:B:479:GLU:HB3    | 1:B:485:LYS:HE2  | 1.92                     | 0.51              |
| 1:A:435:ALA:O      | 1:A:512:PRO:HG3  | 2.10                     | 0.50              |
| 1:B:46:GLU:O       | 1:B:57:CYS:HA    | 2.11                     | 0.50              |
| 1:B:498:ILE:C      | 1:B:500:VAL:H    | 2.19                     | 0.50              |
| 1:A:173:ASP:O      | 1:A:177:VAL:HG23 | 2.11                     | 0.50              |
| 1:A:105(A):ILE:CD1 | 1:A:108:LEU:HD12 | 2.41                     | 0.50              |
| 1:B:424:GLU:O      | 1:B:428:ARG:HD2  | 2.11                     | 0.50              |
| 1:B:176:GLU:O      | 1:B:180:LYS:HG3  | 2.11                     | 0.50              |
| 1:B:178:LEU:HD23   | 1:B:182:LEU:HB2  | 1.94                     | 0.50              |
| 1:A:92:ILE:HA      | 1:A:96:PHE:HE1   | 1.76                     | 0.50              |
| 1:A:117:LEU:HD21   | 1:A:535:MET:HE2  | 1.93                     | 0.50              |
| 1:A:232:HIS:ND1    | 1:A:233:ILE:HG13 | 2.27                     | 0.50              |
| 1:A:546:LYS:HD3    | 1:B:58:ASP:OD2   | 2.11                     | 0.50              |
| 1:B:379:SER:HB3    | 1:B:460:TYR:OH   | 2.12                     | 0.50              |
| 1:B:582:VAL:O      | 1:B:582:VAL:HG13 | 2.11                     | 0.50              |
| 1:B:463:LEU:HD21   | 1:B:475:TYR:HD2  | 1.77                     | 0.50              |
| 1:A:578:THR:CG2    | 1:A:579:SER:H    | 2.24                     | 0.50              |
| 1:B:92:ILE:HA      | 1:B:96:PHE:HE1   | 1.76                     | 0.50              |
| 1:B:134:TYR:HB3    | 1:B:136:TYR:O    | 2.11                     | 0.50              |
| 1:B:574:GLY:O      | 1:B:576:PRO:CD   | 2.58                     | 0.50              |
| 1:A:211:LYS:NZ     | 1:A:236:GLU:HG3  | 2.27                     | 0.50              |
| 1:A:252:LEU:O      | 1:A:310:GLN:NE2  | 2.44                     | 0.50              |
| 1:B:242:HIS:ND1    | 1:B:247:PHE:HZ   | 2.10                     | 0.50              |
| 1:B:379:SER:O      | 1:B:382:ASN:N    | 2.45                     | 0.50              |
| 1:A:97:LYS:HG3     | 1:A:356:HIS:NE2  | 2.26                     | 0.50              |
| 1:A:279:ILE:HG22   | 1:A:284:GLN:HG2  | 1.94                     | 0.50              |
| 1:A:320:HIS:HE1    | 1:A:551:GLY:O    | 1.95                     | 0.49              |
| 1:A:379:SER:HB3    | 1:A:460:TYR:OH   | 2.12                     | 0.49              |
| 1:A:498:ILE:C      | 1:A:500:VAL:H    | 2.20                     | 0.49              |
| 1:A:91:TYR:O       | 1:A:95:HIS:HD2   | 1.95                     | 0.49              |
| 1:A:190:ASP:OD1    | 1:A:517:ILE:HB   | 2.12                     | 0.49              |
| 1:A:230:LEU:HD23   | 1:A:230:LEU:N    | 2.26                     | 0.49              |
| 1:B:72:PRO:HB2     | 1:B:76:THR:HB    | 1.94                     | 0.49              |
| 1:B:226:HIS:CE1    | 1:B:376:ARG:HD2  | 2.47                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:252:LEU:HD22 | 1:A:309:HIS:CG   | 2.47                     | 0.49              |
| 1:B:103:VAL:HG22 | 1:B:108:LEU:HD13 | 1.95                     | 0.49              |
| 1:B:193:GLY:O    | 1:B:582:VAL:N    | 2.41                     | 0.49              |
| 1:B:345:ILE:HD11 | 1:B:534:LEU:HG   | 1.94                     | 0.49              |
| 1:B:134:TYR:HD1  | 1:B:136:TYR:CE1  | 2.30                     | 0.49              |
| 1:B:148:TYR:CD1  | 1:B:377:ILE:HG13 | 2.47                     | 0.49              |
| 1:B:414:LEU:HA   | 1:B:422:PHE:CE2  | 2.48                     | 0.49              |
| 1:A:134:TYR:HD1  | 1:A:136:TYR:CE1  | 2.31                     | 0.49              |
| 1:A:543:GLN:HE22 | 1:B:127:PRO:HD2  | 1.78                     | 0.49              |
| 1:B:306:LEU:HD23 | 1:B:306:LEU:C    | 2.37                     | 0.49              |
| 1:B:344:VAL:O    | 1:B:349:VAL:HG23 | 2.13                     | 0.49              |
| 1:B:413:ILE:O    | 1:B:422:PHE:HE2  | 1.96                     | 0.49              |
| 1:A:389:PRO:HG2  | 1:A:508:LEU:HD22 | 1.94                     | 0.49              |
| 1:A:280:PRO:O    | 1:A:283:LEU:HB3  | 2.13                     | 0.49              |
| 1:B:113:MET:O    | 1:B:117:LEU:HB2  | 2.12                     | 0.49              |
| 1:A:176:GLU:O    | 1:A:180:LYS:HG3  | 2.12                     | 0.49              |
| 1:B:294:LEU:HD22 | 1:B:409:TYR:CD2  | 2.47                     | 0.49              |
| 1:B:479:GLU:HG2  | 1:B:485:LYS:CE   | 2.42                     | 0.49              |
| 1:B:94:THR:O     | 1:B:356:HIS:ND1  | 2.46                     | 0.49              |
| 1:B:132:VAL:HG21 | 1:B:219:GLY:HA3  | 1.95                     | 0.49              |
| 1:B:183:LEU:O    | 1:B:438:ARG:HB3  | 2.13                     | 0.49              |
| 1:A:417:HIS:HB3  | 1:A:421:GLN:O    | 2.13                     | 0.48              |
| 1:A:421:GLN:OE1  | 1:A:424:GLU:HB2  | 2.13                     | 0.48              |
| 1:B:308:GLU:OE1  | 1:B:311:ARG:HD3  | 2.13                     | 0.48              |
| 1:A:131:ASN:ND2  | 1:A:147:TYR:CD2  | 2.81                     | 0.48              |
| 1:A:171:LEU:HB3  | 1:A:456:ARG:HH21 | 1.78                     | 0.48              |
| 1:B:92:ILE:HA    | 1:B:96:PHE:CE1   | 2.48                     | 0.48              |
| 1:B:120:ARG:HG3  | 1:B:120:ARG:NH1  | 2.28                     | 0.48              |
| 1:A:92:ILE:HA    | 1:A:96:PHE:CE1   | 2.48                     | 0.48              |
| 1:B:454:GLN:O    | 1:B:457:GLU:N    | 2.46                     | 0.48              |
| 1:B:108:LEU:O    | 1:B:112:ILE:HG12 | 2.12                     | 0.48              |
| 1:B:490:GLU:O    | 1:B:493:ALA:HB3  | 2.14                     | 0.48              |
| 1:A:85:THR:HB    | 1:A:86:PRO:HD2   | 1.95                     | 0.48              |
| 1:B:230:LEU:N    | 1:B:230:LEU:HD23 | 2.27                     | 0.48              |
| 1:B:398:GLU:O    | 1:B:399:ASP:HB3  | 2.13                     | 0.48              |
| 1:A:251:LYS:HD3  | 1:A:310:GLN:HG3  | 1.96                     | 0.48              |
| 1:A:447:VAL:HG13 | 3:A:682:HEM:HBA2 | 1.94                     | 0.48              |
| 1:A:197:MET:HG3  | 1:A:578:THR:HG23 | 1.94                     | 0.48              |
| 1:A:226:HIS:ND1  | 1:A:376:ARG:HD2  | 2.29                     | 0.48              |
| 1:B:173:ASP:O    | 1:B:177:VAL:HG23 | 2.13                     | 0.48              |
| 1:B:246:LEU:O    | 1:B:247:PHE:HB2  | 2.12                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:95:HIS:HB2    | 1:A:96:PHE:CE1   | 2.49                     | 0.48              |
| 1:B:331:THR:O     | 1:B:334:LEU:HB2  | 2.13                     | 0.48              |
| 1:A:133:HIS:ND1   | 1:A:147:TYR:HE2  | 2.12                     | 0.48              |
| 1:B:113:MET:HG2   | 1:B:360:LYS:HB3  | 1.95                     | 0.48              |
