



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:31 PM UTC

PDB ID : 1UDU / pdb\_00001udu  
Title : Crystal structure of Human Phosphodiesterase 5 complexed with  
tadalafil(Cialis)  
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Y.H.; Hwang, K.Y.; Ro, S.  
Deposited on : 2003-05-06  
Resolution : 2.83 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](#) ①) were used in the production of this report:

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

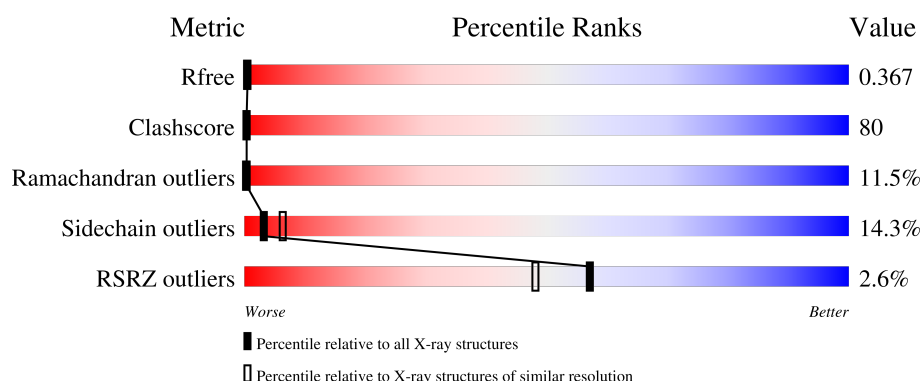
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

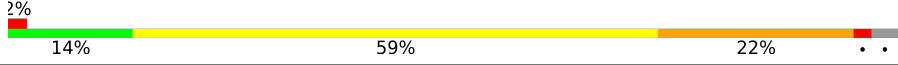
The reported resolution of this entry is 2.83 Å.

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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1520 (2.86-2.82)                                      |
| Clashscore            | 190562                      | 1559 (2.86-2.82)                                      |
| Ramachandran outliers | 187476                      | 1517 (2.86-2.82)                                      |
| Sidechain outliers    | 187428                      | 1518 (2.86-2.82)                                      |
| RSRZ outliers         | 180081                      | 1521 (2.86-2.82)                                      |

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 324    |  |
| 1   | B     | 324    |  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5146 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 cGMP-specific 3',5'-cyclic phosphodiesterase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 313      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2542  | 1617 | 442 | 465 | 18 |         |         |       |
| 1   | B     | 313      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2542  | 1617 | 442 | 465 | 18 |         |         |       |

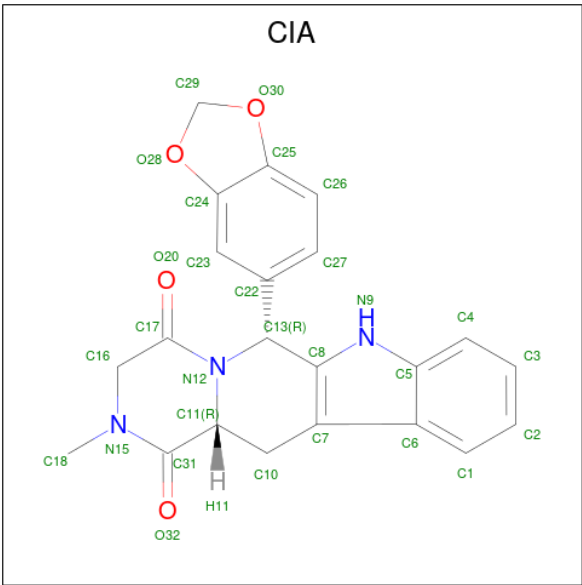
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | B     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

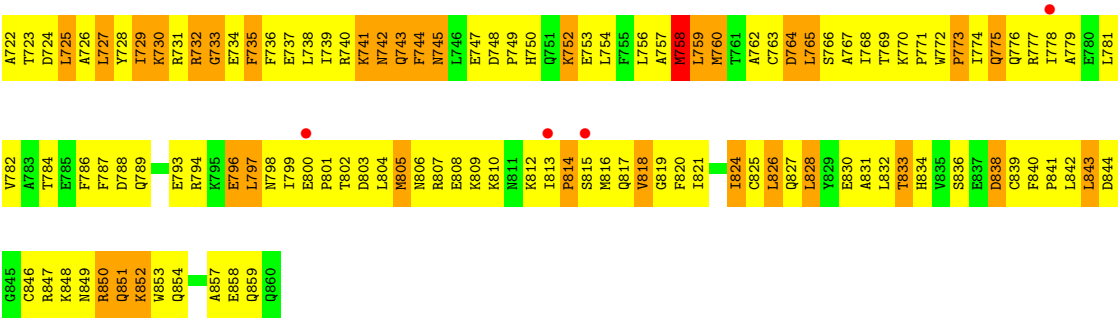
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | B     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 4 is 6-BENZO[1,3]DIOXOL-5-YL-2-METHYL-2,3,6,7,12,12A-HEXAHYDR O-PYRAZINO[1',2':1,6]PYRIDO[3,4-B]INDOLE-1,4-DIONE (CCD ID: CIA) (formula: C<sub>22</sub>H<sub>19</sub>N<sub>3</sub>O<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 4   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 29    | 22 | 3 | 4 |         |         |
| 4   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 29    | 22 | 3 | 4 |         |         |





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 131.35Å 48.56Å 123.86Å<br>90.00° 117.28° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 19.59 – 2.83<br>19.59 – 2.83                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 71.5 (19.59-2.83)<br>71.5 (19.59-2.83)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.52 (at 2.83Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.263 , 0.374<br>0.260 , 0.367                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 627 reflections (4.67%)                                     | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 36.6                                                        | Xtriage          |
| Anisotropy                                                              | 1.008                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 67.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 5146                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 49.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, CIA

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     | 0.60         | 0/2590  | 1.13        | 25/3493 (0.7%) |
| 1   | B     | 0.62         | 0/2590  | 1.15        | 24/3493 (0.7%) |
| All | All   | 0.61         | 0/5180  | 1.14        | 49/6986 (0.7%) |

There are no bond length outliers.

All (49) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 738 | LEU  | N-CA-C | -10.31 | 100.64      | 113.01   |
| 1   | B     | 738 | LEU  | N-CA-C | -9.68  | 101.39      | 113.01   |
| 1   | B     | 595 | LEU  | N-CA-C | -8.17  | 102.37      | 111.28   |
| 1   | A     | 628 | ALA  | N-CA-C | -7.91  | 103.61      | 113.18   |
| 1   | A     | 595 | LEU  | N-CA-C | -7.76  | 102.82      | 111.28   |
| 1   | A     | 622 | ALA  | N-CA-C | -7.58  | 102.37      | 111.69   |
| 1   | B     | 628 | ALA  | N-CA-C | -7.46  | 104.06      | 113.01   |
| 1   | A     | 597 | ARG  | N-CA-C | -7.34  | 103.36      | 111.36   |
| 1   | A     | 852 | LYS  | N-CA-C | -7.32  | 104.48      | 113.41   |
| 1   | A     | 655 | LEU  | N-CA-C | 7.31   | 123.43      | 111.37   |
| 1   | A     | 730 | LYS  | N-CA-C | -7.17  | 105.37      | 112.97   |
| 1   | B     | 655 | LEU  | N-CA-C | 7.11   | 123.02      | 111.37   |
| 1   | B     | 852 | LYS  | N-CA-C | -7.10  | 104.75      | 113.41   |
| 1   | B     | 622 | ALA  | N-CA-C | -6.65  | 103.51      | 111.69   |
| 1   | B     | 730 | LYS  | N-CA-C | -6.62  | 105.95      | 112.97   |
| 1   | A     | 770 | LYS  | CA-C-N | 6.60   | 128.09      | 119.84   |
| 1   | A     | 770 | LYS  | C-N-CA | 6.60   | 128.09      | 119.84   |
| 1   | B     | 625 | MET  | N-CA-C | -6.49  | 103.48      | 111.40   |
| 1   | B     | 586 | GLN  | N-CA-C | 6.36   | 118.01      | 111.14   |
| 1   | B     | 764 | ASP  | N-CA-C | -6.32  | 104.08      | 110.97   |
| 1   | A     | 689 | CYS  | N-CA-C | -5.93  | 104.51      | 110.97   |
| 1   | A     | 805 | MET  | N-CA-C | 5.87   | 120.46      | 112.88   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 621 | THR  | N-CA-C | -5.86 | 106.47      | 113.97   |
| 1   | A     | 816 | MET  | N-CA-C | -5.84 | 105.25      | 112.90   |
| 1   | B     | 610 | VAL  | N-CA-C | -5.83 | 103.62      | 110.21   |
| 1   | B     | 608 | LYS  | N-CA-C | -5.76 | 106.48      | 112.93   |
| 1   | B     | 800 | GLU  | CA-C-N | -5.75 | 113.27      | 120.51   |
| 1   | B     | 800 | GLU  | C-N-CA | -5.75 | 113.27      | 120.51   |
| 1   | A     | 553 | THR  | N-CA-C | -5.72 | 105.13      | 111.71   |
| 1   | B     | 741 | LYS  | N-CA-C | -5.70 | 105.25      | 114.09   |
| 1   | A     | 752 | LYS  | N-CA-C | -5.69 | 105.60      | 112.54   |
| 1   | B     | 796 | GLU  | N-CA-C | -5.56 | 104.91      | 110.97   |
| 1   | A     | 557 | THR  | N-CA-C | 5.50  | 118.98      | 112.72   |
| 1   | A     | 830 | GLU  | N-CA-C | -5.44 | 105.04      | 110.97   |
| 1   | A     | 548 | VAL  | CA-C-N | 5.34  | 126.52      | 119.84   |
| 1   | A     | 548 | VAL  | C-N-CA | 5.34  | 126.52      | 119.84   |
| 1   | B     | 729 | ILE  | N-CA-C | -5.24 | 107.72      | 112.96   |
| 1   | B     | 685 | HIS  | N-CA-C | -5.22 | 105.03      | 111.40   |
| 1   | B     | 621 | THR  | N-CA-C | -5.20 | 107.06      | 113.41   |
| 1   | B     | 851 | GLN  | N-CA-C | -5.20 | 106.74      | 114.64   |
| 1   | A     | 640 | ASP  | N-CA-C | -5.15 | 106.50      | 112.89   |
| 1   | A     | 646 | LEU  | N-CA-C | 5.14  | 116.89      | 111.28   |
| 1   | B     | 752 | LYS  | N-CA-C | -5.11 | 105.89      | 111.82   |
| 1   | A     | 644 | LEU  | N-CA-C | -5.10 | 105.41      | 111.69   |
| 1   | B     | 566 | LEU  | N-CA-C | 5.09  | 118.24      | 110.20   |
| 1   | B     | 805 | MET  | N-CA-C | 5.08  | 120.11      | 113.30   |
| 1   | A     | 564 | PHE  | N-CA-C | 5.08  | 121.61      | 110.80   |
| 1   | B     | 646 | LEU  | N-CA-C | 5.04  | 117.51      | 111.71   |
| 1   | A     | 851 | GLN  | N-CA-C | -5.02 | 107.01      | 114.64   |

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     | 2542  | 0        | 2552     | 420     | 0            |
| 1   | B     | 2542  | 0        | 2552     | 422     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 29    | 0        | 19       | 8       | 0            |
| 4   | B     | 29    | 0        | 19       | 1       | 0            |
| All | All   | 5146  | 0        | 5142     | 828     | 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 80.

All (828) 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:653:HIS:HA   | 1:A:720:ILE:HG23 | 1.26                     | 1.14              |
| 1:B:653:HIS:HA   | 1:B:720:ILE:HG23 | 1.26                     | 1.11              |
| 1:A:801:PRO:HB2  | 1:A:806:ASN:HB3  | 1.34                     | 1.07              |
| 1:B:725:LEU:O    | 1:B:729:ILE:HG13 | 1.58                     | 1.04              |
| 1:B:658:ARG:HG2  | 1:B:658:ARG:HH11 | 1.23                     | 1.02              |
| 1:B:679:SER:HB3  | 1:B:682:GLU:HG3  | 1.39                     | 1.02              |
| 1:B:801:PRO:HB2  | 1:B:806:ASN:HB3  | 1.35                     | 1.02              |
| 1:B:797:LEU:H    | 1:B:797:LEU:HD22 | 1.22                     | 1.02              |
| 1:A:808:GLU:HG3  | 1:A:809:LYS:H    | 1.20                     | 1.01              |
| 1:B:543:LEU:HD11 | 1:B:572:ALA:HB1  | 1.43                     | 0.99              |
| 1:B:808:GLU:HG3  | 1:B:809:LYS:H    | 1.26                     | 0.98              |
| 1:B:572:ALA:O    | 1:B:576:ILE:HG13 | 1.67                     | 0.95              |
| 1:A:821:ILE:HA   | 1:A:825:CYS:HB2  | 1.49                     | 0.94              |
| 1:A:725:LEU:O    | 1:A:729:ILE:HG13 | 1.66                     | 0.94              |
| 1:A:735:PHE:HB2  | 1:A:754:LEU:HD23 | 1.48                     | 0.93              |
| 1:B:559:PHE:HD1  | 1:B:559:PHE:H    | 1.13                     | 0.93              |
| 1:A:718:GLN:HE22 | 1:B:796:GLU:HB3  | 1.34                     | 0.93              |
| 1:B:793:GLU:HA   | 1:B:797:LEU:HD23 | 1.52                     | 0.92              |
| 1:B:652:SER:HB3  | 1:B:655:LEU:HD12 | 1.52                     | 0.92              |
| 1:A:797:LEU:HD22 | 1:A:797:LEU:H    | 1.34                     | 0.91              |
| 1:B:813:ILE:HA   | 1:B:816:MET:HE3  | 1.53                     | 0.91              |
| 1:A:652:SER:HB3  | 1:A:655:LEU:HD12 | 1.50                     | 0.90              |
| 1:B:607:ARG:NH2  | 1:B:658:ARG:HH21 | 1.68                     | 0.90              |
| 1:B:735:PHE:HB2  | 1:B:754:LEU:HD23 | 1.52                     | 0.89              |
| 1:B:765:LEU:O    | 1:B:768:ILE:HG22 | 1.73                     | 0.89              |
| 1:A:830:GLU:HA   | 1:A:843:LEU:HD22 | 1.56                     | 0.88              |
| 1:A:559:PHE:HD1  | 1:A:559:PHE:H    | 1.21                     | 0.87              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:813:ILE:HA   | 1:A:816:MET:HE3   | 1.54                     | 0.87              |
| 1:B:821:ILE:HA   | 1:B:825:CYS:HB2   | 1.58                     | 0.86              |
| 1:A:677:CYS:HA   | 1:B:677:CYS:SG    | 2.16                     | 0.85              |
| 1:B:727:LEU:HD23 | 1:B:728:TYR:N     | 1.89                     | 0.85              |
| 1:B:632:GLY:HA2  | 1:B:838:ASP:HB3   | 1.56                     | 0.85              |
| 1:B:828:LEU:O    | 1:B:828:LEU:HD22  | 1.77                     | 0.85              |
| 1:A:679:SER:HB3  | 1:A:682:GLU:HG3   | 1.57                     | 0.85              |
| 1:A:636:ASN:ND2  | 1:A:637:LYS:HG3   | 1.91                     | 0.85              |
| 1:B:543:LEU:HD11 | 1:B:572:ALA:CB    | 2.08                     | 0.84              |
| 1:A:661:ASN:C    | 1:A:662:ASN:HD22  | 1.85                     | 0.84              |
| 1:B:653:HIS:HB2  | 1:B:723:THR:HG21  | 1.56                     | 0.84              |
| 1:B:770:LYS:NZ   | 1:B:774:ILE:HG21  | 1.93                     | 0.84              |
| 1:A:604:LYS:HB2  | 1:A:604:LYS:NZ    | 1.93                     | 0.83              |
| 1:A:787:PHE:HB3  | 1:A:807:ARG:HD2   | 1.59                     | 0.83              |
| 1:A:793:GLU:HA   | 1:A:797:LEU:HD23  | 1.61                     | 0.83              |
| 1:A:658:ARG:HG2  | 1:A:658:ARG:HH11  | 1.42                     | 0.83              |
| 1:B:566:LEU:H    | 1:B:566:LEU:HD23  | 1.44                     | 0.82              |
| 1:A:543:LEU:HD11 | 1:A:572:ALA:HB1   | 1.60                     | 0.82              |
| 1:B:636:ASN:HD22 | 1:B:636:ASN:C     | 1.87                     | 0.82              |
| 1:B:693:LEU:HD22 | 1:B:701:LEU:HD12  | 1.61                     | 0.82              |
| 1:B:712:THR:O    | 1:B:716:ILE:HG13  | 1.80                     | 0.81              |
| 1:A:727:LEU:HD23 | 1:A:728:TYR:N     | 1.94                     | 0.81              |
| 1:B:642:GLU:O    | 1:B:646:LEU:HD23  | 1.79                     | 0.81              |
| 1:B:679:SER:HB3  | 1:B:682:GLU:CG    | 2.10                     | 0.81              |
| 1:A:607:ARG:NH2  | 1:A:658:ARG:HH21  | 1.77                     | 0.81              |
| 1:B:604:LYS:HB2  | 1:B:604:LYS:NZ    | 1.96                     | 0.80              |
| 1:A:663:SER:HA   | 4:A:1003:CIA:H182 | 1.64                     | 0.80              |
| 1:A:572:ALA:O    | 1:A:576:ILE:HG13  | 1.81                     | 0.79              |
| 1:B:603:LYS:HG3  | 1:B:615:TRP:CD1   | 2.17                     | 0.79              |
| 1:B:569:LEU:O    | 1:B:572:ALA:HB3   | 1.81                     | 0.79              |
| 1:A:693:LEU:HD22 | 1:A:701:LEU:HD12  | 1.64                     | 0.79              |
| 1:A:770:LYS:NZ   | 1:A:774:ILE:HG21  | 1.97                     | 0.79              |
| 1:A:539:GLU:HG2  | 1:A:600:LEU:HD11  | 1.63                     | 0.79              |
| 1:B:827:GLN:HA   | 1:B:830:GLU:HG2   | 1.63                     | 0.78              |
| 1:A:632:GLY:HA2  | 1:A:838:ASP:HB3   | 1.64                     | 0.78              |
| 1:A:653:HIS:HB2  | 1:A:723:THR:HG21  | 1.63                     | 0.78              |
| 1:B:734:GLU:C    | 1:B:736:PHE:H     | 1.86                     | 0.78              |
| 1:B:820:PHE:CE1  | 1:B:824:ILE:HD12  | 2.19                     | 0.78              |
| 1:B:563:ASP:HB3  | 1:B:620:ASN:HD21  | 1.49                     | 0.78              |
| 1:B:770:LYS:HZ3  | 1:B:774:ILE:HG21  | 1.49                     | 0.77              |
| 1:A:765:LEU:O    | 1:A:768:ILE:HG22  | 1.84                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:636:ASN:C    | 1:A:636:ASN:HD22 | 1.91                     | 0.77              |
| 1:B:549:PRO:HG2  | 1:B:554:LEU:HD21 | 1.67                     | 0.77              |
| 1:B:787:PHE:HB3  | 1:B:807:ARG:HD2  | 1.67                     | 0.77              |
| 1:A:543:LEU:HD11 | 1:A:572:ALA:CB   | 2.14                     | 0.77              |
| 1:A:566:LEU:HD23 | 1:A:566:LEU:H    | 1.48                     | 0.77              |
| 1:A:582:LEU:HD21 | 1:A:629:LEU:HD23 | 1.66                     | 0.77              |
| 1:B:636:ASN:ND2  | 1:B:637:LYS:HG3  | 2.01                     | 0.76              |
| 1:A:705:SER:HB2  | 1:A:708:GLU:HG2  | 1.68                     | 0.76              |
| 1:A:712:THR:O    | 1:A:716:ILE:HG13 | 1.85                     | 0.75              |
| 1:A:630:LYS:O    | 1:A:632:GLY:N    | 2.18                     | 0.75              |
| 1:B:806:ASN:HD21 | 1:B:809:LYS:HG2  | 1.50                     | 0.74              |
| 1:A:759:LEU:O    | 1:A:759:LEU:HD12 | 1.87                     | 0.74              |
| 1:A:742:ASN:C    | 1:A:744:PHE:H    | 1.94                     | 0.74              |
| 1:B:639:THR:OG1  | 1:B:642:GLU:HG3  | 1.87                     | 0.74              |
| 1:B:826:LEU:HD23 | 1:B:827:GLN:N    | 2.01                     | 0.74              |
| 1:B:559:PHE:CD2  | 1:B:841:PRO:HB2  | 2.23                     | 0.74              |
| 1:B:586:GLN:HA   | 1:B:586:GLN:HE21 | 1.52                     | 0.74              |
| 1:A:586:GLN:HA   | 1:A:586:GLN:HE21 | 1.51                     | 0.74              |
| 1:B:692:ILE:O    | 1:B:695:SER:N    | 2.21                     | 0.73              |
| 1:B:630:LYS:O    | 1:B:632:GLY:N    | 2.21                     | 0.73              |
| 1:A:642:GLU:O    | 1:A:646:LEU:HD23 | 1.89                     | 0.73              |
| 1:A:808:GLU:HG3  | 1:A:809:LYS:N    | 2.00                     | 0.73              |
| 1:A:558:ASP:N    | 1:A:558:ASP:OD2  | 2.20                     | 0.73              |
| 1:A:734:GLU:C    | 1:A:736:PHE:H    | 1.95                     | 0.73              |
| 1:B:661:ASN:C    | 1:B:662:ASN:HD22 | 1.96                     | 0.73              |
| 1:A:696:PRO:HA   | 1:A:699:GLN:HE21 | 1.54                     | 0.72              |
| 1:A:717:LYS:HG2  | 1:A:721:LEU:HD11 | 1.71                     | 0.72              |
| 1:A:787:PHE:HB2  | 1:A:807:ARG:NH1  | 2.03                     | 0.72              |
| 1:B:607:ARG:HH21 | 1:B:658:ARG:HH21 | 1.35                     | 0.72              |
| 1:B:704:LEU:HB3  | 1:B:708:GLU:HB2  | 1.72                     | 0.72              |
| 1:B:705:SER:HB2  | 1:B:708:GLU:HG2  | 1.71                     | 0.72              |
| 1:B:658:ARG:HH11 | 1:B:658:ARG:CG   | 2.02                     | 0.71              |
| 1:B:762:ALA:HA   | 1:B:828:LEU:HD11 | 1.70                     | 0.71              |
| 1:B:575:THR:O    | 1:B:578:MET:HB2  | 1.90                     | 0.71              |
| 1:B:658:ARG:HG2  | 1:B:658:ARG:NH1  | 2.00                     | 0.71              |
| 1:B:742:ASN:C    | 1:B:744:PHE:H    | 1.99                     | 0.71              |
| 1:A:663:SER:HA   | 4:A:1003:CIA:C18 | 2.21                     | 0.71              |
| 1:A:826:LEU:HD23 | 1:A:827:GLN:N    | 2.06                     | 0.70              |
| 1:A:711:THR:O    | 1:A:715:ILE:HG13 | 1.91                     | 0.70              |
| 1:B:584:LEU:HD13 | 1:B:644:LEU:HD12 | 1.72                     | 0.70              |
| 1:A:652:SER:HB3  | 1:A:655:LEU:CD1  | 2.21                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:759:LEU:HD12 | 1:B:759:LEU:O    | 1.91                     | 0.70              |
| 1:A:767:ALA:HA   | 1:A:770:LYS:CG   | 2.22                     | 0.70              |
| 1:B:833:THR:HG22 | 1:B:834:HIS:N    | 2.06                     | 0.70              |
| 1:A:636:ASN:HD21 | 1:A:637:LYS:HG3  | 1.56                     | 0.70              |
| 1:B:801:PRO:HB2  | 1:B:806:ASN:CB   | 2.19                     | 0.69              |
| 1:B:734:GLU:C    | 1:B:736:PHE:N    | 2.50                     | 0.69              |
| 1:A:770:LYS:HZ3  | 1:A:774:ILE:HG21 | 1.57                     | 0.69              |
| 1:A:828:LEU:HD22 | 1:A:828:LEU:O    | 1.92                     | 0.69              |
| 1:A:718:GLN:NE2  | 1:B:796:GLU:HB3  | 2.07                     | 0.69              |
| 1:B:571:THR:HA   | 1:B:619:PHE:CZ   | 2.28                     | 0.69              |
| 1:A:716:ILE:O    | 1:A:719:ALA:HB3  | 1.93                     | 0.69              |
| 1:A:563:ASP:HB2  | 1:A:616:ARG:HH11 | 1.58                     | 0.69              |
| 1:A:597:ARG:HG2  | 1:A:698:ASN:OD1  | 1.93                     | 0.69              |
| 1:A:695:SER:HB2  | 1:A:698:ASN:HD22 | 1.57                     | 0.69              |
| 1:B:558:ASP:OD2  | 1:B:558:ASP:N    | 2.24                     | 0.69              |
| 1:B:745:ASN:ND2  | 1:B:748:ASP:HB2  | 2.08                     | 0.69              |
| 1:A:639:THR:OG1  | 1:A:642:GLU:HG3  | 1.93                     | 0.69              |
| 1:A:658:ARG:HG2  | 1:A:658:ARG:NH1  | 2.08                     | 0.68              |
| 1:B:574:CYS:O    | 1:B:577:ARG:HB3  | 1.93                     | 0.68              |
| 1:B:584:LEU:HD13 | 1:B:644:LEU:CD1  | 2.23                     | 0.68              |
| 1:B:559:PHE:CD1  | 1:B:559:PHE:N    | 2.59                     | 0.68              |
| 1:B:597:ARG:HG2  | 1:B:698:ASN:OD1  | 1.94                     | 0.68              |
| 1:B:716:ILE:O    | 1:B:719:ALA:HB3  | 1.94                     | 0.68              |
| 1:B:717:LYS:HG2  | 1:B:721:LEU:HD11 | 1.75                     | 0.68              |
| 1:A:636:ASN:HD22 | 1:A:637:LYS:N    | 1.92                     | 0.68              |
| 1:A:679:SER:HB3  | 1:A:682:GLU:CG   | 2.23                     | 0.68              |
| 1:A:704:LEU:HB3  | 1:A:708:GLU:HB2  | 1.75                     | 0.68              |
| 1:A:692:ILE:O    | 1:A:695:SER:N    | 2.26                     | 0.68              |
| 1:B:583:ASN:HB3  | 1:B:587:ASN:HD21 | 1.57                     | 0.68              |