| 1:A:306:LEU:HD23  | 1:A:306:LEU:C    | 2.39                     | 0.48              |
| 1:A:103:VAL:HG22  | 1:A:108:LEU:HD13 | 1.96                     | 0.47              |
| 1:A:546:LYS:HD2   | 1:B:46:GLU:OE2   | 2.14                     | 0.47              |
| 1:A:544:TYR:O     | 1:A:549:THR:OG1  | 2.25                     | 0.47              |
| 1:B:255:GLN:HG2   | 1:B:263:PRO:O    | 2.14                     | 0.47              |
| 1:B:521:THR:O     | 1:B:522:MET:C    | 2.56                     | 0.47              |
| 1:B:513:ARG:O     | 1:B:514:PRO:C    | 2.58                     | 0.47              |
| 1:B:546:LYS:HB2   | 1:B:547:PRO:HD2  | 1.95                     | 0.47              |
| 1:A:85:THR:OG1    | 1:A:88:THR:HG23  | 2.15                     | 0.47              |
| 1:A:308:GLU:O     | 1:A:309:HIS:C    | 2.54                     | 0.47              |
| 1:A:479:GLU:HG3   | 1:A:488:ALA:HB1  | 1.95                     | 0.47              |
| 1:A:582:VAL:O     | 1:A:583:GLN:HB2  | 2.14                     | 0.47              |
| 4:A:701:S58:H10   | 4:A:701:S58:C11  | 2.44                     | 0.47              |
| 1:B:367:PHE:C     | 1:B:369:GLN:H    | 2.22                     | 0.47              |
| 1:A:254:TYR:HD2   | 1:A:310:GLN:HE21 | 1.61                     | 0.47              |
| 1:A:495:TYR:O     | 1:A:496:SER:HB2  | 2.14                     | 0.47              |
| 1:A:519:GLY:O     | 1:A:523:VAL:HG23 | 2.14                     | 0.47              |
| 1:B:190:ASP:OD1   | 1:B:517:ILE:HB   | 2.14                     | 0.47              |
| 1:B:264:PRO:HB2   | 1:B:269:THR:HG23 | 1.96                     | 0.47              |
| 1:A:35:PRO:HB2    | 1:A:55:TYR:HB3   | 1.97                     | 0.47              |
| 1:A:72:PRO:HB2    | 1:A:76:THR:HB    | 1.95                     | 0.47              |
| 1:A:105(A):ILE:CB | 1:A:108:LEU:HB2  | 2.44                     | 0.47              |
| 1:A:178:LEU:HD23  | 1:A:182:LEU:HB2  | 1.96                     | 0.47              |
| 1:A:264:PRO:HG2   | 1:A:286:ALA:CB   | 2.45                     | 0.47              |
| 1:B:91:TYR:O      | 1:B:95:HIS:CD2   | 2.67                     | 0.47              |
| 1:B:222:ARG:NH2   | 1:B:236:GLU:HG2  | 2.29                     | 0.47              |
| 1:A:114:LYS:O     | 1:A:118:THR:HG23 | 2.15                     | 0.47              |
| 1:A:232:HIS:CE1   | 1:A:233:ILE:HG13 | 2.49                     | 0.47              |
| 1:A:413:ILE:O     | 1:A:422:PHE:HE2  | 1.97                     | 0.47              |
| 1:A:454:GLN:O     | 1:A:457:GLU:N    | 2.48                     | 0.47              |
| 1:B:130:TYR:CE1   | 1:B:135:GLY:O    | 2.68                     | 0.47              |
| 1:B:403:SER:HB2   | 1:B:405:LYS:NZ   | 2.29                     | 0.47              |
| 1:A:132:VAL:HG21  | 1:A:219:GLY:HA3  | 1.97                     | 0.47              |
| 1:A:495:TYR:CE2   | 1:A:501:MET:SD   | 3.07                     | 0.47              |
| 1:B:133:HIS:ND1   | 1:B:147:TYR:CE2  | 2.82                     | 0.47              |
| 1:B:197:MET:HG3   | 1:B:578:THR:HG23 | 1.97                     | 0.47              |
| 1:A:222:ARG:NH2   | 1:A:236:GLU:HG2  | 2.29                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:100:TRP:O    | 1:B:104:ASN:HB2  | 2.15                     | 0.46              |
| 1:B:454:GLN:HA   | 1:B:457:GLU:HG3  | 1.96                     | 0.46              |
| 1:A:113:MET:HA   | 1:A:116:VAL:HG13 | 1.97                     | 0.46              |
| 1:A:442:ILE:O    | 1:A:445:GLN:HG2  | 2.16                     | 0.46              |
| 1:A:472:LEU:HD22 | 1:A:520:GLU:CD   | 2.40                     | 0.46              |
| 1:B:495:TYR:O    | 1:B:496:SER:HB2  | 2.16                     | 0.46              |
| 1:B:581:ASN:C    | 1:B:583:GLN:H    | 2.23                     | 0.46              |
| 1:A:130:TYR:CE1  | 1:A:135:GLY:O    | 2.68                     | 0.46              |
| 1:A:140:GLU:OE2  | 1:A:144:ASN:HB2  | 2.16                     | 0.46              |
| 1:A:521:THR:O    | 1:A:522:MET:C    | 2.58                     | 0.46              |
| 1:B:291:VAL:HG22 | 1:B:294:LEU:HD12 | 1.98                     | 0.46              |
| 1:B:297:GLY:O    | 1:B:300:MET:HB3  | 2.14                     | 0.46              |
| 1:A:185:ARG:NE   | 1:A:438:ARG:HD3  | 2.27                     | 0.46              |
| 1:A:490:GLU:O    | 1:A:493:ALA:HB3  | 2.15                     | 0.46              |
| 1:B:232:HIS:ND1  | 1:B:233:ILE:HG13 | 2.30                     | 0.46              |
| 1:A:230:LEU:HG   | 1:A:337:ILE:HG12 | 1.97                     | 0.46              |
| 1:B:230:LEU:HD13 | 1:B:233:ILE:HD12 | 1.98                     | 0.46              |
| 1:B:402:TYR:OH   | 1:B:417:HIS:HE1  | 1.98                     | 0.46              |
| 1:A:139:TRP:CZ3  | 1:B:538:PRO:HG2  | 2.51                     | 0.46              |
| 1:A:159:CYS:HB3  | 1:A:164:GLY:O    | 2.16                     | 0.46              |
| 1:A:548:SER:OG   | 1:B:58:ASP:CB    | 2.64                     | 0.46              |
| 1:B:513:ARG:O    | 1:B:514:PRO:O    | 2.32                     | 0.46              |
| 1:A:226:HIS:CE1  | 1:A:376:ARG:HD2  | 2.51                     | 0.46              |
| 1:B:151:ALA:HB3  | 1:B:380:GLU:HG3  | 1.96                     | 0.46              |
| 1:B:232:HIS:CE1  | 1:B:233:ILE:HG13 | 2.51                     | 0.46              |
| 1:B:521:THR:O    | 1:B:523:VAL:N    | 2.49                     | 0.46              |
| 1:A:388:HIS:N    | 1:A:389:PRO:CD   | 2.79                     | 0.46              |
| 1:A:437:GLY:O    | 1:A:438:ARG:C    | 2.58                     | 0.46              |
| 1:A:546:LYS:HB2  | 1:A:547:PRO:HD2  | 1.98                     | 0.46              |
| 1:B:35:PRO:HB2   | 1:B:55:TYR:HB3   | 1.98                     | 0.46              |
| 1:B:568:ILE:HG22 | 1:B:576:PRO:HD2  | 1.98                     | 0.46              |
| 1:B:578:THR:HG22 | 1:B:579:SER:H    | 1.78                     | 0.46              |
| 1:A:184:ARG:HB2  | 1:A:439:ASN:HA   | 1.98                     | 0.46              |
| 1:A:242:HIS:ND1  | 1:A:247:PHE:HZ   | 2.14                     | 0.46              |
| 1:A:513:ARG:O    | 1:A:514:PRO:C    | 2.59                     | 0.46              |
| 1:B:251:LYS:HD3  | 1:B:310:GLN:HG3  | 1.98                     | 0.46              |
| 1:B:433:ARG:H    | 1:B:439:ASN:ND2  | 2.14                     | 0.46              |
| 1:B:91:TYR:CD1   | 1:B:95:HIS:CD2   | 3.03                     | 0.45              |
| 1:B:479:GLU:HG3  | 1:B:488:ALA:CB   | 2.45                     | 0.45              |
| 1:A:189:PRO:HB2  | 1:A:430:ILE:HD13 | 1.98                     | 0.45              |
| 1:A:193:GLY:O    | 1:A:582:VAL:N    | 2.46                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:337:ILE:O    | 1:A:341:ILE:HG13 | 2.16                     | 0.45              |
| 1:B:184:ARG:HA   | 1:B:438:ARG:O    | 2.17                     | 0.45              |
| 1:A:295:VAL:HB   | 1:A:298:LEU:HD22 | 1.97                     | 0.45              |
| 1:A:240:ARG:CZ   | 1:A:271:VAL:HG23 | 2.46                     | 0.45              |
| 1:A:379:SER:O    | 1:A:382:ASN:N    | 2.49                     | 0.45              |
| 1:B:437:GLY:O    | 1:B:438:ARG:C    | 2.58                     | 0.45              |
| 1:B:578:THR:CG2  | 1:B:579:SER:H    | 2.29                     | 0.45              |
| 1:A:295:VAL:HG22 | 1:A:408:LEU:HD22 | 1.99                     | 0.45              |
| 1:B:240:ARG:CZ   | 1:B:271:VAL:HG23 | 2.46                     | 0.45              |
| 1:B:507:LEU:HD21 | 1:B:521:THR:HG22 | 1.99                     | 0.45              |
| 1:A:285:PHE:HD2  | 1:A:299:MET:SD   | 2.40                     | 0.45              |
| 1:B:149:THR:O    | 1:B:378:ALA:HA   | 2.17                     | 0.45              |
| 1:B:266:VAL:HG12 | 1:B:266:VAL:O    | 2.16                     | 0.45              |
| 1:B:156:ALA:C    | 1:B:158:ASP:H    | 2.25                     | 0.45              |
| 1:B:198:PHE:HZ   | 1:B:352:LEU:HD13 | 1.79                     | 0.45              |
| 1:B:211:LYS:NZ   | 1:B:236:GLU:HG3  | 2.32                     | 0.45              |
| 1:B:468:LYS:HG2  | 1:B:474:PRO:HG3  | 1.99                     | 0.45              |
| 1:B:470:PHE:O    | 1:B:471:SER:HB2  | 2.17                     | 0.45              |
| 1:B:412:SER:O    | 1:B:413:ILE:C    | 2.59                     | 0.45              |
| 1:B:283:LEU:HD13 | 1:B:411:ASN:CA   | 2.46                     | 0.44              |
| 1:A:403:SER:O    | 1:A:406:GLN:HG2  | 2.17                     | 0.44              |
| 1:B:417:HIS:HB2  | 1:B:422:PHE:CD2  | 2.53                     | 0.44              |
| 1:A:283:LEU:HD13 | 1:A:411:ASN:HA   | 1.99                     | 0.44              |
| 1:B:142:PHE:CD1  | 1:B:142:PHE:C    | 2.94                     | 0.44              |
| 1:A:384:LEU:C    | 1:A:384:LEU:HD12 | 2.42                     | 0.44              |
| 1:A:454:GLN:O    | 1:A:457:GLU:HB2  | 2.18                     | 0.44              |
| 1:A:513:ARG:O    | 1:A:514:PRO:O    | 2.35                     | 0.44              |
| 1:B:308:GLU:O    | 1:B:309:HIS:C    | 2.59                     | 0.44              |
| 1:B:479:GLU:HG2  | 1:B:485:LYS:CD   | 2.47                     | 0.44              |
| 1:A:105(A):ILE:O | 1:A:108:LEU:N    | 2.50                     | 0.44              |
| 1:A:345:ILE:HD11 | 1:A:534:LEU:HG   | 1.99                     | 0.44              |
| 1:A:414:LEU:HD11 | 1:A:419:LEU:HD22 | 2.00                     | 0.44              |
| 1:B:434:VAL:HG23 | 1:B:517:ILE:HD11 | 2.00                     | 0.44              |
| 1:A:275:TYR:CE2  | 1:A:284:GLN:HA   | 2.53                     | 0.44              |
| 1:A:58:ASP:CB    | 1:B:548:SER:OG   | 2.66                     | 0.44              |
| 1:B:156:ALA:C    | 1:B:158:ASP:N    | 2.76                     | 0.44              |
| 1:B:171:LEU:HB3  | 1:B:456:ARG:HH21 | 1.83                     | 0.44              |
| 1:B:182:LEU:CD1  | 1:B:452:ILE:HD11 | 2.48                     | 0.44              |
| 1:A:230:LEU:HD23 | 1:A:230:LEU:H    | 1.83                     | 0.44              |
| 1:A:367:PHE:C    | 1:A:369:GLN:H    | 2.26                     | 0.44              |
| 1:A:472:LEU:HD11 | 1:A:524:GLU:HB2  | 2.00                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:105(A):ILE:CB | 1:B:108:LEU:HB2  | 2.47                     | 0.44              |
| 1:B:254:TYR:HD2   | 1:B:310:GLN:HE21 | 1.65                     | 0.44              |
| 1:A:211:LYS:HZ3   | 1:A:236:GLU:HG3  | 1.81                     | 0.44              |
| 1:A:297:GLY:O     | 1:A:300:MET:HB3  | 2.18                     | 0.44              |
| 1:B:328:LEU:HD23  | 1:B:328:LEU:HA   | 1.86                     | 0.44              |
| 1:A:322:GLU:HB3   | 1:B:52:PHE:CE1   | 2.53                     | 0.43              |
| 1:B:184:ARG:HB2   | 1:B:439:ASN:HA   | 1.99                     | 0.43              |
| 1:A:564:ILE:O     | 1:A:568:ILE:HD13 | 2.19                     | 0.43              |
| 1:B:185:ARG:NE    | 1:B:438:ARG:HD3  | 2.28                     | 0.43              |
| 1:B:222:ARG:HH22  | 1:B:236:GLU:HG2  | 1.83                     | 0.43              |
| 1:B:327:GLN:O     | 1:B:331:THR:OG1  | 2.34                     | 0.43              |
| 1:A:184:ARG:NE    | 1:A:439:ASN:OD1  | 2.49                     | 0.43              |
| 1:B:105(A):ILE:O  | 1:B:108:LEU:N    | 2.51                     | 0.43              |
| 1:B:131:ASN:ND2   | 1:B:147:TYR:CD2  | 2.86                     | 0.43              |
| 1:B:283:LEU:HD12  | 1:B:283:LEU:C    | 2.44                     | 0.43              |
| 1:A:131:ASN:ND2   | 1:A:147:TYR:CG   | 2.86                     | 0.43              |
| 1:A:184:ARG:HA    | 1:A:438:ARG:O    | 2.18                     | 0.43              |
| 1:B:384:LEU:HD12  | 1:B:384:LEU:C    | 2.44                     | 0.43              |
| 1:B:403:SER:O     | 1:B:406:GLN:HG2  | 2.17                     | 0.43              |
| 1:A:222:ARG:HH22  | 1:A:236:GLU:HG2  | 1.84                     | 0.43              |
| 1:A:448:ALA:O     | 1:A:452:ILE:HG13 | 2.18                     | 0.43              |
| 1:B:435:ALA:O     | 1:B:512:PRO:HG3  | 2.18                     | 0.43              |
| 1:A:412:SER:O     | 1:A:413:ILE:C    | 2.62                     | 0.43              |
| 1:A:40:PRO:HB3    | 2:A:661:NAG:H62  | 1.99                     | 0.43              |
| 1:A:100:TRP:O     | 1:A:104:ASN:HB2  | 2.17                     | 0.43              |
| 1:A:242:HIS:HE1   | 1:A:245:ARG:NH2  | 2.17                     | 0.43              |
| 1:B:85:THR:OG1    | 1:B:88:THR:HG23  | 2.19                     | 0.43              |
| 1:B:198:PHE:CD1   | 1:B:198:PHE:C    | 2.96                     | 0.43              |
| 1:A:350:GLN:HE22  | 1:A:358:LYS:HA   | 1.84                     | 0.43              |
| 1:A:87:ASN:O      | 1:A:89:VAL:N     | 2.52                     | 0.43              |
| 1:A:388:HIS:N     | 1:A:389:PRO:HD2  | 2.34                     | 0.42              |
| 1:B:185:ARG:NH2   | 1:B:438:ARG:HD3  | 2.34                     | 0.42              |
| 1:B:447:VAL:HG13  | 3:B:682:HEM:HBA2 | 2.00                     | 0.42              |
| 1:A:463:LEU:HD21  | 1:A:475:TYR:CD2  | 2.54                     | 0.42              |
| 1:A:538:PRO:HG2   | 1:B:139:TRP:CZ3  | 2.54                     | 0.42              |
| 1:B:322:GLU:H     | 1:B:322:GLU:HG3  | 1.45                     | 0.42              |
| 1:B:564:ILE:O     | 1:B:568:ILE:HD13 | 2.19                     | 0.42              |
| 1:A:402:TYR:OH    | 1:A:417:HIS:HE1  | 2.02                     | 0.42              |
| 1:A:479:GLU:HG3   | 1:A:485:LYS:HG3  | 2.00                     | 0.42              |
| 1:B:159:CYS:HB3   | 1:B:164:GLY:O    | 2.19                     | 0.42              |
| 1:B:230:LEU:HD23  | 1:B:230:LEU:H    | 1.83                     | 0.42              |