| 1:B:844:ASP:O    | 1:B:848:LYS:HG3  | 1.93                     | 0.68              |
| 1:B:770:LYS:HZ3  | 1:B:774:ILE:CG2  | 2.07                     | 0.68              |
| 1:A:549:PRO:HG2  | 1:A:554:LEU:HD21 | 1.77                     | 0.67              |
| 1:B:839:CYS:C    | 1:B:841:PRO:HD2  | 2.20                     | 0.67              |
| 1:A:725:LEU:HD12 | 1:A:725:LEU:H    | 1.60                     | 0.67              |
| 1:B:582:LEU:HD21 | 1:B:629:LEU:HD23 | 1.76                     | 0.67              |
| 1:B:830:GLU:O    | 1:B:833:THR:HB   | 1.94                     | 0.67              |
| 1:A:818:VAL:HG12 | 1:A:819:GLY:N    | 2.07                     | 0.67              |
| 1:B:578:MET:O    | 1:B:582:LEU:HD12 | 1.95                     | 0.67              |
| 1:A:779:ALA:HB1  | 1:A:817:GLN:NE2  | 2.09                     | 0.66              |
| 1:B:724:ASP:OD2  | 1:B:726:ALA:HB3  | 1.96                     | 0.66              |
| 1:B:695:SER:HB2  | 1:B:698:ASN:HD22 | 1.61                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:636:ASN:HD22 | 1:B:637:LYS:N    | 1.93                     | 0.66              |
| 1:B:549:PRO:HB2  | 1:B:554:LEU:HG   | 1.78                     | 0.66              |
| 1:B:630:LYS:C    | 1:B:632:GLY:H    | 2.04                     | 0.66              |
| 1:B:585:VAL:O    | 1:B:589:GLN:HA   | 1.96                     | 0.66              |
| 1:A:568:ASP:O    | 1:A:571:THR:N    | 2.29                     | 0.65              |
| 1:A:724:ASP:OD2  | 1:A:726:ALA:HB3  | 1.97                     | 0.65              |
| 1:A:761:THR:O    | 1:A:765:LEU:HD13 | 1.96                     | 0.65              |
| 1:B:727:LEU:O    | 1:B:731:ARG:HG3  | 1.95                     | 0.65              |
| 1:B:731:ARG:O    | 1:B:733:GLY:N    | 2.29                     | 0.65              |
| 1:A:709:TYR:CE2  | 1:A:713:LEU:HD11 | 2.32                     | 0.65              |
| 1:A:821:ILE:HA   | 1:A:825:CYS:CB   | 2.26                     | 0.65              |
| 1:A:563:ASP:HB2  | 1:A:616:ARG:NH1  | 2.12                     | 0.65              |
| 1:B:797:LEU:HD22 | 1:B:797:LEU:N    | 2.05                     | 0.65              |
| 1:B:583:ASN:O    | 1:B:587:ASN:ND2  | 2.29                     | 0.65              |
| 1:B:717:LYS:HE2  | 1:B:721:LEU:HD11 | 1.79                     | 0.65              |
| 1:B:632:GLY:CA   | 1:B:838:ASP:HB3  | 2.26                     | 0.65              |
| 1:B:806:ASN:ND2  | 1:B:809:LYS:HG2  | 2.13                     | 0.64              |
| 1:B:806:ASN:ND2  | 1:B:808:GLU:HB3  | 2.12                     | 0.64              |
| 1:B:808:GLU:HG3  | 1:B:809:LYS:N    | 2.06                     | 0.64              |
| 1:A:796:GLU:HB2  | 1:B:717:LYS:HZ3  | 1.62                     | 0.64              |
| 1:B:779:ALA:HB1  | 1:B:817:GLN:NE2  | 2.12                     | 0.64              |
| 1:A:630:LYS:C    | 1:A:632:GLY:H    | 2.05                     | 0.64              |
| 1:A:654:ASP:HA   | 1:A:685:HIS:CE1  | 2.32                     | 0.64              |
| 1:A:731:ARG:O    | 1:A:733:GLY:N    | 2.31                     | 0.64              |
| 1:A:695:SER:O    | 1:A:699:GLN:HG3  | 1.98                     | 0.64              |
| 1:A:745:ASN:ND2  | 1:A:748:ASP:HB2  | 2.13                     | 0.64              |
| 1:B:598:TRP:HA   | 1:B:698:ASN:HB3  | 1.80                     | 0.64              |
| 1:B:603:LYS:O    | 1:B:606:TYR:HB2  | 1.97                     | 0.64              |
| 1:A:814:PRO:HB2  | 1:A:857:ALA:HB2  | 1.79                     | 0.64              |
| 1:B:833:THR:HG22 | 1:B:834:HIS:HD2  | 1.62                     | 0.63              |
| 1:B:582:LEU:O    | 1:B:583:ASN:HB2  | 1.98                     | 0.63              |
| 1:A:578:MET:O    | 1:A:582:LEU:HD12 | 1.98                     | 0.63              |
| 1:B:696:PRO:HA   | 1:B:699:GLN:HE21 | 1.63                     | 0.63              |
| 1:A:767:ALA:HA   | 1:A:770:LYS:HG3  | 1.79                     | 0.63              |
| 1:A:813:ILE:CG1  | 1:A:814:PRO:HD3  | 2.29                     | 0.63              |
| 1:B:709:TYR:CE2  | 1:B:713:LEU:HD11 | 2.34                     | 0.63              |
| 1:B:652:SER:HB3  | 1:B:655:LEU:CD1  | 2.27                     | 0.63              |
| 1:B:821:ILE:HA   | 1:B:825:CYS:CB   | 2.28                     | 0.63              |
| 1:B:711:THR:O    | 1:B:715:ILE:HG13 | 1.99                     | 0.63              |
| 1:B:830:GLU:HA   | 1:B:843:LEU:HD22 | 1.81                     | 0.63              |
| 1:A:759:LEU:HD12 | 1:A:759:LEU:C    | 2.24                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:779:ALA:HB1  | 1:B:817:GLN:HE22 | 1.63                     | 0.63              |
| 1:A:806:ASN:ND2  | 1:A:808:GLU:HB3  | 2.14                     | 0.63              |
| 1:B:598:TRP:O    | 1:B:602:VAL:HG23 | 1.98                     | 0.63              |
| 1:B:725:LEU:HD12 | 1:B:725:LEU:H    | 1.64                     | 0.63              |
| 1:B:683:HIS:O    | 1:B:687:ASP:OD1  | 2.17                     | 0.62              |
| 1:B:787:PHE:HB2  | 1:B:807:ARG:NH1  | 2.14                     | 0.62              |
| 1:A:778:ILE:HA   | 1:A:781:LEU:HD12 | 1.81                     | 0.62              |
| 1:B:580:THR:C    | 1:B:582:LEU:H    | 2.08                     | 0.62              |
| 1:B:689:CYS:SG   | 1:B:720:ILE:HD11 | 2.40                     | 0.62              |
| 1:A:734:GLU:C    | 1:A:736:PHE:N    | 2.56                     | 0.62              |
| 1:B:767:ALA:HA   | 1:B:770:LYS:CG   | 2.30                     | 0.62              |
| 1:A:621:THR:HG23 | 1:A:763:CYS:O    | 2.00                     | 0.62              |
| 1:A:679:SER:O    | 1:A:683:HIS:ND1  | 2.30                     | 0.62              |
| 1:A:779:ALA:HB1  | 1:A:817:GLN:HE22 | 1.62                     | 0.62              |
| 1:B:590:MET:HE1  | 1:B:644:LEU:HD11 | 1.80                     | 0.62              |
| 1:A:735:PHE:CE2  | 1:A:758:MET:HG2  | 2.34                     | 0.62              |
| 1:B:604:LYS:HB2  | 1:B:604:LYS:HZ3  | 1.63                     | 0.62              |
| 1:A:563:ASP:HB3  | 1:A:620:ASN:HD21 | 1.65                     | 0.62              |
| 1:A:604:LYS:HB2  | 1:A:604:LYS:HZ3  | 1.65                     | 0.62              |
| 1:A:628:ALA:O    | 1:A:634:ILE:HB   | 1.99                     | 0.62              |
| 1:A:578:MET:O    | 1:A:582:LEU:HB2  | 1.99                     | 0.61              |
| 1:B:813:ILE:CG1  | 1:B:814:PRO:HD3  | 2.30                     | 0.61              |
| 1:A:786:PHE:HD1  | 1:A:804:LEU:HG   | 1.64                     | 0.61              |
| 1:B:562:SER:OG   | 1:B:777:ARG:NH2  | 2.30                     | 0.61              |
| 1:B:827:GLN:HA   | 1:B:830:GLU:CG   | 2.30                     | 0.61              |
| 1:A:571:THR:HA   | 1:A:619:PHE:CZ   | 2.35                     | 0.61              |
| 1:A:683:HIS:O    | 1:A:687:ASP:OD1  | 2.18                     | 0.61              |
| 1:B:583:ASN:HB3  | 1:B:587:ASN:ND2  | 2.15                     | 0.61              |
| 1:B:820:PHE:HE1  | 1:B:824:ILE:HD12 | 1.63                     | 0.61              |
| 1:A:769:THR:HG22 | 1:A:846:CYS:HB2  | 1.80                     | 0.61              |
| 1:B:570:GLU:C    | 1:B:572:ALA:H    | 2.08                     | 0.61              |
| 1:B:778:ILE:HA   | 1:B:781:LEU:HD12 | 1.81                     | 0.61              |
| 1:A:559:PHE:CD2  | 1:A:841:PRO:HB2  | 2.34                     | 0.61              |
| 1:B:563:ASP:HB2  | 1:B:616:ARG:HH11 | 1.66                     | 0.61              |
| 1:A:539:GLU:HG2  | 1:A:600:LEU:CD1  | 2.31                     | 0.61              |
| 1:A:583:ASN:O    | 1:A:587:ASN:ND2  | 2.33                     | 0.61              |
| 1:A:844:ASP:O    | 1:A:848:LYS:HG3  | 2.01                     | 0.61              |
| 1:B:679:SER:CB   | 1:B:682:GLU:HG3  | 2.24                     | 0.61              |
| 1:B:814:PRO:HB2  | 1:B:857:ALA:HB2  | 1.83                     | 0.61              |
| 1:A:582:LEU:HD11 | 1:A:626:PHE:HD1  | 1.64                     | 0.61              |
| 1:B:562:SER:HG   | 1:B:777:ARG:HH22 | 1.48                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:763:CYS:O    | 1:B:766:SER:HB3  | 2.00                     | 0.61              |
| 1:A:549:PRO:HB2  | 1:A:554:LEU:HG   | 1.84                     | 0.60              |
| 1:B:597:ARG:HD2  | 1:B:697:GLY:O    | 2.01                     | 0.60              |
| 1:B:636:ASN:C    | 1:B:636:ASN:ND2  | 2.59                     | 0.60              |
| 1:B:762:ALA:CA   | 1:B:828:LEU:HD11 | 2.31                     | 0.60              |
| 1:B:684:HIS:O    | 1:B:688:GLN:HB2  | 2.02                     | 0.60              |
| 1:B:750:HIS:O    | 1:B:753:GLU:HB2  | 2.02                     | 0.60              |
| 1:B:830:GLU:CG   | 1:B:831:ALA:H    | 2.14                     | 0.60              |
| 1:A:692:ILE:O    | 1:A:694:ASN:N    | 2.34                     | 0.60              |
| 1:A:585:VAL:O    | 1:A:589:GLN:HA   | 2.01                     | 0.60              |
| 1:A:786:PHE:CD1  | 1:A:804:LEU:HG   | 2.37                     | 0.60              |
| 1:B:712:THR:HA   | 1:B:715:ILE:HD12 | 1.83                     | 0.60              |
| 1:A:693:LEU:HD22 | 1:A:701:LEU:CD1  | 2.32                     | 0.59              |
| 1:B:658:ARG:CG   | 1:B:658:ARG:NH1  | 2.63                     | 0.59              |
| 1:A:597:ARG:HD2  | 1:A:697:GLY:O    | 2.01                     | 0.59              |
| 1:A:575:THR:O    | 1:A:578:MET:HB2  | 2.02                     | 0.59              |
| 1:B:695:SER:O    | 1:B:699:GLN:HG3  | 2.02                     | 0.59              |
| 1:A:604:LYS:HB2  | 1:A:604:LYS:HZ2  | 1.68                     | 0.59              |
| 1:A:623:GLN:O    | 1:A:625:MET:N    | 2.36                     | 0.59              |
| 1:A:762:ALA:HA   | 1:A:828:LEU:HD11 | 1.84                     | 0.59              |
| 1:A:559:PHE:CD1  | 1:A:559:PHE:N    | 2.61                     | 0.59              |
| 1:A:742:ASN:C    | 1:A:744:PHE:N    | 2.61                     | 0.59              |
| 1:A:677:CYS:C    | 1:A:678:HIS:CG   | 2.80                     | 0.59              |
| 1:B:551:ALA:HB2  | 1:B:581:ASP:OD1  | 2.03                     | 0.59              |
| 1:A:813:ILE:HG12 | 1:A:814:PRO:HD3  | 1.84                     | 0.59              |
| 1:A:624:CYS:O    | 1:A:624:CYS:SG   | 2.61                     | 0.58              |
| 1:A:684:HIS:O    | 1:A:688:GLN:HB2  | 2.02                     | 0.58              |
| 1:B:578:MET:O    | 1:B:582:LEU:HB2  | 2.03                     | 0.58              |
| 1:A:559:PHE:HD2  | 1:A:842:LEU:HG   | 1.69                     | 0.58              |
| 1:B:636:ASN:HD21 | 1:B:637:LYS:HG3  | 1.67                     | 0.58              |
| 1:B:775:GLN:HG3  | 1:B:776:GLN:N    | 2.18                     | 0.58              |
| 1:A:607:ARG:HH21 | 1:A:658:ARG:HH21 | 1.48                     | 0.58              |
| 1:A:857:ALA:C    | 1:A:859:GLN:H    | 2.11                     | 0.58              |
| 1:A:709:TYR:HE2  | 1:A:713:LEU:HD11 | 1.66                     | 0.58              |
| 1:A:847:ARG:O    | 1:A:851:GLN:HG3  | 2.03                     | 0.58              |
| 1:A:644:LEU:HG   | 1:A:648:ILE:HD12 | 1.86                     | 0.58              |
| 1:B:615:TRP:O    | 1:B:615:TRP:CE3  | 2.57                     | 0.58              |
| 1:B:540:LEU:CD2  | 1:B:597:ARG:HE   | 2.16                     | 0.58              |
| 1:B:559:PHE:CD2  | 1:B:842:LEU:HG   | 2.39                     | 0.58              |
| 1:B:590:MET:HE1  | 1:B:644:LEU:CD1  | 2.34                     | 0.58              |
| 1:B:622:ALA:O    | 1:B:625:MET:HB3  | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:679:SER:C    | 1:B:682:GLU:HG2  | 2.29                     | 0.57              |
| 1:B:630:LYS:HD3  | 1:B:635:GLN:NE2  | 2.19                     | 0.57              |
| 1:B:759:LEU:HD12 | 1:B:759:LEU:C    | 2.28                     | 0.57              |
| 1:A:570:GLU:C    | 1:A:572:ALA:H    | 2.11                     | 0.57              |