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| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 1:A:93:LEU:HB3      | 1:A:355:TYR:CD1  | 2.55                     | 0.42              |
| 1:A:255:GLN:HG2     | 1:A:263:PRO:O    | 2.18                     | 0.42              |
| 1:A:433:ARG:H       | 1:A:439:ASN:ND2  | 2.16                     | 0.42              |
| 1:A:453:ASP:O       | 1:A:457:GLU:HG3  | 2.19                     | 0.42              |
| 1:B:451:SER:HB2     | 1:B:504:TYR:CE2  | 2.54                     | 0.42              |
| 1:A:74:PHE:O        | 1:A:77:ARG:HB2   | 2.20                     | 0.42              |
| 1:B:472:LEU:HD11    | 1:B:524:GLU:HB2  | 2.02                     | 0.42              |
| 1:B:495:TYR:CE2     | 1:B:501:MET:SD   | 3.12                     | 0.42              |
| 1:A:242:HIS:CE1     | 1:A:245:ARG:NH2  | 2.88                     | 0.42              |
| 1:A:308:GLU:OE1     | 1:A:311:ARG:HD3  | 2.19                     | 0.42              |
| 1:A:331:THR:O       | 1:A:334:LEU:HB2  | 2.19                     | 0.42              |
| 1:B:87:ASN:C        | 1:B:89:VAL:N     | 2.78                     | 0.42              |
| 1:A:126:SER:HA      | 1:A:127:PRO:HA   | 1.85                     | 0.42              |
| 1:A:470:PHE:O       | 1:A:471:SER:HB2  | 2.20                     | 0.42              |
| 1:A:521:THR:O       | 1:A:523:VAL:N    | 2.52                     | 0.42              |
| 1:B:278:HIS:CD2     | 1:B:278:HIS:O    | 2.73                     | 0.42              |
| 1:B:343:ILE:O       | 1:B:345:ILE:N    | 2.53                     | 0.42              |
| 1:B:403:SER:O       | 1:B:404:PHE:C    | 2.62                     | 0.42              |
| 1:B:544:TYR:O       | 1:B:549:THR:OG1  | 2.29                     | 0.42              |
| 1:A:105(A):ILE:HG23 | 1:A:107:PHE:CD2  | 2.54                     | 0.42              |
| 1:A:581:ASN:C       | 1:A:583:GLN:H    | 2.27                     | 0.42              |
| 1:B:62:THR:OG1      | 1:B:63:GLY:N     | 2.51                     | 0.42              |
| 1:B:67:GLU:HG2      | 1:B:68:ASN:OD1   | 2.20                     | 0.42              |
| 1:B:202:ALA:HB2     | 1:B:348:TYR:HE1  | 1.84                     | 0.42              |
| 1:B:275:TYR:CE2     | 1:B:284:GLN:HA   | 2.55                     | 0.42              |
| 1:B:347:ASP:O       | 1:B:348:TYR:C    | 2.63                     | 0.42              |
| 1:B:582:VAL:O       | 1:B:583:GLN:HB2  | 2.20                     | 0.42              |
| 1:A:65:TYR:N        | 1:A:65:TYR:CD1   | 2.88                     | 0.41              |
| 1:A:224:LEU:HA      | 1:A:224:LEU:HD23 | 1.79                     | 0.41              |
| 1:B:180:LYS:HD3     | 1:B:490:GLU:CD   | 2.44                     | 0.41              |
| 1:B:453:ASP:O       | 1:B:457:GLU:HG3  | 2.19                     | 0.41              |
| 1:B:500:VAL:O       | 1:B:500:VAL:CG1  | 2.67                     | 0.41              |
| 1:A:330:GLN:HB3     | 1:B:138:SER:HB2  | 2.02                     | 0.41              |
| 1:A:447:VAL:O       | 1:A:448:ALA:C    | 2.63                     | 0.41              |
| 1:B:150:ARG:HD2     | 1:B:380:GLU:OE1  | 2.19                     | 0.41              |
| 1:B:189:PRO:HB2     | 1:B:430:ILE:HD13 | 2.02                     | 0.41              |
| 1:A:100:TRP:C       | 1:A:102:ILE:H    | 2.28                     | 0.41              |
| 1:A:244:LEU:HD21    | 1:A:271:VAL:HG11 | 2.01                     | 0.41              |
| 1:A:283:LEU:HD12    | 1:A:283:LEU:C    | 2.43                     | 0.41              |
| 1:B:316:LEU:HD12    | 1:B:316:LEU:HA   | 1.92                     | 0.41              |
| 1:B:388:HIS:N       | 1:B:389:PRO:CD   | 2.84                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:557:LYS:HE3  | 1:B:557:LYS:HA   | 2.01                     | 0.41              |
| 1:A:120:ARG:HB3  | 1:A:528:PRO:HG3  | 2.02                     | 0.41              |
| 1:B:113:MET:HA   | 1:B:116:VAL:HG13 | 2.02                     | 0.41              |
| 1:B:370:GLN:O    | 1:B:371:PHE:HB2  | 2.20                     | 0.41              |
| 1:A:34:ASN:HA    | 1:A:35:PRO:HD2   | 1.70                     | 0.41              |
| 1:A:97:LYS:HB2   | 1:A:356:HIS:CE1  | 2.56                     | 0.41              |
| 1:A:283:LEU:HD13 | 1:A:411:ASN:CB   | 2.51                     | 0.41              |
| 1:A:468:LYS:HG2  | 1:A:474:PRO:HG3  | 2.03                     | 0.41              |
| 1:B:93:LEU:HB3   | 1:B:355:TYR:CD1  | 2.55                     | 0.41              |
| 1:B:248:LYS:HD2  | 1:B:249:ASP:CG   | 2.46                     | 0.41              |
| 1:A:87:ASN:C     | 1:A:89:VAL:N     | 2.75                     | 0.41              |
| 1:A:276:PRO:HD2  | 1:A:279:ILE:HD13 | 2.03                     | 0.41              |
| 1:A:428:ARG:O    | 1:A:429:GLN:HB2  | 2.20                     | 0.41              |
| 1:B:421:GLN:OE1  | 1:B:424:GLU:HB2  | 2.20                     | 0.41              |
| 1:A:64:PHE:HD2   | 1:A:70:THR:O     | 2.04                     | 0.41              |
| 1:A:173:ASP:OD1  | 1:A:175:LYS:HB3  | 2.21                     | 0.41              |
| 1:A:184:ARG:CZ   | 1:A:187:PHE:HD1  | 2.34                     | 0.41              |
| 1:A:291:VAL:HG22 | 1:A:294:LEU:HD12 | 2.02                     | 0.41              |
| 1:A:479:GLU:HG2  | 1:A:485:LYS:CE   | 2.51                     | 0.41              |
| 1:A:500:VAL:O    | 1:A:500:VAL:CG1  | 2.68                     | 0.41              |
| 1:A:507:LEU:HD21 | 1:A:521:THR:HG22 | 2.02                     | 0.41              |
| 1:B:195:ASN:HB2  | 1:B:196:MET:H    | 1.78                     | 0.41              |
| 1:B:230:LEU:HB3  | 1:B:233:ILE:HD12 | 2.02                     | 0.41              |
| 1:B:388:HIS:O    | 1:B:389:PRO:C    | 2.64                     | 0.41              |
| 1:B:509:VAL:O    | 1:B:510:GLU:C    | 2.64                     | 0.41              |
| 1:A:130:TYR:HB3  | 1:A:134:TYR:O    | 2.21                     | 0.41              |
| 1:A:248:LYS:HD2  | 1:A:249:ASP:CG   | 2.46                     | 0.41              |
| 1:A:320:HIS:CE1  | 1:A:551:GLY:O    | 2.74                     | 0.41              |
| 1:A:518:PHE:CG   | 1:A:522:MET:HG2  | 2.56                     | 0.41              |
| 1:B:97:LYS:HB2   | 1:B:356:HIS:CE1  | 2.56                     | 0.41              |
| 1:B:339:GLU:O    | 1:B:340:THR:C    | 2.64                     | 0.41              |
| 1:B:351:HIS:ND1  | 1:B:351:HIS:C    | 2.79                     | 0.41              |
| 1:A:110:SER:HB2  | 1:A:365:LEU:CD2  | 2.48                     | 0.40              |
| 1:A:174:SER:HB3  | 1:A:456:ARG:NH1  | 2.36                     | 0.40              |
| 1:A:334:LEU:HD13 | 1:A:549:THR:HG22 | 2.03                     | 0.40              |
| 1:A:182:LEU:CD1  | 1:A:452:ILE:HD11 | 2.51                     | 0.40              |
| 1:B:112:ILE:HB   | 1:B:357:PHE:CE1  | 2.55                     | 0.40              |