| 1:A:661:ASN:C    | 1:A:662:ASN:ND2  | 2.60                     | 0.57              |
| 1:A:741:LYS:C    | 1:A:743:GLN:H    | 2.12                     | 0.57              |
| 1:B:814:PRO:O    | 1:B:817:GLN:N    | 2.35                     | 0.57              |
| 1:A:582:LEU:O    | 1:A:583:ASN:HB2  | 2.03                     | 0.57              |
| 1:A:634:ILE:HD13 | 1:A:836:SER:HB2  | 1.86                     | 0.57              |
| 1:B:677:CYS:C    | 1:B:678:HIS:CG   | 2.80                     | 0.57              |
| 1:B:767:ALA:HA   | 1:B:770:LYS:HG3  | 1.85                     | 0.57              |
| 1:A:547:VAL:O    | 1:A:549:PRO:HD3  | 2.05                     | 0.57              |
| 1:A:557:THR:HG22 | 1:A:557:THR:O    | 2.04                     | 0.57              |
| 1:A:801:PRO:HB2  | 1:A:806:ASN:CB   | 2.22                     | 0.57              |
| 1:B:654:ASP:HA   | 1:B:685:HIS:CE1  | 2.40                     | 0.57              |
| 1:B:584:LEU:HD12 | 1:B:647:LEU:CD1  | 2.35                     | 0.57              |
| 1:B:769:THR:HG22 | 1:B:846:CYS:HB2  | 1.86                     | 0.57              |
| 1:A:750:HIS:O    | 1:A:753:GLU:HB2  | 2.05                     | 0.57              |
| 1:A:843:LEU:HD12 | 1:A:843:LEU:O    | 2.03                     | 0.57              |
| 1:B:705:SER:H    | 1:B:708:GLU:HB2  | 1.70                     | 0.57              |
| 1:A:623:GLN:O    | 1:A:626:PHE:N    | 2.37                     | 0.57              |
| 1:A:787:PHE:CB   | 1:A:807:ARG:HH11 | 2.17                     | 0.57              |
| 1:A:830:GLU:O    | 1:A:833:THR:HB   | 2.05                     | 0.57              |
| 1:A:679:SER:C    | 1:A:682:GLU:HG2  | 2.29                     | 0.57              |
| 1:A:559:PHE:CD2  | 1:A:842:LEU:HG   | 2.40                     | 0.56              |
| 1:A:632:GLY:CA   | 1:A:838:ASP:HB3  | 2.35                     | 0.56              |
| 1:B:537:THR:C    | 1:B:539:GLU:H    | 2.13                     | 0.56              |
| 1:A:843:LEU:HD11 | 1:A:847:ARG:NE   | 2.20                     | 0.56              |
| 1:B:656:ASP:H    | 1:B:685:HIS:HD2  | 1.53                     | 0.56              |
| 1:B:720:ILE:O    | 1:B:723:THR:HG23 | 2.06                     | 0.56              |
| 1:B:735:PHE:CE2  | 1:B:758:MET:HG2  | 2.40                     | 0.56              |
| 1:B:847:ARG:O    | 1:B:851:GLN:HG3  | 2.05                     | 0.56              |
| 1:A:725:LEU:O    | 1:A:729:ILE:CG1  | 2.49                     | 0.56              |
| 1:A:833:THR:HG22 | 1:A:834:HIS:N    | 2.21                     | 0.56              |
| 1:B:818:VAL:HG12 | 1:B:819:GLY:N    | 2.21                     | 0.56              |
| 1:A:705:SER:H    | 1:A:708:GLU:CG   | 2.19                     | 0.56              |
| 1:B:770:LYS:HZ1  | 1:B:774:ILE:HG21 | 1.69                     | 0.56              |
| 1:A:727:LEU:O    | 1:A:731:ARG:HG3  | 2.04                     | 0.56              |
| 1:A:767:ALA:HA   | 1:A:770:LYS:HG2  | 1.85                     | 0.56              |
| 1:B:559:PHE:CE2  | 1:B:841:PRO:HB2  | 2.41                     | 0.56              |
| 1:A:770:LYS:HZ1  | 1:A:774:ILE:HG21 | 1.68                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:562:SER:HG   | 1:A:777:ARG:HH22 | 1.51                     | 0.56              |
| 1:A:625:MET:HE2  | 1:A:763:CYS:SG   | 2.46                     | 0.56              |
| 1:B:609:ASN:N    | 1:B:609:ASN:ND2  | 2.52                     | 0.56              |
| 1:A:540:LEU:CD2  | 1:A:597:ARG:HE   | 2.19                     | 0.56              |
| 1:A:787:PHE:CB   | 1:A:807:ARG:NH1  | 2.68                     | 0.56              |
| 1:A:796:GLU:CB   | 1:B:717:LYS:HZ3  | 2.19                     | 0.56              |
| 1:B:830:GLU:HG3  | 1:B:831:ALA:H    | 1.70                     | 0.56              |
| 1:A:839:CYS:C    | 1:A:841:PRO:HD2  | 2.31                     | 0.56              |
| 1:B:692:ILE:O    | 1:B:694:ASN:N    | 2.38                     | 0.56              |
| 1:B:758:MET:HG3  | 1:B:828:LEU:HD23 | 1.88                     | 0.56              |
| 1:B:810:LYS:HA   | 1:B:813:ILE:HG23 | 1.88                     | 0.56              |
| 1:B:539:GLU:HG2  | 1:B:600:LEU:HD11 | 1.87                     | 0.55              |
| 1:B:588:PHE:CD2  | 1:B:704:LEU:HD21 | 2.40                     | 0.55              |
| 1:B:734:GLU:O    | 1:B:736:PHE:N    | 2.39                     | 0.55              |
| 1:B:742:ASN:O    | 1:B:744:PHE:N    | 2.39                     | 0.55              |
| 1:A:639:THR:HG1  | 1:A:642:GLU:HG3  | 1.71                     | 0.55              |
| 1:A:820:PHE:CE1  | 1:A:824:ILE:HD12 | 2.41                     | 0.55              |
| 1:A:609:ASN:N    | 1:A:609:ASN:HD22 | 2.05                     | 0.55              |
| 1:A:636:ASN:ND2  | 1:A:636:ASN:C    | 2.62                     | 0.55              |
| 1:A:742:ASN:O    | 1:A:744:PHE:N    | 2.39                     | 0.55              |
| 1:A:763:CYS:O    | 1:A:766:SER:HB3  | 2.06                     | 0.55              |
| 1:A:771:PRO:O    | 1:A:773:PRO:N    | 2.38                     | 0.55              |
| 1:B:628:ALA:O    | 1:B:634:ILE:HB   | 2.06                     | 0.55              |
| 1:A:712:THR:HA   | 1:A:715:ILE:HD12 | 1.87                     | 0.55              |
| 1:A:588:PHE:O    | 1:A:589:GLN:C    | 2.49                     | 0.55              |
| 1:A:642:GLU:CD   | 1:A:752:LYS:HZ3  | 2.15                     | 0.55              |
| 1:A:717:LYS:HZ3  | 1:B:796:GLU:CB   | 2.20                     | 0.55              |
| 1:A:802:THR:O    | 1:A:804:LEU:N    | 2.38                     | 0.55              |
| 1:B:679:SER:O    | 1:B:683:HIS:ND1  | 2.37                     | 0.55              |
| 1:B:559:PHE:HD2  | 1:B:842:LEU:HG   | 1.72                     | 0.55              |
| 1:A:584:LEU:HD12 | 1:A:647:LEU:CD1  | 2.37                     | 0.54              |
| 1:A:601:SER:O    | 1:A:602:VAL:C    | 2.50                     | 0.54              |
| 1:A:840:PHE:N    | 1:A:841:PRO:CD   | 2.70                     | 0.54              |
| 1:B:609:ASN:N    | 1:B:609:ASN:HD22 | 2.04                     | 0.54              |
| 1:A:571:THR:O    | 1:A:619:PHE:CE1  | 2.60                     | 0.54              |
| 1:A:808:GLU:C    | 1:A:810:LYS:H    | 2.15                     | 0.54              |
| 1:A:832:LEU:O    | 1:A:833:THR:C    | 2.50                     | 0.54              |
| 1:B:802:THR:O    | 1:B:804:LEU:N    | 2.40                     | 0.54              |
| 1:A:801:PRO:CB   | 1:A:806:ASN:HB3  | 2.24                     | 0.54              |
| 1:B:582:LEU:HD11 | 1:B:626:PHE:HD1  | 1.72                     | 0.54              |
| 1:B:724:ASP:O    | 1:B:726:ALA:N    | 2.41                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:701:LEU:HD23 | 1:A:704:LEU:CD1  | 2.37                     | 0.54              |
| 1:A:775:GLN:HG3  | 1:A:776:GLN:N    | 2.21                     | 0.54              |
| 1:B:727:LEU:HG   | 1:B:731:ARG:HD2  | 1.90                     | 0.54              |
| 1:B:731:ARG:O    | 1:B:732:ARG:C    | 2.50                     | 0.54              |
| 1:B:742:ASN:C    | 1:B:744:PHE:N    | 2.65                     | 0.54              |
| 1:A:695:SER:CB   | 1:A:698:ASN:HD22 | 2.21                     | 0.54              |
| 1:A:735:PHE:CB   | 1:A:754:LEU:HD23 | 2.30                     | 0.54              |
| 1:A:765:LEU:CD1  | 1:A:765:LEU:H    | 2.21                     | 0.54              |
| 1:B:797:LEU:H    | 1:B:797:LEU:CD2  | 2.02                     | 0.54              |
| 1:A:584:LEU:HD13 | 1:A:644:LEU:CD1  | 2.37                     | 0.54              |
| 1:A:598:TRP:HA   | 1:A:698:ASN:HB3  | 1.89                     | 0.54              |
| 1:A:609:ASN:N    | 1:A:609:ASN:ND2  | 2.52                     | 0.54              |
| 1:A:737:GLU:C    | 1:A:739:ILE:H    | 2.15                     | 0.54              |
| 1:A:759:LEU:O    | 1:A:762:ALA:HB3  | 2.08                     | 0.54              |
| 1:B:762:ALA:HA   | 1:B:828:LEU:CD1  | 2.38                     | 0.54              |
| 1:A:551:ALA:HB2  | 1:A:581:ASP:OD1  | 2.08                     | 0.54              |
| 1:A:574:CYS:O    | 1:A:577:ARG:HB3  | 2.08                     | 0.54              |
| 1:A:765:LEU:CD1  | 1:A:765:LEU:N    | 2.71                     | 0.54              |
| 1:B:607:ARG:NE   | 1:B:658:ARG:HE   | 2.06                     | 0.54              |
| 1:A:603:LYS:O    | 1:A:606:TYR:HB2  | 2.09                     | 0.53              |
| 1:A:737:GLU:C    | 1:A:739:ILE:N    | 2.64                     | 0.53              |
| 1:A:611:ALA:O    | 1:A:781:LEU:HB3  | 2.08                     | 0.53              |
| 1:A:705:SER:H    | 1:A:708:GLU:HB2  | 1.73                     | 0.53              |
| 1:A:808:GLU:C    | 1:A:810:LYS:N    | 2.66                     | 0.53              |
| 1:B:720:ILE:C    | 1:B:722:ALA:H    | 2.16                     | 0.53              |
| 1:B:810:LYS:O    | 1:B:813:ILE:HG12 | 2.08                     | 0.53              |
| 1:A:568:ASP:O    | 1:A:569:LEU:C    | 2.51                     | 0.53              |
| 1:A:709:TYR:O    | 1:A:713:LEU:HG   | 2.09                     | 0.53              |
| 1:A:758:MET:HG3  | 1:A:828:LEU:HD23 | 1.90                     | 0.53              |
| 1:A:827:GLN:HA   | 1:A:830:GLU:HG2  | 1.90                     | 0.53              |
| 1:A:717:LYS:HE2  | 1:A:721:LEU:HD11 | 1.90                     | 0.53              |
| 1:A:737:GLU:O    | 1:A:741:LYS:HB2  | 2.08                     | 0.53              |
| 1:B:686:PHE:HA   | 1:B:689:CYS:HB2  | 1.89                     | 0.53              |
| 1:B:574:CYS:O    | 1:B:577:ARG:N    | 2.42                     | 0.53              |
| 1:B:812:LYS:O    | 1:B:816:MET:HG3  | 2.08                     | 0.53              |
| 1:B:832:LEU:O    | 1:B:833:THR:C    | 2.51                     | 0.53              |
| 1:B:563:ASP:HB2  | 1:B:616:ARG:NH1  | 2.22                     | 0.53              |
| 1:B:646:LEU:N    | 1:B:646:LEU:CD2  | 2.71                     | 0.53              |
| 1:A:642:GLU:OE1  | 1:A:752:LYS:NZ   | 2.41                     | 0.53              |
| 1:A:725:LEU:H    | 1:A:725:LEU:CD1  | 2.22                     | 0.53              |
| 1:A:704:LEU:HB3  | 1:A:708:GLU:CB   | 2.39                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:740:ARG:HG3  | 1:B:740:ARG:HH11 | 1.73                     | 0.53              |
| 1:B:840:PHE:N    | 1:B:841:PRO:CD   | 2.71                     | 0.53              |
| 1:A:657:HIS:O    | 1:A:658:ARG:HD3  | 2.09                     | 0.52              |
| 1:B:813:ILE:HG13 | 1:B:814:PRO:HD3  | 1.90                     | 0.52              |
| 1:B:854:GLN:HA   | 1:B:854:GLN:OE1  | 2.09                     | 0.52              |
| 1:A:728:TYR:OH   | 1:A:828:LEU:HB2  | 2.09                     | 0.52              |
| 1:B:646:LEU:N    | 1:B:646:LEU:HD22 | 2.23                     | 0.52              |
| 1:B:732:ARG:HG3  | 1:B:733:GLY:N    | 2.24                     | 0.52              |
| 1:B:737:GLU:C    | 1:B:739:ILE:N    | 2.62                     | 0.52              |
| 1:A:752:LYS:O    | 1:A:756:LEU:HB2  | 2.10                     | 0.52              |
| 1:A:797:LEU:HD22 | 1:A:797:LEU:N    | 2.16                     | 0.52              |
| 1:B:704:LEU:HB3  | 1:B:708:GLU:CB   | 2.40                     | 0.52              |
| 1:A:657:HIS:CE1  | 1:A:681:MET:HE3  | 2.44                     | 0.52              |
| 1:B:639:THR:HG23 | 1:B:642:GLU:OE1  | 2.09                     | 0.52              |
| 1:B:815:SER:HA   | 1:B:818:VAL:HB   | 1.92                     | 0.52              |
| 1:A:598:TRP:O    | 1:A:599:ILE:C    | 2.53                     | 0.52              |
| 1:A:621:THR:HG23 | 1:A:763:CYS:C    | 2.34                     | 0.52              |
| 1:A:622:ALA:O    | 1:A:625:MET:HB3  | 2.10                     | 0.52              |
| 1:A:731:ARG:O    | 1:A:732:ARG:C    | 2.52                     | 0.52              |
| 1:A:810:LYS:HA   | 1:A:813:ILE:HG23 | 1.92                     | 0.52              |