| 1:B:210:PHE:HB3  | 1:B:382:ASN:ND2  | 2.35                     | 0.40              |
| 1:A:80:LEU:HD23  | 1:A:80:LEU:HA    | 1.94                     | 0.40              |
| 1:A:230:LEU:CD1  | 1:A:336:LEU:HB3  | 2.51                     | 0.40              |
| 1:B:537:ASN:O    | 1:B:538:PRO:C    | 2.63                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:91:TYR:O     | 1:A:95:HIS:CD2  | 2.73                     | 0.40              |
| 1:B:320:HIS:HE1  | 1:B:551:GLY:O   | 2.05                     | 0.40              |
| 1:A:67:GLU:HG2   | 1:A:68:ASN:OD1  | 2.21                     | 0.40              |
| 1:A:363:PRO:HG2  | 1:A:545:TRP:CD2 | 2.57                     | 0.40              |
| 1:A:387:TRP:HB2  | 3:A:682:HEM:HAC | 2.03                     | 0.40              |
| 1:B:334:LEU:HD23 | 1:B:334:LEU:HA  | 1.80                     | 0.40              |
| 1:B:348:TYR:O    | 1:B:349:VAL:C   | 2.63                     | 0.40              |
| 1:B:442:ILE:O    | 1:B:445:GLN:HB3 | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 550/587 (94%)   | 435 (79%) | 84 (15%)  | 31 (6%)  | <b>1</b>    | <b>4</b> |
| 1   | B     | 550/587 (94%)   | 431 (78%) | 86 (16%)  | 33 (6%)  | <b>1</b>    | <b>3</b> |
| All | All   | 1100/1174 (94%) | 866 (79%) | 170 (16%) | 64 (6%)  | <b>1</b>    | <b>4</b> |

All (64) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 138 | SER  |
| 1   | A     | 348 | TYR  |
| 1   | A     | 398 | GLU  |
| 1   | A     | 510 | GLU  |
| 1   | A     | 514 | PRO  |
| 1   | A     | 573 | LYS  |
| 1   | B     | 138 | SER  |
| 1   | B     | 348 | TYR  |
| 1   | B     | 398 | GLU  |
| 1   | B     | 459 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 510 | GLU  |
| 1   | B     | 514 | PRO  |
| 1   | B     | 573 | LYS  |
| 1   | A     | 51  | GLY  |
| 1   | A     | 82  | LEU  |
| 1   | A     | 96  | PHE  |
| 1   | A     | 212 | THR  |
| 1   | A     | 422 | PHE  |
| 1   | A     | 429 | GLN  |
| 1   | A     | 459 | LYS  |
| 1   | A     | 582 | VAL  |
| 1   | B     | 51  | GLY  |
| 1   | B     | 82  | LEU  |
| 1   | B     | 96  | PHE  |
| 1   | B     | 212 | THR  |
| 1   | B     | 429 | GLN  |
| 1   | B     | 554 | VAL  |
| 1   | B     | 582 | VAL  |
| 1   | A     | 67  | GLU  |
| 1   | A     | 329 | PHE  |
| 1   | A     | 399 | ASP  |
| 1   | A     | 554 | VAL  |
| 1   | B     | 67  | GLU  |
| 1   | B     | 144 | ASN  |
| 1   | B     | 399 | ASP  |
| 1   | B     | 422 | PHE  |
| 1   | B     | 522 | MET  |
| 1   | A     | 88  | THR  |
| 1   | A     | 132 | VAL  |
| 1   | A     | 352 | LEU  |
| 1   | A     | 496 | SER  |
| 1   | A     | 499 | ASP  |
| 1   | B     | 132 | VAL  |
| 1   | B     | 309 | HIS  |
| 1   | B     | 329 | PHE  |
| 1   | B     | 352 | LEU  |
| 1   | B     | 412 | SER  |
| 1   | A     | 144 | ASN  |
| 1   | A     | 522 | MET  |
| 1   | B     | 44  | ARG  |
| 1   | B     | 172 | PRO  |
| 1   | B     | 344 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 380 | GLU  |
| 1   | B     | 496 | SER  |
| 1   | B     | 575 | CYS  |
| 1   | A     | 104 | ASN  |
| 1   | A     | 172 | PRO  |
| 1   | A     | 412 | SER  |
| 1   | B     | 88  | THR  |
| 1   | A     | 575 | CYS  |
| 1   | B     | 413 | ILE  |
| 1   | B     | 287 | VAL  |
| 1   | A     | 413 | ILE  |
| 1   | A     | 344 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |    |
|-----|-------|----------------|-----------|-----------|-------------|----|
| 1   | A     | 493/525 (94%)  | 428 (87%) | 65 (13%)  | 4           | 14 |
| 1   | B     | 493/525 (94%)  | 430 (87%) | 63 (13%)  | 4           | 15 |
| All | All   | 986/1050 (94%) | 858 (87%) | 128 (13%) | 4           | 14 |

All (128) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 39  | ASN  |
| 1   | A     | 65  | TYR  |
| 1   | A     | 71  | THR  |
| 1   | A     | 93  | LEU  |
| 1   | A     | 96  | PHE  |
| 1   | A     | 97  | LYS  |
| 1   | A     | 101 | ASN  |
| 1   | A     | 107 | PHE  |
| 1   | A     | 108 | LEU  |
| 1   | A     | 111 | LEU  |
| 1   | A     | 116 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 117 | LEU  |
| 1   | A     | 126 | SER  |
| 1   | A     | 150 | ARG  |
| 1   | A     | 152 | LEU  |
| 1   | A     | 172 | PRO  |
| 1   | A     | 175 | LYS  |
| 1   | A     | 176 | GLU  |
| 1   | A     | 178 | LEU  |
| 1   | A     | 181 | VAL  |
| 1   | A     | 186 | GLU  |
| 1   | A     | 230 | LEU  |
| 1   | A     | 232 | HIS  |
| 1   | A     | 238 | LEU  |
| 1   | A     | 241 | GLN  |
| 1   | A     | 245 | ARG  |
| 1   | A     | 252 | LEU  |
| 1   | A     | 253 | LYS  |
| 1   | A     | 271 | VAL  |
| 1   | A     | 279 | ILE  |
| 1   | A     | 280 | PRO  |
| 1   | A     | 283 | LEU  |
| 1   | A     | 290 | GLU  |
| 1   | A     | 291 | VAL  |
| 1   | A     | 298 | LEU  |
| 1   | A     | 307 | ARG  |
| 1   | A     | 310 | GLN  |
| 1   | A     | 311 | ARG  |
| 1   | A     | 316 | LEU  |
| 1   | A     | 322 | GLU  |
| 1   | A     | 356 | HIS  |
| 1   | A     | 369 | GLN  |
| 1   | A     | 376 | ARG  |
| 1   | A     | 377 | ILE  |
| 1   | A     | 380 | GLU  |
| 1   | A     | 385 | TYR  |
| 1   | A     | 389 | PRO  |
| 1   | A     | 396 | ASN  |
| 1   | A     | 405 | LYS  |
| 1   | A     | 412 | SER  |
| 1   | A     | 422 | PHE  |
| 1   | A     | 428 | ARG  |
| 1   | A     | 442 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 454 | GLN  |
| 1   | A     | 463 | LEU  |
| 1   | A     | 469 | ARG  |
| 1   | A     | 484 | GLU  |
| 1   | A     | 485 | LYS  |
| 1   | A     | 509 | VAL  |
| 1   | A     | 512 | PRO  |
| 1   | A     | 514 | PRO  |
| 1   | A     | 528 | PRO  |
| 1   | A     | 534 | LEU  |
| 1   | A     | 539 | ILE  |
| 1   | A     | 557 | LYS  |
| 1   | B     | 38  | SER  |
| 1   | B     | 65  | TYR  |
| 1   | B     | 71  | THR  |
| 1   | B     | 93  | LEU  |
| 1   | B     | 96  | PHE  |
| 1   | B     | 97  | LYS  |
| 1   | B     | 101 | ASN  |
| 1   | B     | 107 | PHE  |
| 1   | B     | 108 | LEU  |
| 1   | B     | 111 | LEU  |
| 1   | B     | 116 | VAL  |
| 1   | B     | 117 | LEU  |
| 1   | B     | 126 | SER  |
| 1   | B     | 150 | ARG  |
| 1   | B     | 152 | LEU  |
| 1   | B     | 172 | PRO  |
| 1   | B     | 175 | LYS  |
| 1   | B     | 176 | GLU  |
| 1   | B     | 178 | LEU  |
| 1   | B     | 181 | VAL  |
| 1   | B     | 230 | LEU  |
| 1   | B     | 232 | HIS  |
| 1   | B     | 238 | LEU  |
| 1   | B     | 241 | GLN  |
| 1   | B     | 252 | LEU  |
| 1   | B     | 253 | LYS  |
| 1   | B     | 271 | VAL  |
| 1   | B     | 279 | ILE  |
| 1   | B     | 280 | PRO  |
| 1   | B     | 283 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 290 | GLU  |
| 1   | B     | 291 | VAL  |
| 1   | B     | 298 | LEU  |
| 1   | B     | 307 | ARG  |
| 1   | B     | 310 | GLN  |
| 1   | B     | 316 | LEU  |
| 1   | B     | 322 | GLU  |
| 1   | B     | 340 | THR  |
| 1   | B     | 356 | HIS  |
| 1   | B     | 369 | GLN  |
| 1   | B     | 377 | ILE  |
| 1   | B     | 380 | GLU  |
| 1   | B     | 385 | TYR  |
| 1   | B     | 389 | PRO  |
| 1   | B     | 396 | ASN  |
| 1   | B     | 400 | GLN  |
| 1   | B     | 405 | LYS  |
| 1   | B     | 412 | SER  |
| 1   | B     | 422 | PHE  |
| 1   | B     | 442 | ILE  |
| 1   | B     | 444 | VAL  |
| 1   | B     | 454 | GLN  |
| 1   | B     | 463 | LEU  |
| 1   | B     | 469 | ARG  |
| 1   | B     | 484 | GLU  |
| 1   | B     | 485 | LYS  |
| 1   | B     | 509 | VAL  |
| 1   | B     | 512 | PRO  |
| 1   | B     | 514 | PRO  |
| 1   | B     | 534 | LEU  |
| 1   | B     | 539 | ILE  |
| 1   | B     | 557 | LYS  |
| 1   | B     | 583 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 43  | ASN  |
| 1   | A     | 95  | HIS  |
| 1   | A     | 208 | GLN  |
| 1   | A     | 278 | HIS  |
| 1   | A     | 320 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 350 | GLN  |
| 1   | A     | 351 | HIS  |
| 1   | A     | 369 | GLN  |
| 1   | A     | 417 | HIS  |
| 1   | A     | 583 | GLN  |
| 1   | B     | 43  | ASN  |
| 1   | B     | 95  | HIS  |
| 1   | B     | 208 | GLN  |
| 1   | B     | 278 | HIS  |
| 1   | B     | 320 | HIS  |
| 1   | B     | 350 | GLN  |
| 1   | B     | 351 | HIS  |
| 1   | B     | 369 | GLN  |
| 1   | B     | 417 | HIS  |
| 1   | B     | 454 | GLN  |
| 1   | B     | 543 | GLN  |
| 1   | B     | 565 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | S58  | B     | 701 | -    | 28,28,28     | 2.33 | 7 (25%)  | 43,43,43    | 2.29 | 11 (25%) |
| 2   | NAG  | B     | 671 | 1    | 14,14,15     | 0.58 | 0        | 17,19,21    | 0.94 | 1 (5%)   |
| 2   | NAG  | B     | 661 | 1    | 14,14,15     | 0.57 | 0        | 17,19,21    | 0.59 | 0        |
| 2   | NAG  | B     | 681 | 1    | 14,14,15     | 0.71 | 0        | 17,19,21    | 0.86 | 0        |
| 3   | HEM  | B     | 682 | 1    | 50,50,50     | 1.21 | 4 (8%)   | 67,82,82    | 0.94 | 2 (2%)   |
| 4   | S58  | A     | 701 | -    | 28,28,28     | 2.41 | 7 (25%)  | 43,43,43    | 2.45 | 13 (30%) |
| 2   | NAG  | A     | 671 | 1    | 14,14,15     | 0.42 | 0        | 17,19,21    | 0.85 | 1 (5%)   |
| 2   | NAG  | A     | 681 | 1    | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.98 | 1 (5%)   |
| 3   | HEM  | A     | 682 | 1    | 50,50,50     | 1.21 | 4 (8%)   | 67,82,82    | 0.86 | 0        |
| 2   | NAG  | A     | 661 | 1    | 14,14,15     | 0.67 | 0        | 17,19,21    | 0.54 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 4   | S58  | B     | 701 | -    | -       | 2/20/20/20 | 0/3/3/3 |
| 2   | NAG  | B     | 671 | 1    | -       | 2/6/23/26  | 0/1/1/1 |
| 2   | NAG  | B     | 661 | 1    | -       | 2/6/23/26  | 0/1/1/1 |
| 2   | NAG  | B     | 681 | 1    | -       | 0/6/23/26  | 0/1/1/1 |
| 3   | HEM  | B     | 682 | 1    | -       | 7/14/54/54 | -       |
| 4   | S58  | A     | 701 | -    | -       | 2/20/20/20 | 0/3/3/3 |
| 2   | NAG  | A     | 671 | 1    | -       | 2/6/23/26  | 0/1/1/1 |
| 2   | NAG  | A     | 681 | 1    | -       | 0/6/23/26  | 0/1/1/1 |
| 3   | HEM  | A     | 682 | 1    | -       | 7/14/54/54 | -       |
| 2   | NAG  | A     | 661 | 1    | -       | 2/6/23/26  | 0/1/1/1 |

All (22) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | A     | 701 | S58  | S1-N3   | 8.19  | 1.76        | 1.60     |
| 4   | B     | 701 | S58  | S1-N3   | 7.40  | 1.74        | 1.60     |
| 4   | B     | 701 | S58  | C1-C3   | 5.07  | 1.47        | 1.39     |
| 4   | A     | 701 | S58  | C1-C3   | 4.83  | 1.47        | 1.39     |
| 4   | B     | 701 | S58  | C8-S1   | 4.25  | 1.83        | 1.77     |
| 4   | B     | 701 | S58  | BR1-C14 | -3.84 | 1.82        | 1.90     |
| 4   | A     | 701 | S58  | BR1-C14 | -3.71 | 1.83        | 1.90     |
| 4   | B     | 701 | S58  | N1-N2   | 3.62  | 1.46        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | B     | 682 | HEM  | CAB-C3B | -3.53 | 1.38        | 1.47     |
| 4   | A     | 701 | S58  | C3-N2   | -3.49 | 1.28        | 1.34     |
| 3   | A     | 682 | HEM  | CAB-C3B | -3.37 | 1.38        | 1.47     |
| 3   | A     | 682 | HEM  | CAC-C3C | -3.36 | 1.38        | 1.47     |
| 4   | A     | 701 | S58  | C1-C2   | -3.26 | 1.32        | 1.38     |
| 3   | A     | 682 | HEM  | CBC-CAC | 3.24  | 1.45        | 1.30     |
| 3   | B     | 682 | HEM  | CAC-C3C | -3.19 | 1.38        | 1.47     |
| 3   | B     | 682 | HEM  | CBB-CAB | 3.00  | 1.44        | 1.30     |
| 3   | A     | 682 | HEM  | CBB-CAB | 2.98  | 1.44        | 1.30     |
| 4   | A     | 701 | S58  | N1-N2   | 2.78  | 1.44        | 1.39     |
| 3   | B     | 682 | HEM  | CBC-CAC | 2.78  | 1.43        | 1.30     |
| 4   | A     | 701 | S58  | C8-S1   | 2.68  | 1.81        | 1.77     |
| 4   | B     | 701 | S58  | C3-N2   | -2.63 | 1.30        | 1.34     |
| 4   | B     | 701 | S58  | C1-C2   | -2.22 | 1.34        | 1.38     |

All (29) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | B     | 701 | S58  | C2-N1-N2    | -7.43 | 107.47      | 112.19   |
| 4   | A     | 701 | S58  | C2-N1-N2    | -7.36 | 107.52      | 112.19   |
| 4   | A     | 701 | S58  | O2-S1-O1    | -5.65 | 110.11      | 118.80   |
| 4   | B     | 701 | S58  | C4-C3-N2    | 5.29  | 126.29      | 119.20   |
| 4   | A     | 701 | S58  | C4-C3-N2    | 5.11  | 126.05      | 119.20   |
| 4   | B     | 701 | S58  | O2-S1-O1    | -4.85 | 111.34      | 118.80   |
| 4   | A     | 701 | S58  | C3-N2-N1    | 4.66  | 108.17      | 104.27   |
| 4   | B     | 701 | S58  | C3-N2-N1    | 4.53  | 108.06      | 104.27   |
| 4   | A     | 701 | S58  | O1-S1-N3    | 4.48  | 113.81      | 107.35   |
| 4   | A     | 701 | S58  | C1-C3-N2    | -3.56 | 107.66      | 111.86   |
| 4   | B     | 701 | S58  | C1-C3-N2    | -3.49 | 107.73      | 111.86   |
| 4   | B     | 701 | S58  | C2-C1-C3    | 3.49  | 107.92      | 104.05   |
| 4   | A     | 701 | S58  | O2-S1-C8    | 3.45  | 111.25      | 107.35   |
| 4   | A     | 701 | S58  | C1-C2-N1    | 3.43  | 108.84      | 105.84   |
| 4   | B     | 701 | S58  | C1-C2-N1    | 3.37  | 108.79      | 105.84   |
| 4   | A     | 701 | S58  | C2-C1-C3    | 3.37  | 107.79      | 104.05   |
| 4   | B     | 701 | S58  | C5-N1-N2    | 3.33  | 123.49      | 118.67   |
| 2   | B     | 671 | NAG  | C2-N2-C7    | -2.95 | 118.94      | 122.90   |
| 4   | A     | 701 | S58  | C5-N1-N2    | 2.91  | 122.89      | 118.67   |
| 2   | A     | 671 | NAG  | C2-N2-C7    | -2.70 | 119.28      | 122.90   |
| 4   | B     | 701 | S58  | F2-C4-C3    | -2.62 | 107.49      | 112.86   |
| 3   | B     | 682 | HEM  | CMD-C2D-C1D | 2.56  | 129.03      | 125.03   |
| 4   | A     | 701 | S58  | F2-C4-C3    | -2.41 | 107.91      | 112.86   |
| 4   | B     | 701 | S58  | O1-S1-N3    | 2.32  | 110.70      | 107.35   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | A     | 701 | S58  | C11-C2-C1  | -2.29 | 123.39      | 128.09   |
| 2   | A     | 681 | NAG  | C1-C2-N2   | -2.27 | 106.85      | 110.43   |
| 4   | B     | 701 | S58  | O2-S1-C8   | 2.15  | 109.78      | 107.35   |
| 4   | A     | 701 | S58  | C11-C2-N1  | 2.12  | 127.74      | 125.01   |
| 3   | B     | 682 | HEM  | C3B-C4B-NB | 2.12  | 110.99      | 109.47   |

There are no chirality outliers.