| 1:B:705:SER:H    | 1:B:708:GLU:CG   | 2.23                     | 0.52              |
| 1:A:717:LYS:NZ   | 1:B:796:GLU:HG2  | 2.25                     | 0.52              |
| 1:B:557:THR:HG22 | 1:B:557:THR:O    | 2.10                     | 0.52              |
| 1:B:793:GLU:HA   | 1:B:797:LEU:CD2  | 2.32                     | 0.52              |
| 1:A:549:PRO:HB2  | 1:A:554:LEU:CG   | 2.39                     | 0.52              |
| 1:A:580:THR:C    | 1:A:582:LEU:H    | 2.18                     | 0.52              |
| 1:B:657:HIS:O    | 1:B:658:ARG:HD3  | 2.09                     | 0.52              |
| 1:A:582:LEU:HG   | 1:A:626:PHE:CE1  | 2.45                     | 0.52              |
| 1:A:740:ARG:HG3  | 1:A:740:ARG:HH11 | 1.74                     | 0.52              |
| 1:B:741:LYS:C    | 1:B:743:GLN:H    | 2.18                     | 0.52              |
| 1:B:648:ILE:CD1  | 1:B:700:ILE:HD11 | 2.40                     | 0.52              |
| 1:B:639:THR:HG1  | 1:B:642:GLU:HG3  | 1.76                     | 0.51              |
| 1:A:570:GLU:C    | 1:A:572:ALA:N    | 2.68                     | 0.51              |
| 1:A:717:LYS:HG2  | 1:A:721:LEU:CD1  | 2.38                     | 0.51              |
| 1:A:757:ALA:O    | 1:A:760:MET:N    | 2.43                     | 0.51              |
| 1:B:571:THR:HG22 | 1:B:619:PHE:CE2  | 2.46                     | 0.51              |
| 1:B:623:GLN:O    | 1:B:626:PHE:N    | 2.43                     | 0.51              |
| 1:B:737:GLU:C    | 1:B:739:ILE:H    | 2.18                     | 0.51              |
| 1:A:564:PHE:CE1  | 1:A:777:ARG:HD3  | 2.46                     | 0.51              |
| 1:B:630:LYS:C    | 1:B:632:GLY:N    | 2.67                     | 0.51              |
| 1:B:715:ILE:O    | 1:B:719:ALA:HB2  | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:813:ILE:N    | 1:B:814:PRO:CD   | 2.74                     | 0.51              |
| 1:B:830:GLU:HG3  | 1:B:831:ALA:N    | 2.26                     | 0.51              |
| 1:A:720:ILE:C    | 1:A:722:ALA:H    | 2.19                     | 0.51              |
| 1:B:663:SER:HG   | 1:B:664:TYR:HD1  | 1.58                     | 0.51              |
| 1:B:548:VAL:HG23 | 1:B:548:VAL:O    | 2.09                     | 0.51              |
| 1:B:607:ARG:HG2  | 1:B:607:ARG:HH11 | 1.75                     | 0.51              |
| 1:B:611:ALA:O    | 1:B:781:LEU:HB3  | 2.10                     | 0.51              |
| 1:B:653:HIS:CA   | 1:B:720:ILE:HG23 | 2.19                     | 0.51              |
| 1:B:737:GLU:O    | 1:B:741:LYS:HG3  | 2.11                     | 0.51              |
| 1:A:537:THR:C    | 1:A:539:GLU:H    | 2.17                     | 0.51              |
| 1:A:806:ASN:OD1  | 1:A:809:LYS:HB2  | 2.10                     | 0.51              |
| 1:B:568:ASP:O    | 1:B:569:LEU:C    | 2.53                     | 0.51              |
| 1:A:623:GLN:C    | 1:A:625:MET:N    | 2.68                     | 0.51              |
| 1:B:547:VAL:O    | 1:B:549:PRO:HD3  | 2.11                     | 0.51              |
| 1:B:649:ALA:O    | 1:B:652:SER:N    | 2.44                     | 0.51              |
| 1:B:715:ILE:O    | 1:B:719:ALA:CB   | 2.59                     | 0.51              |
| 1:A:569:LEU:O    | 1:A:572:ALA:HB3  | 2.11                     | 0.50              |
| 1:B:578:MET:HA   | 1:B:626:PHE:CE1  | 2.45                     | 0.50              |
| 1:B:830:GLU:CG   | 1:B:831:ALA:N    | 2.73                     | 0.50              |
| 1:B:604:LYS:HB2  | 1:B:604:LYS:HZ2  | 1.75                     | 0.50              |
| 1:A:583:ASN:HB3  | 1:A:587:ASN:ND2  | 2.27                     | 0.50              |
| 1:A:585:VAL:HG13 | 1:A:590:MET:HB2  | 1.93                     | 0.50              |
| 1:A:814:PRO:O    | 1:A:817:GLN:N    | 2.42                     | 0.50              |
| 1:B:696:PRO:HA   | 1:B:699:GLN:NE2  | 2.25                     | 0.50              |
| 1:A:574:CYS:O    | 1:A:577:ARG:N    | 2.44                     | 0.50              |
| 1:B:695:SER:CB   | 1:B:698:ASN:HD22 | 2.23                     | 0.50              |
| 1:B:720:ILE:O    | 1:B:722:ALA:N    | 2.45                     | 0.50              |
| 1:A:690:LEU:O    | 1:A:691:MET:C    | 2.55                     | 0.50              |
| 1:A:714:LYS:O    | 1:A:718:GLN:HB2  | 2.12                     | 0.50              |
| 1:B:818:VAL:HG23 | 1:B:853:TRP:HB3  | 1.93                     | 0.50              |
| 1:A:582:LEU:CD1  | 1:A:626:PHE:HD1  | 2.25                     | 0.50              |
| 1:B:770:LYS:O    | 1:B:775:GLN:HB3  | 2.12                     | 0.50              |
| 1:A:717:LYS:O    | 1:A:721:LEU:HG   | 2.12                     | 0.50              |
| 1:B:563:ASP:HB3  | 1:B:620:ASN:ND2  | 2.23                     | 0.50              |
| 1:B:621:THR:HG23 | 1:B:763:CYS:O    | 2.10                     | 0.50              |
| 1:A:548:VAL:HG23 | 1:A:548:VAL:O    | 2.11                     | 0.50              |
| 1:B:709:TYR:HE2  | 1:B:713:LEU:HD11 | 1.76                     | 0.50              |
| 1:B:771:PRO:O    | 1:B:772:TRP:C    | 2.55                     | 0.50              |
| 1:B:820:PHE:CZ   | 4:B:2003:CIA:H11 | 2.47                     | 0.50              |
| 1:A:813:ILE:N    | 1:A:814:PRO:CD   | 2.76                     | 0.49              |
| 1:B:559:PHE:HD2  | 1:B:842:LEU:CD2  | 2.24                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:661:ASN:C    | 1:B:662:ASN:ND2  | 2.69                     | 0.49              |
| 1:B:828:LEU:HD22 | 1:B:828:LEU:C    | 2.37                     | 0.49              |
| 1:A:815:SER:HA   | 1:A:818:VAL:HB   | 1.94                     | 0.49              |
| 1:B:735:PHE:CB   | 1:B:754:LEU:HD23 | 2.34                     | 0.49              |
| 1:B:541:GLN:O    | 1:B:544:ALA:HB3  | 2.12                     | 0.49              |
| 1:A:705:SER:HB2  | 1:A:708:GLU:CG   | 2.41                     | 0.49              |
| 1:A:854:GLN:OE1  | 1:A:854:GLN:HA   | 2.12                     | 0.49              |
| 1:B:607:ARG:HG2  | 1:B:607:ARG:NH1  | 2.27                     | 0.49              |
| 1:B:623:GLN:O    | 1:B:625:MET:N    | 2.45                     | 0.49              |
| 1:A:548:VAL:HG11 | 1:A:576:ILE:CG2  | 2.42                     | 0.49              |
| 1:A:793:GLU:HA   | 1:A:797:LEU:CD2  | 2.37                     | 0.49              |
| 1:B:757:ALA:O    | 1:B:760:MET:N    | 2.45                     | 0.49              |
| 1:A:635:GLN:C    | 1:A:637:LYS:H    | 2.20                     | 0.49              |
| 1:B:537:THR:C    | 1:B:539:GLU:N    | 2.70                     | 0.49              |
| 1:B:634:ILE:HD13 | 1:B:836:SER:HB2  | 1.93                     | 0.49              |
| 1:A:584:LEU:HD13 | 1:A:644:LEU:HD12 | 1.94                     | 0.49              |
| 1:A:765:LEU:HD13 | 1:A:765:LEU:H    | 1.77                     | 0.49              |
| 1:B:750:HIS:CD2  | 1:B:754:LEU:HD13 | 2.48                     | 0.49              |
| 1:B:757:ALA:C    | 1:B:759:LEU:N    | 2.70                     | 0.49              |
| 1:A:644:LEU:HG   | 1:A:648:ILE:CD1  | 2.42                     | 0.49              |
| 1:B:632:GLY:O    | 1:B:836:SER:OG   | 2.18                     | 0.49              |
| 1:B:727:LEU:HD23 | 1:B:728:TYR:H    | 1.75                     | 0.49              |
| 1:B:687:ASP:O    | 1:B:691:MET:HB2  | 2.13                     | 0.49              |
| 1:B:808:GLU:CG   | 1:B:809:LYS:H    | 2.10                     | 0.49              |
| 1:A:583:ASN:HB3  | 1:A:587:ASN:HD21 | 1.77                     | 0.49              |
| 1:A:630:LYS:C    | 1:A:632:GLY:N    | 2.67                     | 0.49              |
| 1:A:732:ARG:HG3  | 1:A:733:GLY:N    | 2.28                     | 0.49              |
| 1:B:588:PHE:O    | 1:B:589:GLN:C    | 2.55                     | 0.49              |
| 1:B:653:HIS:HD2  | 1:B:764:ASP:OD2  | 1.96                     | 0.49              |
| 1:A:719:ALA:HB1  | 1:A:760:MET:HE3  | 1.95                     | 0.48              |
| 1:A:765:LEU:N    | 1:A:765:LEU:HD12 | 2.28                     | 0.48              |
| 1:B:679:SER:CA   | 1:B:682:GLU:HG2  | 2.42                     | 0.48              |
| 1:B:745:ASN:HD22 | 1:B:748:ASP:HB2  | 1.75                     | 0.48              |
| 1:B:767:ALA:HA   | 1:B:770:LYS:HG2  | 1.93                     | 0.48              |
| 1:B:717:LYS:HG2  | 1:B:721:LEU:CD1  | 2.43                     | 0.48              |
| 1:A:607:ARG:CZ   | 1:A:658:ARG:HE   | 2.25                     | 0.48              |
| 1:A:656:ASP:H    | 1:A:685:HIS:HD2  | 1.59                     | 0.48              |
| 1:A:808:GLU:O    | 1:A:810:LYS:N    | 2.46                     | 0.48              |
| 1:B:570:GLU:C    | 1:B:572:ALA:N    | 2.67                     | 0.48              |
| 1:B:736:PHE:O    | 1:B:737:GLU:OE1  | 2.31                     | 0.48              |
| 1:B:623:GLN:C    | 1:B:625:MET:N    | 2.70                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:705:SER:H    | 1:A:708:GLU:HG3   | 1.77                     | 0.48              |
| 1:A:610:VAL:HG11 | 1:A:613:HIS:HB2   | 1.95                     | 0.48              |
| 1:A:770:LYS:HZ3  | 1:A:774:ILE:CG2   | 2.25                     | 0.48              |
| 1:B:586:GLN:HE21 | 1:B:586:GLN:CA    | 2.16                     | 0.48              |
| 1:B:735:PHE:O    | 1:B:735:PHE:CD2   | 2.67                     | 0.48              |
| 1:A:656:ASP:H    | 1:A:685:HIS:CD2   | 2.32                     | 0.48              |
| 1:A:771:PRO:O    | 1:A:772:TRP:C     | 2.56                     | 0.48              |
| 1:B:813:ILE:HG12 | 1:B:814:PRO:HD3   | 1.96                     | 0.48              |
| 1:A:783:ALA:HA   | 4:A:1003:CIA:H291 | 1.95                     | 0.48              |
| 1:B:549:PRO:HB2  | 1:B:554:LEU:CG    | 2.42                     | 0.48              |
| 1:B:715:ILE:O    | 1:B:719:ALA:N     | 2.46                     | 0.48              |
| 1:B:857:ALA:C    | 1:B:859:GLN:H     | 2.21                     | 0.48              |
| 1:A:582:LEU:HD11 | 1:A:626:PHE:CD1   | 2.48                     | 0.47              |
| 1:A:808:GLU:CG   | 1:A:809:LYS:H     | 2.03                     | 0.47              |
| 1:B:539:GLU:HG2  | 1:B:600:LEU:CD1   | 2.43                     | 0.47              |
| 1:B:705:SER:H    | 1:B:708:GLU:HG3   | 1.79                     | 0.47              |
| 1:B:772:TRP:HB3  | 1:B:773:PRO:HD3   | 1.96                     | 0.47              |
| 1:B:717:LYS:HE2  | 1:B:721:LEU:CD1   | 2.43                     | 0.47              |
| 1:A:717:LYS:HZ3  | 1:B:796:GLU:CG    | 2.28                     | 0.47              |
| 1:B:584:LEU:HD12 | 1:B:647:LEU:HD13  | 1.96                     | 0.47              |
| 1:B:607:ARG:CZ   | 1:B:658:ARG:HE    | 2.26                     | 0.47              |
| 1:B:729:ILE:C    | 1:B:731:ARG:H     | 2.22                     | 0.47              |
| 1:A:705:SER:H    | 1:A:708:GLU:CB    | 2.27                     | 0.47              |
| 1:B:808:GLU:C    | 1:B:810:LYS:H     | 2.21                     | 0.47              |
| 1:B:820:PHE:CD1  | 1:B:824:ILE:HD12  | 2.49                     | 0.47              |
| 1:B:709:TYR:O    | 1:B:713:LEU:HG    | 2.14                     | 0.47              |
| 1:B:749:PRO:O    | 1:B:752:LYS:N     | 2.47                     | 0.47              |
| 1:B:756:LEU:HD23 | 1:B:759:LEU:HD23  | 1.97                     | 0.47              |
| 1:B:808:GLU:C    | 1:B:810:LYS:N     | 2.73                     | 0.47              |
| 1:A:646:LEU:O    | 1:A:650:ALA:CB    | 2.62                     | 0.47              |
| 1:A:816:MET:HB2  | 4:A:1003:CIA:H26  | 1.94                     | 0.47              |
| 1:A:825:CYS:O    | 1:A:826:LEU:C     | 2.57                     | 0.47              |
| 1:B:717:LYS:O    | 1:B:718:GLN:C     | 2.54                     | 0.47              |
| 1:A:612:TYR:OH   | 4:A:1003:CIA:H2   | 2.14                     | 0.47              |
| 1:A:719:ALA:HB1  | 1:A:760:MET:CE    | 2.45                     | 0.47              |
| 1:A:736:PHE:O    | 1:A:737:GLU:OE1   | 2.33                     | 0.47              |