All (26) torsion outliers are listed below:

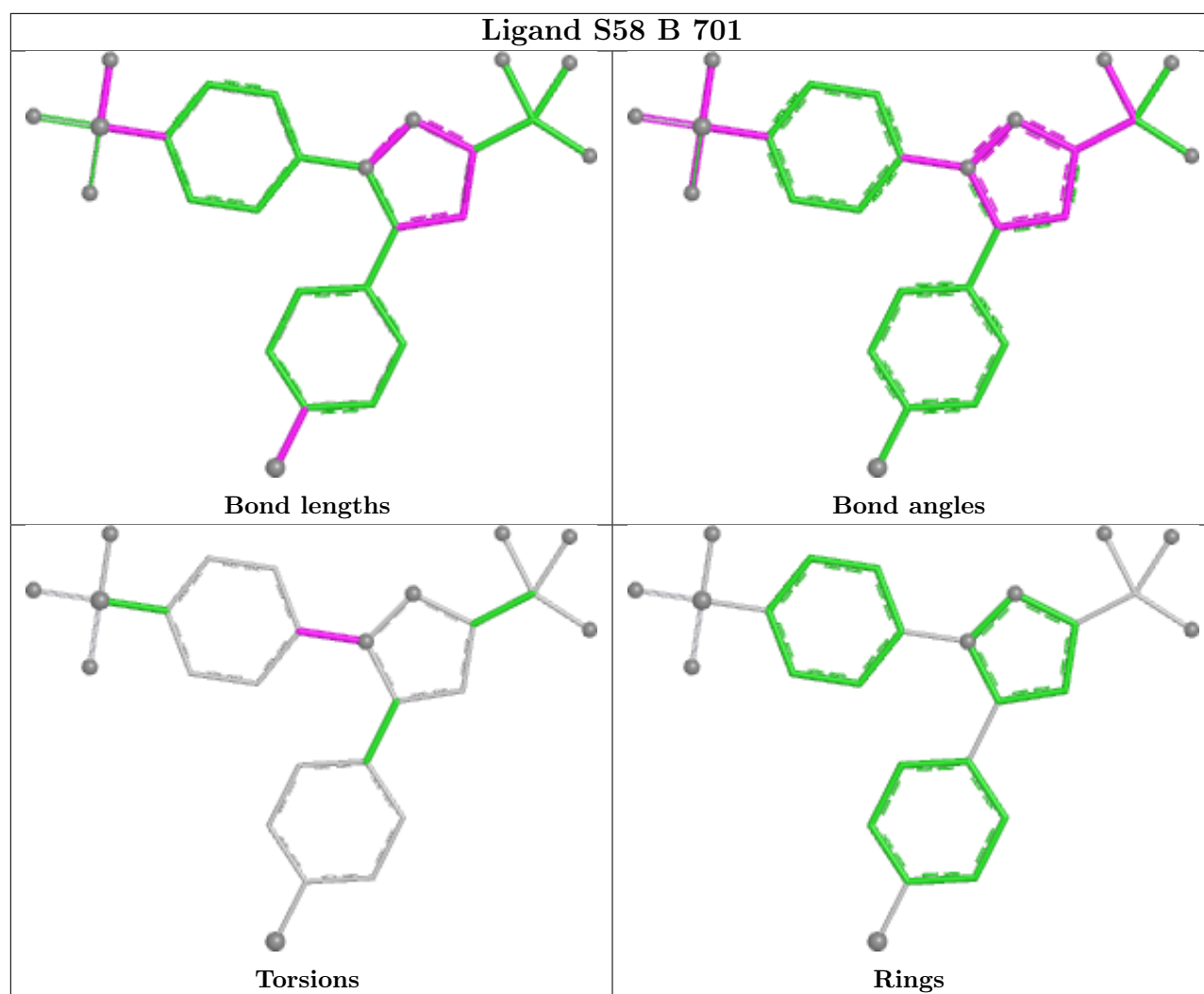
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | A     | 682 | HEM  | C2B-C3B-CAB-CBB |
| 3   | B     | 682 | HEM  | C2A-CAA-CBA-CGA |
| 3   | B     | 682 | HEM  | C2B-C3B-CAB-CBB |
| 3   | A     | 682 | HEM  | C2A-CAA-CBA-CGA |
| 2   | A     | 671 | NAG  | O5-C5-C6-O6     |
| 2   | B     | 671 | NAG  | O5-C5-C6-O6     |
| 2   | A     | 671 | NAG  | C4-C5-C6-O6     |
| 2   | A     | 661 | NAG  | O5-C5-C6-O6     |
| 2   | B     | 671 | NAG  | C4-C5-C6-O6     |
| 2   | A     | 661 | NAG  | C4-C5-C6-O6     |
| 2   | B     | 661 | NAG  | C4-C5-C6-O6     |
| 2   | B     | 661 | NAG  | O5-C5-C6-O6     |
| 3   | A     | 682 | HEM  | C2C-C3C-CAC-CBC |
| 3   | B     | 682 | HEM  | C2C-C3C-CAC-CBC |
| 4   | B     | 701 | S58  | C6-C5-N1-C2     |
| 4   | B     | 701 | S58  | C10-C5-N1-C2    |
| 4   | A     | 701 | S58  | C6-C5-N1-C2     |
| 4   | A     | 701 | S58  | C10-C5-N1-C2    |
| 3   | A     | 682 | HEM  | CAA-CBA-CGA-O2A |
| 3   | A     | 682 | HEM  | C4B-C3B-CAB-CBB |
| 3   | A     | 682 | HEM  | C4C-C3C-CAC-CBC |
| 3   | B     | 682 | HEM  | C4B-C3B-CAB-CBB |
| 3   | B     | 682 | HEM  | C4C-C3C-CAC-CBC |
| 3   | B     | 682 | HEM  | CAA-CBA-CGA-O2A |
| 3   | A     | 682 | HEM  | CAA-CBA-CGA-O1A |
| 3   | B     | 682 | HEM  | CAA-CBA-CGA-O1A |

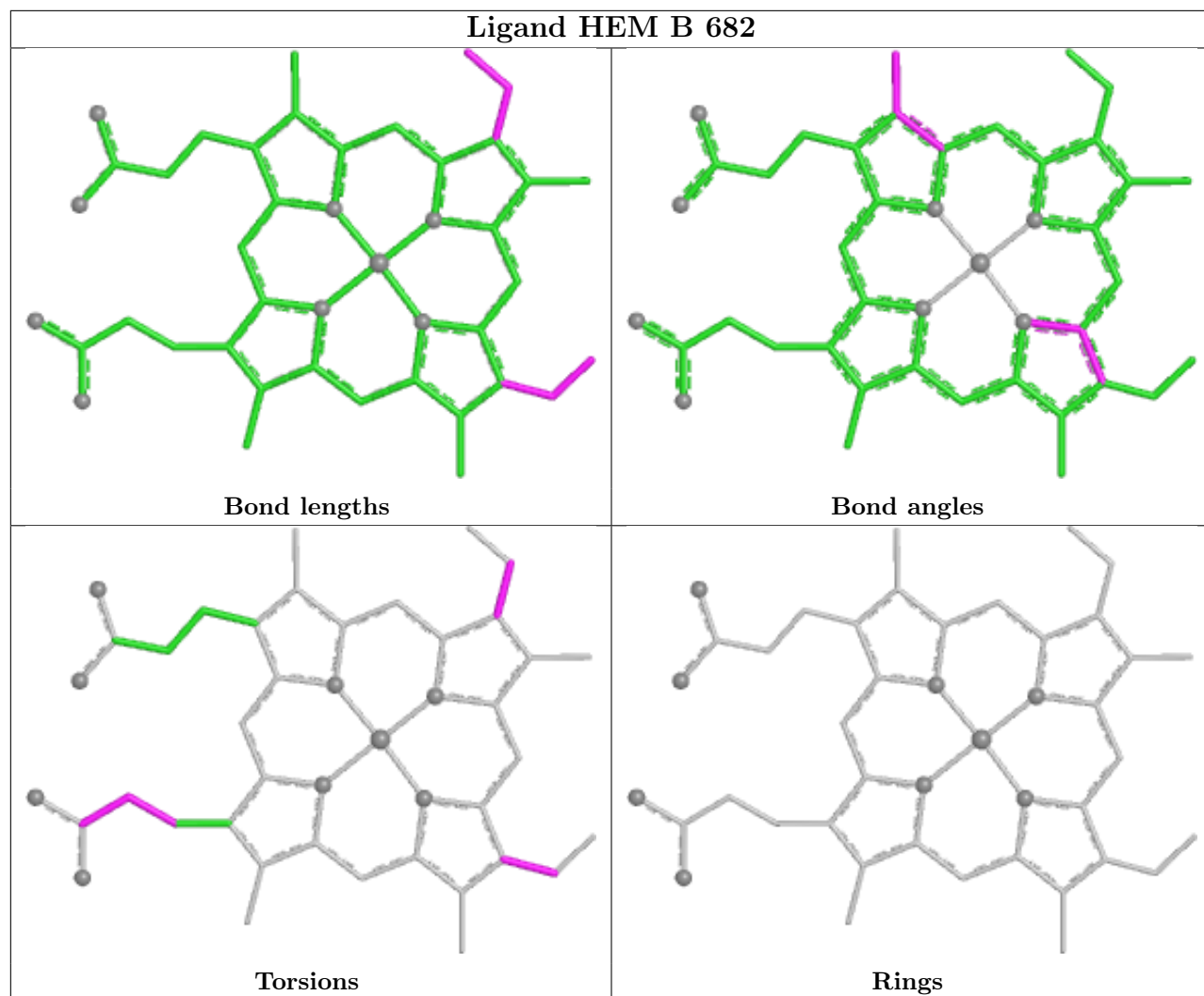
There are no ring outliers.