| 1:A:797:LEU:HD13 | 1:B:718:GLN:NE2   | 2.30                     | 0.47              |
| 1:B:543:LEU:HD22 | 1:B:576:ILE:HD11  | 1.96                     | 0.47              |
| 1:B:645:ALA:O    | 1:B:649:ALA:CB    | 2.62                     | 0.47              |
| 1:B:849:ASN:C    | 1:B:851:GLN:H     | 2.23                     | 0.47              |
| 1:A:679:SER:CA   | 1:A:682:GLU:HG2   | 2.45                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:561:PHE:CD2  | 1:A:623:GLN:HG3  | 2.50                     | 0.47              |
| 1:A:629:LEU:HG   | 1:A:635:GLN:HB2  | 1.96                     | 0.47              |
| 1:A:757:ALA:C    | 1:A:759:LEU:N    | 2.72                     | 0.47              |
| 1:B:641:LEU:O    | 1:B:644:LEU:N    | 2.47                     | 0.47              |
| 1:B:646:LEU:O    | 1:B:650:ALA:HB3  | 2.15                     | 0.47              |
| 1:B:728:TYR:OH   | 1:B:828:LEU:HB2  | 2.15                     | 0.47              |
| 1:A:623:GLN:C    | 1:A:625:MET:H    | 2.23                     | 0.47              |
| 1:A:797:LEU:HD11 | 1:B:717:LYS:NZ   | 2.30                     | 0.47              |
| 1:B:656:ASP:HB3  | 1:B:684:HIS:NE2  | 2.30                     | 0.47              |
| 1:B:717:LYS:CE   | 1:B:721:LEU:HD11 | 2.45                     | 0.47              |
| 1:A:849:ASN:C    | 1:A:851:GLN:H    | 2.23                     | 0.46              |
| 1:B:690:LEU:O    | 1:B:691:MET:C    | 2.58                     | 0.46              |
| 1:B:705:SER:H    | 1:B:708:GLU:CB   | 2.28                     | 0.46              |
| 1:B:788:ASP:OD1  | 1:B:807:ARG:NH1  | 2.48                     | 0.46              |
| 1:A:654:ASP:HA   | 1:A:685:HIS:ND1  | 2.31                     | 0.46              |
| 1:A:663:SER:HG   | 1:A:664:TYR:HD1  | 1.56                     | 0.46              |
| 1:B:692:ILE:HA   | 1:B:695:SER:OG   | 2.14                     | 0.46              |
| 1:A:793:GLU:CA   | 1:A:797:LEU:HD23 | 2.41                     | 0.46              |
| 1:B:789:GLN:NE2  | 1:B:805:MET:SD   | 2.88                     | 0.46              |
| 1:B:830:GLU:O    | 1:B:831:ALA:C    | 2.56                     | 0.46              |
| 1:A:732:ARG:HH12 | 1:A:824:ILE:HA   | 1.79                     | 0.46              |
| 1:A:812:LYS:O    | 1:A:816:MET:HG3  | 2.15                     | 0.46              |
| 1:B:568:ASP:O    | 1:B:571:THR:N    | 2.48                     | 0.46              |
| 1:B:632:GLY:HA2  | 1:B:838:ASP:O    | 2.15                     | 0.46              |
| 1:B:750:HIS:NE2  | 1:B:754:LEU:HD13 | 2.30                     | 0.46              |
| 1:B:772:TRP:CZ2  | 1:B:852:LYS:HB3  | 2.50                     | 0.46              |
| 1:B:774:ILE:HG23 | 1:B:777:ARG:NH2  | 2.30                     | 0.46              |
| 1:B:656:ASP:H    | 1:B:685:HIS:CD2  | 2.32                     | 0.46              |
| 1:A:564:PHE:HB2  | 1:A:777:ARG:NH2  | 2.31                     | 0.46              |
| 1:A:771:PRO:C    | 1:A:773:PRO:CD   | 2.89                     | 0.46              |
| 1:B:540:LEU:HD21 | 1:B:597:ARG:HB2  | 1.97                     | 0.46              |
| 1:B:639:THR:HG23 | 1:B:642:GLU:CD   | 2.39                     | 0.46              |
| 1:A:577:ARG:NH1  | 1:A:581:ASP:OD2  | 2.44                     | 0.46              |
| 1:A:605:ASN:O    | 1:A:605:ASN:ND2  | 2.49                     | 0.46              |
| 1:A:735:PHE:CD2  | 1:A:758:MET:HG2  | 2.51                     | 0.46              |
| 1:A:820:PHE:CE1  | 4:A:1003:CIA:H11 | 2.51                     | 0.46              |
| 1:B:591:LYS:O    | 1:B:592:HIS:C    | 2.57                     | 0.46              |
| 1:A:590:MET:HE1  | 1:A:644:LEU:HD11 | 1.97                     | 0.46              |
| 1:A:685:HIS:O    | 1:A:689:CYS:N    | 2.48                     | 0.46              |
| 1:B:653:HIS:NE2  | 1:B:654:ASP:OD2  | 2.48                     | 0.46              |
| 1:B:732:ARG:HB3  | 1:B:758:MET:SD   | 2.56                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:639:THR:O    | 1:A:643:ILE:HD12 | 2.16                     | 0.46              |
| 1:B:604:LYS:NZ   | 1:B:604:LYS:CB   | 2.74                     | 0.46              |
| 1:B:786:PHE:HD1  | 1:B:804:LEU:HG   | 1.80                     | 0.46              |
| 1:B:826:LEU:CD2  | 1:B:827:GLN:N    | 2.77                     | 0.46              |
| 1:A:537:THR:C    | 1:A:539:GLU:N    | 2.73                     | 0.45              |
| 1:A:603:LYS:O    | 1:A:604:LYS:C    | 2.59                     | 0.45              |
| 1:A:695:SER:O    | 1:A:699:GLN:CG   | 2.64                     | 0.45              |
| 1:B:765:LEU:N    | 1:B:765:LEU:CD1  | 2.78                     | 0.45              |
| 1:B:549:PRO:CG   | 1:B:554:LEU:HD21 | 2.42                     | 0.45              |
| 1:A:563:ASP:HB3  | 1:A:620:ASN:ND2  | 2.31                     | 0.45              |
| 1:A:584:LEU:HB3  | 1:A:590:MET:HE3  | 1.98                     | 0.45              |
| 1:A:554:LEU:HB2  | 1:A:556:ILE:HG23 | 1.99                     | 0.45              |
| 1:B:580:THR:C    | 1:B:582:LEU:N    | 2.73                     | 0.45              |
| 1:B:784:THR:O    | 1:B:788:ASP:OD1  | 2.35                     | 0.45              |
| 1:A:603:LYS:O    | 1:A:605:ASN:N    | 2.50                     | 0.45              |
| 1:A:603:LYS:C    | 1:A:605:ASN:N    | 2.74                     | 0.45              |
| 1:A:615:TRP:O    | 1:A:615:TRP:CE3  | 2.69                     | 0.45              |
| 1:A:692:ILE:O    | 1:A:693:LEU:C    | 2.59                     | 0.45              |
| 1:A:701:LEU:HD23 | 1:A:704:LEU:HD11 | 1.98                     | 0.45              |
| 1:A:783:ALA:HA   | 4:A:1003:CIA:C29 | 2.46                     | 0.45              |
| 1:B:839:CYS:C    | 1:B:841:PRO:CD   | 2.88                     | 0.45              |
| 1:A:540:LEU:O    | 1:A:541:GLN:C    | 2.58                     | 0.45              |
| 1:A:612:TYR:C    | 1:A:614:ASN:H    | 2.24                     | 0.45              |
| 1:A:781:LEU:O    | 1:A:784:THR:HB   | 2.17                     | 0.45              |
| 1:A:598:TRP:O    | 1:A:601:SER:N    | 2.50                     | 0.45              |
| 1:A:607:ARG:NE   | 1:A:658:ARG:HE   | 2.15                     | 0.45              |
| 1:A:622:ALA:HB2  | 1:A:651:LEU:CD2  | 2.46                     | 0.45              |
| 1:A:843:LEU:HD11 | 1:A:847:ARG:HE   | 1.82                     | 0.45              |
| 1:A:590:MET:HE1  | 1:A:644:LEU:CD1  | 2.47                     | 0.45              |
| 1:A:715:ILE:O    | 1:A:719:ALA:HB2  | 2.17                     | 0.45              |
| 1:B:540:LEU:O    | 1:B:541:GLN:C    | 2.59                     | 0.45              |
| 1:B:692:ILE:O    | 1:B:693:LEU:C    | 2.60                     | 0.45              |
| 1:B:813:ILE:HG13 | 1:B:814:PRO:CD   | 2.47                     | 0.45              |
| 1:A:701:LEU:HD23 | 1:A:704:LEU:HD12 | 1.99                     | 0.44              |
| 1:A:758:MET:N    | 1:A:758:MET:HE2  | 2.32                     | 0.44              |
| 1:A:727:LEU:HG   | 1:A:731:ARG:HD2  | 1.98                     | 0.44              |
| 1:A:806:ASN:HD21 | 1:A:809:LYS:HD3  | 1.82                     | 0.44              |
| 1:B:595:LEU:O    | 1:B:595:LEU:HD23 | 2.16                     | 0.44              |
| 1:B:627:ALA:C    | 1:B:629:LEU:H    | 2.24                     | 0.44              |
| 1:B:732:ARG:CB   | 1:B:758:MET:SD   | 3.05                     | 0.44              |
| 1:B:786:PHE:CD1  | 1:B:804:LEU:HG   | 2.52                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:548:VAL:HG11 | 1:A:576:ILE:HG21 | 1.98                     | 0.44              |
| 1:B:584:LEU:HD12 | 1:B:647:LEU:HD12 | 1.99                     | 0.44              |
| 1:B:605:ASN:O    | 1:B:605:ASN:ND2  | 2.50                     | 0.44              |
| 1:A:741:LYS:C    | 1:A:743:GLN:N    | 2.75                     | 0.44              |
| 1:A:758:MET:HE2  | 1:A:758:MET:H    | 1.82                     | 0.44              |
| 1:A:797:LEU:H    | 1:A:797:LEU:CD2  | 2.13                     | 0.44              |
| 1:B:686:PHE:O    | 1:B:689:CYS:N    | 2.50                     | 0.44              |
| 1:B:695:SER:O    | 1:B:699:GLN:CG   | 2.65                     | 0.44              |
| 1:B:740:ARG:O    | 1:B:740:ARG:HG2  | 2.17                     | 0.44              |
| 1:A:544:ALA:O    | 1:A:592:HIS:HE1  | 2.01                     | 0.44              |
| 1:A:559:PHE:CE2  | 1:A:841:PRO:HB2  | 2.53                     | 0.44              |
| 1:A:788:ASP:OD1  | 1:A:807:ARG:NH1  | 2.49                     | 0.44              |
| 1:A:814:PRO:O    | 1:A:817:GLN:HB2  | 2.17                     | 0.44              |
| 1:B:607:ARG:HH21 | 1:B:658:ARG:NH2  | 2.09                     | 0.44              |
| 1:B:621:THR:HG23 | 1:B:763:CYS:C    | 2.42                     | 0.44              |
| 1:B:725:LEU:O    | 1:B:729:ILE:CG1  | 2.46                     | 0.44              |
| 1:B:787:PHE:CB   | 1:B:807:ARG:HH11 | 2.31                     | 0.44              |
| 1:A:810:LYS:C    | 1:A:813:ILE:HG23 | 2.43                     | 0.44              |
| 1:B:584:LEU:HD13 | 1:B:644:LEU:HD13 | 1.98                     | 0.44              |
| 1:B:615:TRP:CE3  | 1:B:618:ALA:HB3  | 2.53                     | 0.44              |
| 1:B:820:PHE:O    | 1:B:824:ILE:N    | 2.47                     | 0.44              |
| 1:A:584:LEU:HD12 | 1:A:647:LEU:HD12 | 1.98                     | 0.44              |
| 1:A:727:LEU:HD23 | 1:A:728:TYR:H    | 1.78                     | 0.44              |
| 1:B:646:LEU:O    | 1:B:650:ALA:CB   | 2.66                     | 0.44              |
| 1:A:539:GLU:O    | 1:A:542:SER:HB3  | 2.18                     | 0.44              |
| 1:A:741:LYS:O    | 1:A:743:GLN:N    | 2.51                     | 0.44              |
| 1:B:582:LEU:CD1  | 1:B:626:PHE:HD1  | 2.31                     | 0.44              |
| 1:B:720:ILE:C    | 1:B:722:ALA:N    | 2.76                     | 0.44              |
| 1:B:842:LEU:O    | 1:B:844:ASP:N    | 2.51                     | 0.44              |
| 1:A:540:LEU:HD11 | 1:A:596:CYS:HB2  | 2.00                     | 0.43              |
| 1:A:634:ILE:CD1  | 1:A:836:SER:HB2  | 2.47                     | 0.43              |
| 1:A:681:MET:HG3  | 1:A:685:HIS:CE1  | 2.52                     | 0.43              |
| 1:B:548:VAL:O    | 1:B:549:PRO:O    | 2.36                     | 0.43              |
| 1:B:842:LEU:C    | 1:B:844:ASP:N    | 2.76                     | 0.43              |
| 1:A:813:ILE:HG13 | 1:A:814:PRO:HD3  | 1.98                     | 0.43              |
| 1:B:623:GLN:C    | 1:B:625:MET:H    | 2.26                     | 0.43              |
| 1:B:685:HIS:O    | 1:B:689:CYS:N    | 2.43                     | 0.43              |
| 1:B:692:ILE:C    | 1:B:694:ASN:N    | 2.76                     | 0.43              |
| 1:A:612:TYR:O    | 1:A:614:ASN:N    | 2.42                     | 0.43              |
| 1:A:771:PRO:C    | 1:A:773:PRO:HD2  | 2.43                     | 0.43              |
| 1:B:827:GLN:HA   | 1:B:830:GLU:CD   | 2.43                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:559:PHE:HD2  | 1:A:842:LEU:CD2  | 2.31                     | 0.43              |
| 1:A:653:HIS:HA   | 1:A:720:ILE:CG2  | 2.19                     | 0.43              |
| 1:A:692:ILE:C    | 1:A:694:ASN:N    | 2.76                     | 0.43              |
| 1:A:734:GLU:O    | 1:A:736:PHE:N    | 2.51                     | 0.43              |
| 1:A:753:GLU:O    | 1:A:754:LEU:C    | 2.62                     | 0.43              |
| 1:B:598:TRP:C    | 1:B:602:VAL:HG23 | 2.44                     | 0.43              |
| 1:A:646:LEU:HD11 | 1:A:756:LEU:HD22 | 2.00                     | 0.43              |
| 1:A:648:ILE:HG12 | 1:A:700:ILE:HD11 | 2.00                     | 0.43              |
| 1:A:696:PRO:HA   | 1:A:699:GLN:NE2  | 2.27                     | 0.43              |
| 1:A:728:TYR:HE2  | 1:A:824:ILE:CG2  | 2.32                     | 0.43              |
| 1:A:758:MET:HG3  | 1:A:828:LEU:CD2  | 2.48                     | 0.43              |