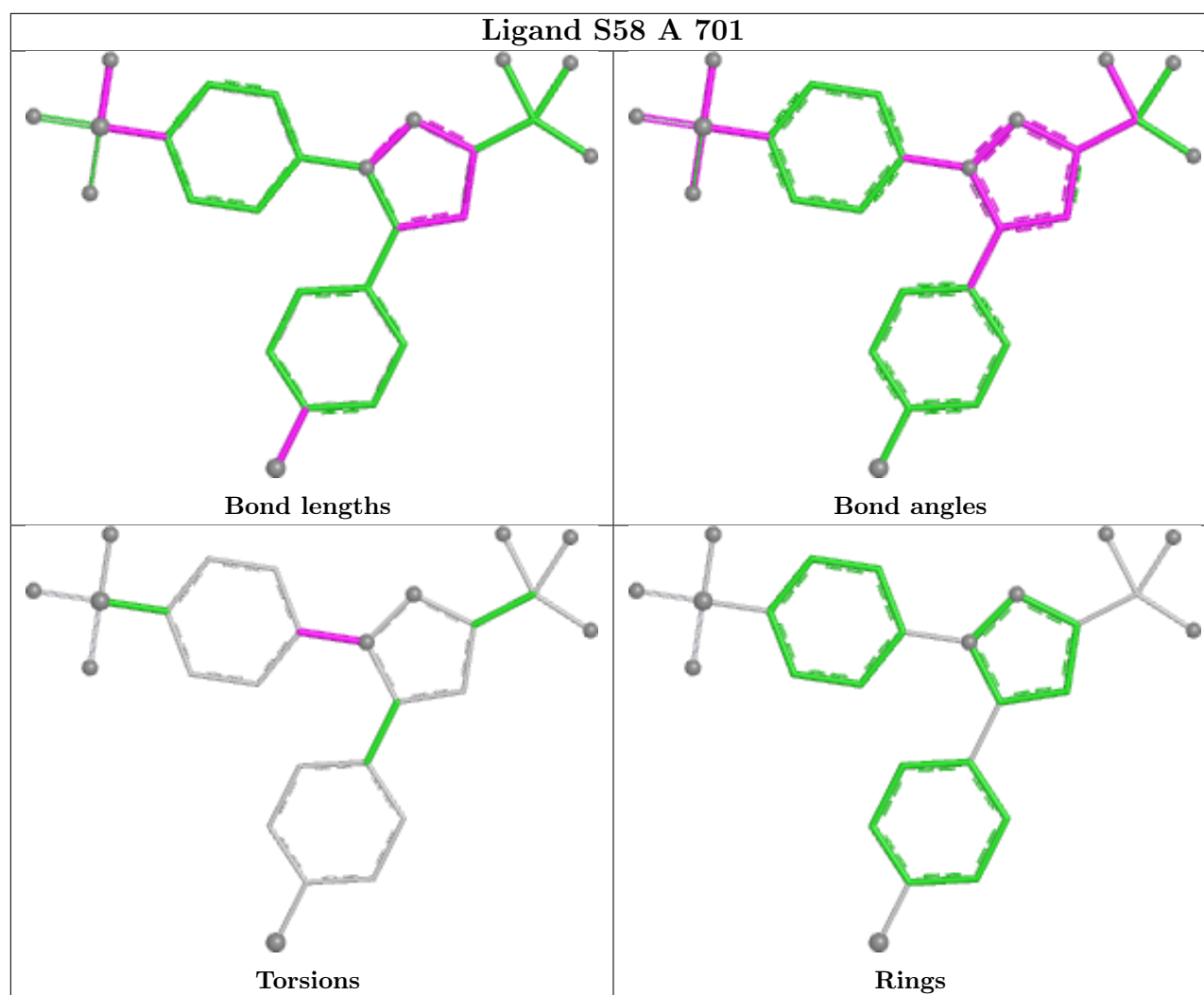
5 monomers are involved in 9 short contacts:

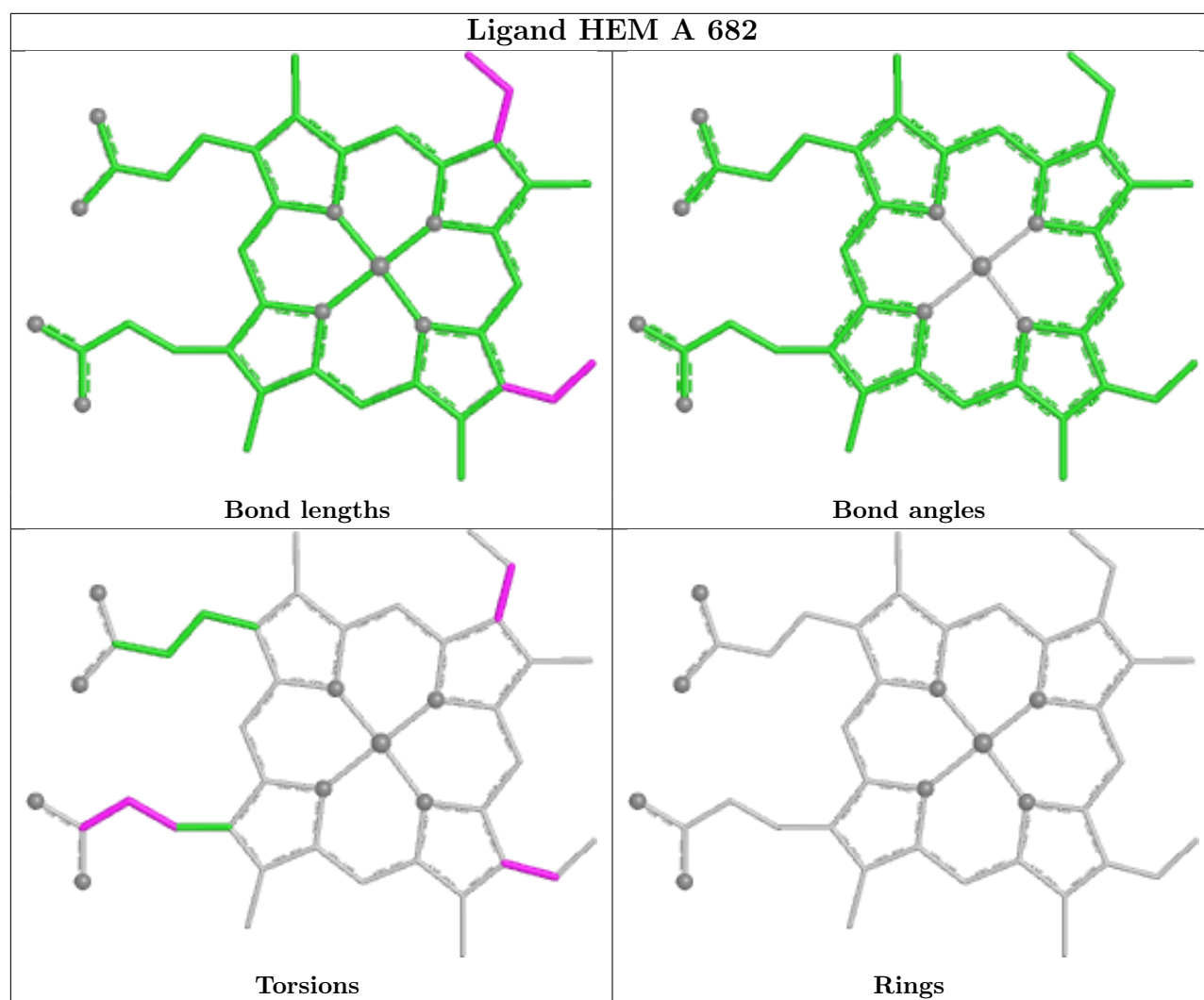
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | B     | 701 | S58  | 2       | 0            |
| 3   | B     | 682 | HEM  | 1       | 0            |
| 4   | A     | 701 | S58  | 3       | 0            |
| 3   | A     | 682 | HEM  | 2       | 0            |
| 2   | A     | 661 | NAG  | 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.









## 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.