| 1:A:768:ILE:HD11 | 1:A:821:ILE:HD11 | 2.01                     | 0.43              |
| 1:A:786:PHE:HE1  | 1:A:804:LEU:HD21 | 1.83                     | 0.43              |
| 1:B:598:TRP:O    | 1:B:601:SER:HB3  | 2.19                     | 0.43              |
| 1:B:614:ASN:O    | 1:B:615:TRP:C    | 2.61                     | 0.43              |
| 1:B:787:PHE:CB   | 1:B:807:ARG:NH1  | 2.81                     | 0.43              |
| 1:A:662:ASN:HD22 | 1:A:662:ASN:N    | 2.09                     | 0.43              |
| 1:B:607:ARG:NE   | 1:B:658:ARG:NE   | 2.65                     | 0.43              |
| 1:B:740:ARG:HG3  | 1:B:740:ARG:NH1  | 2.33                     | 0.43              |
| 1:B:810:LYS:O    | 1:B:813:ILE:HG23 | 2.18                     | 0.43              |
| 1:A:582:LEU:CD1  | 1:A:626:PHE:CD1  | 3.02                     | 0.43              |
| 1:A:820:PHE:HE1  | 1:A:824:ILE:HD12 | 1.83                     | 0.43              |
| 1:A:636:ASN:HD22 | 1:A:637:LYS:HG3  | 1.77                     | 0.43              |
| 1:A:645:ALA:O    | 1:A:649:ALA:CB   | 2.66                     | 0.43              |
| 1:A:656:ASP:HB3  | 1:A:684:HIS:NE2  | 2.33                     | 0.43              |
| 1:A:694:ASN:O    | 1:A:695:SER:C    | 2.61                     | 0.43              |
| 1:A:717:LYS:O    | 1:A:718:GLN:C    | 2.61                     | 0.43              |
| 1:A:830:GLU:CG   | 1:A:831:ALA:H    | 2.31                     | 0.43              |
| 1:B:571:THR:O    | 1:B:619:PHE:CE1  | 2.72                     | 0.43              |
| 1:B:580:THR:O    | 1:B:582:LEU:N    | 2.52                     | 0.43              |
| 1:A:562:SER:OG   | 1:A:777:ARG:NH2  | 2.33                     | 0.43              |
| 1:A:578:MET:HA   | 1:A:626:PHE:CE1  | 2.53                     | 0.43              |
| 1:A:584:LEU:HD12 | 1:A:647:LEU:HD13 | 2.00                     | 0.43              |
| 1:B:556:ILE:HG13 | 1:B:626:PHE:CE2  | 2.53                     | 0.43              |
| 1:B:612:TYR:O    | 1:B:614:ASN:N    | 2.46                     | 0.43              |
| 1:A:690:LEU:HD12 | 1:A:690:LEU:HA   | 1.87                     | 0.43              |
| 1:A:810:LYS:O    | 1:A:813:ILE:HG23 | 2.19                     | 0.42              |
| 1:B:717:LYS:C    | 1:B:719:ALA:N    | 2.76                     | 0.42              |
| 1:B:724:ASP:O    | 1:B:725:LEU:C    | 2.61                     | 0.42              |
| 1:B:779:ALA:CB   | 1:B:817:GLN:HE22 | 2.29                     | 0.42              |
| 1:B:840:PHE:N    | 1:B:841:PRO:HD2  | 2.34                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:857:ALA:C    | 1:A:859:GLN:N    | 2.76                     | 0.42              |
| 1:A:676:TYR:CZ   | 1:A:678:HIS:HA   | 2.54                     | 0.42              |
| 1:B:543:LEU:HD22 | 1:B:576:ILE:CD1  | 2.49                     | 0.42              |
| 1:B:584:LEU:CD1  | 1:B:647:LEU:HD12 | 2.49                     | 0.42              |
| 1:A:622:ALA:HB2  | 1:A:651:LEU:HD23 | 2.00                     | 0.42              |
| 1:A:722:ALA:HA   | 1:A:727:LEU:HD22 | 2.01                     | 0.42              |
| 1:A:735:PHE:CD2  | 1:A:735:PHE:O    | 2.72                     | 0.42              |
| 1:A:840:PHE:N    | 1:A:841:PRO:HD2  | 2.34                     | 0.42              |
| 1:B:601:SER:O    | 1:B:602:VAL:C    | 2.62                     | 0.42              |
| 1:A:735:PHE:CE1  | 1:A:755:PHE:HA   | 2.54                     | 0.42              |
| 1:A:740:ARG:HG3  | 1:A:740:ARG:NH1  | 2.34                     | 0.42              |
| 1:B:714:LYS:O    | 1:B:718:GLN:HB2  | 2.20                     | 0.42              |
| 1:A:757:ALA:O    | 1:A:758:MET:C    | 2.61                     | 0.42              |
| 1:A:779:ALA:CB   | 1:A:817:GLN:HE22 | 2.30                     | 0.42              |
| 1:A:787:PHE:HB3  | 1:A:807:ARG:HH11 | 1.82                     | 0.42              |
| 1:B:607:ARG:C    | 1:B:609:ASN:H    | 2.26                     | 0.42              |
| 1:B:627:ALA:C    | 1:B:629:LEU:N    | 2.75                     | 0.42              |
| 1:A:803:ASP:O    | 1:A:804:LEU:C    | 2.62                     | 0.42              |
| 1:B:663:SER:OG   | 1:B:664:TYR:HD1  | 2.03                     | 0.42              |
| 1:B:694:ASN:O    | 1:B:695:SER:C    | 2.63                     | 0.42              |
| 1:B:735:PHE:O    | 1:B:735:PHE:CG   | 2.73                     | 0.42              |
| 1:B:810:LYS:C    | 1:B:813:ILE:HG23 | 2.44                     | 0.42              |
| 1:A:832:LEU:O    | 1:A:835:VAL:N    | 2.41                     | 0.42              |
| 1:B:634:ILE:O    | 1:B:635:GLN:C    | 2.63                     | 0.42              |
| 1:B:814:PRO:C    | 1:B:816:MET:N    | 2.77                     | 0.42              |
| 1:B:833:THR:CG2  | 1:B:834:HIS:N    | 2.73                     | 0.42              |
| 1:A:711:THR:O    | 1:A:715:ILE:CG1  | 2.66                     | 0.42              |
| 1:B:642:GLU:OE2  | 1:B:752:LYS:HE2  | 2.20                     | 0.42              |
| 1:B:690:LEU:HA   | 1:B:690:LEU:HD12 | 1.82                     | 0.42              |
| 1:B:771:PRO:O    | 1:B:773:PRO:N    | 2.53                     | 0.42              |
| 1:B:821:ILE:HA   | 1:B:825:CYS:SG   | 2.60                     | 0.42              |
| 1:B:825:CYS:O    | 1:B:826:LEU:C    | 2.62                     | 0.42              |
| 1:B:843:LEU:HD12 | 1:B:843:LEU:O    | 2.20                     | 0.42              |
| 1:A:574:CYS:HB2  | 1:A:619:PHE:CZ   | 2.55                     | 0.42              |
| 1:A:586:GLN:HE21 | 1:A:586:GLN:CA   | 2.17                     | 0.42              |
| 1:A:750:HIS:NE2  | 1:A:754:LEU:HD13 | 2.35                     | 0.42              |
| 1:A:764:ASP:C    | 1:A:766:SER:H    | 2.27                     | 0.42              |
| 1:B:652:SER:CB   | 1:B:655:LEU:CD1  | 2.96                     | 0.42              |
| 1:B:758:MET:HG3  | 1:B:828:LEU:CD2  | 2.48                     | 0.42              |
| 1:A:646:LEU:CD2  | 1:A:646:LEU:N    | 2.83                     | 0.41              |
| 1:B:653:HIS:CD2  | 1:B:764:ASP:OD2  | 2.72                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:830:GLU:HB3  | 1:B:843:LEU:HD13 | 2.03                     | 0.41              |
| 1:A:686:PHE:O    | 1:A:689:CYS:N    | 2.53                     | 0.41              |
| 1:A:717:LYS:NZ   | 1:B:796:GLU:CG   | 2.82                     | 0.41              |
| 1:B:648:ILE:HD13 | 1:B:700:ILE:HD11 | 2.02                     | 0.41              |
| 1:A:717:LYS:HZ3  | 1:B:796:GLU:HG2  | 1.86                     | 0.41              |
| 1:B:765:LEU:N    | 1:B:765:LEU:HD12 | 2.34                     | 0.41              |
| 1:A:720:ILE:O    | 1:A:722:ALA:N    | 2.53                     | 0.41              |
| 1:B:757:ALA:C    | 1:B:759:LEU:H    | 2.27                     | 0.41              |
| 1:A:563:ASP:CG   | 1:A:564:PHE:N    | 2.79                     | 0.41              |
| 1:A:715:ILE:O    | 1:A:719:ALA:CB   | 2.69                     | 0.41              |
| 1:A:770:LYS:O    | 1:A:775:GLN:HB3  | 2.20                     | 0.41              |
| 1:A:830:GLU:CG   | 1:A:831:ALA:N    | 2.84                     | 0.41              |
| 1:A:830:GLU:HG3  | 1:A:831:ALA:N    | 2.36                     | 0.41              |
| 1:B:564:PHE:HB2  | 1:B:777:ARG:NH2  | 2.35                     | 0.41              |
| 1:B:635:GLN:C    | 1:B:637:LYS:H    | 2.28                     | 0.41              |
| 1:B:662:ASN:ND2  | 1:B:662:ASN:N    | 2.68                     | 0.41              |
| 1:B:711:THR:O    | 1:B:715:ILE:CG1  | 2.66                     | 0.41              |
| 1:B:717:LYS:O    | 1:B:721:LEU:HG   | 2.19                     | 0.41              |
| 1:B:778:ILE:HA   | 1:B:781:LEU:CD1  | 2.48                     | 0.41              |
| 1:B:801:PRO:CB   | 1:B:806:ASN:HB3  | 2.26                     | 0.41              |
| 1:A:634:ILE:CD1  | 1:A:836:SER:CB   | 2.99                     | 0.41              |
| 1:A:724:ASP:O    | 1:A:726:ALA:N    | 2.53                     | 0.41              |
| 1:A:725:LEU:HA   | 1:A:728:TYR:HB3  | 2.02                     | 0.41              |
| 1:A:797:LEU:CD1  | 1:B:718:GLN:HE21 | 2.34                     | 0.41              |
| 1:A:813:ILE:HG13 | 1:A:814:PRO:CD   | 2.50                     | 0.41              |
| 1:B:658:ARG:HD2  | 1:B:658:ARG:HA   | 1.79                     | 0.41              |
| 1:A:603:LYS:O    | 1:A:606:TYR:N    | 2.54                     | 0.41              |
| 1:A:604:LYS:C    | 1:A:606:TYR:H    | 2.29                     | 0.41              |
| 1:A:639:THR:HG23 | 1:A:642:GLU:OE1  | 2.20                     | 0.41              |
| 1:A:756:LEU:HD23 | 1:A:756:LEU:HA   | 1.85                     | 0.41              |
| 1:B:612:TYR:C    | 1:B:614:ASN:H    | 2.27                     | 0.41              |
| 1:B:847:ARG:O    | 1:B:851:GLN:CG   | 2.69                     | 0.41              |
| 1:B:850:ARG:HH21 | 1:B:854:GLN:NE2  | 2.19                     | 0.41              |
| 1:B:629:LEU:O    | 1:B:635:GLN:HB2  | 2.21                     | 0.41              |
| 1:B:691:MET:HE2  | 1:B:691:MET:O    | 2.20                     | 0.41              |
| 1:A:630:LYS:O    | 1:A:633:LYS:N    | 2.41                     | 0.41              |
| 1:A:641:LEU:C    | 1:A:643:ILE:N    | 2.79                     | 0.41              |
| 1:A:717:LYS:CG   | 1:A:721:LEU:HD11 | 2.46                     | 0.41              |
| 1:A:787:PHE:HB2  | 1:A:807:ARG:HH11 | 1.77                     | 0.41              |
| 1:A:803:ASP:C    | 1:A:805:MET:N    | 2.78                     | 0.41              |
| 1:B:624:CYS:O    | 1:B:624:CYS:SG   | 2.78                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:730:LYS:O    | 1:B:730:LYS:HG2  | 2.21                     | 0.41              |
| 1:A:623:GLN:O    | 1:A:624:CYS:C    | 2.64                     | 0.40              |
| 1:A:717:LYS:C    | 1:A:719:ALA:N    | 2.79                     | 0.40              |
| 1:B:756:LEU:HD23 | 1:B:756:LEU:HA   | 1.90                     | 0.40              |
| 1:A:687:ASP:O    | 1:A:691:MET:HB2  | 2.21                     | 0.40              |
| 1:A:796:GLU:HB2  | 1:B:717:LYS:NZ   | 2.33                     | 0.40              |
| 1:A:821:ILE:CA   | 1:A:825:CYS:HB2  | 2.35                     | 0.40              |
| 1:B:582:LEU:HD11 | 1:B:626:PHE:CD1  | 2.53                     | 0.40              |
| 1:B:796:GLU:H    | 1:B:796:GLU:CD   | 2.30                     | 0.40              |
| 1:A:549:PRO:CG   | 1:A:554:LEU:HD21 | 2.48                     | 0.40              |
| 1:A:612:TYR:CZ   | 4:A:1003:CIA:H2  | 2.56                     | 0.40              |
| 1:A:724:ASP:O    | 1:A:725:LEU:C    | 2.64                     | 0.40              |
| 1:B:732:ARG:O    | 1:B:733:GLY:C    | 2.63                     | 0.40              |
| 1:B:752:LYS:O    | 1:B:756:LEU:HB2  | 2.21                     | 0.40              |
| 1:A:566:LEU:HD23 | 1:A:566:LEU:N    | 2.26                     | 0.40              |
| 1:A:645:ALA:O    | 1:A:649:ALA:N    | 2.39                     | 0.40              |
| 1:A:646:LEU:O    | 1:A:650:ALA:HB3  | 2.21                     | 0.40              |
| 1:A:658:ARG:NH1  | 1:A:658:ARG:CG   | 2.76                     | 0.40              |
| 1:A:720:ILE:C    | 1:A:722:ALA:N    | 2.77                     | 0.40              |
| 1:B:732:ARG:HH12 | 1:B:824:ILE:HA   | 1.85                     | 0.40              |
| 1:A:657:HIS:ND1  | 1:A:681:MET:HE3  | 2.37                     | 0.40              |
| 1:B:712:THR:HA   | 1:B:715:ILE:CD1  | 2.49                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed   | Outliers | Percentiles |   |
|-----|-------|---------------|-----------|-----------|----------|-------------|---|
| 1   | A     | 309/324 (95%) | 194 (63%) | 78 (25%)  | 37 (12%) | 0           | 0 |
| 1   | B     | 309/324 (95%) | 196 (63%) | 79 (26%)  | 34 (11%) | 0           | 0 |
| All | All   | 618/648 (95%) | 390 (63%) | 157 (25%) | 71 (12%) | 0           | 0 |



All (71) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 549 | PRO  |
| 1   | A     | 564 | PHE  |
| 1   | A     | 631 | ALA  |
| 1   | A     | 693 | LEU  |
| 1   | A     | 732 | ARG  |
| 1   | A     | 826 | LEU  |
| 1   | B     | 549 | PRO  |
| 1   | B     | 631 | ALA  |
| 1   | B     | 650 | ALA  |
| 1   | B     | 732 | ARG  |
| 1   | B     | 743 | GLN  |
| 1   | B     | 826 | LEU  |
| 1   | A     | 589 | GLN  |
| 1   | A     | 598 | TRP  |
| 1   | A     | 599 | ILE  |
| 1   | A     | 624 | CYS  |
| 1   | A     | 721 | LEU  |
| 1   | A     | 742 | ASN  |
| 1   | A     | 743 | GLN  |
| 1   | A     | 745 | ASN  |
| 1   | A     | 794 | ARG  |
| 1   | B     | 589 | GLN  |
| 1   | B     | 649 | ALA  |
| 1   | B     | 663 | SER  |
| 1   | B     | 693 | LEU  |
| 1   | B     | 721 | LEU  |
| 1   | B     | 725 | LEU  |
| 1   | B     | 742 | ASN  |
| 1   | B     | 744 | PHE  |
| 1   | B     | 745 | ASN  |
| 1   | B     | 794 | ARG  |
| 1   | A     | 602 | VAL  |
| 1   | A     | 604 | LYS  |
| 1   | A     | 612 | TYR  |
| 1   | A     | 650 | ALA  |
| 1   | A     | 663 | SER  |
| 1   | A     | 725 | LEU  |
| 1   | A     | 744 | PHE  |
| 1   | A     | 803 | ASP  |
| 1   | B     | 581 | ASP  |
| 1   | B     | 604 | LYS  |
| 1   | B     | 612 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 735 | PHE  |
| 1   | B     | 803 | ASP  |
| 1   | A     | 601 | SER  |
| 1   | A     | 623 | GLN  |
| 1   | A     | 703 | GLY  |
| 1   | A     | 756 | LEU  |
| 1   | A     | 772 | TRP  |
| 1   | A     | 809 | LYS  |
| 1   | B     | 564 | PHE  |
| 1   | B     | 642 | GLU  |
| 1   | B     | 703 | GLY  |
| 1   | B     | 717 | LYS  |
| 1   | B     | 773 | PRO  |
| 1   | A     | 649 | ALA  |
| 1   | A     | 692 | ILE  |
| 1   | A     | 717 | LYS  |
| 1   | A     | 733 | GLY  |
| 1   | A     | 735 | PHE  |
| 1   | A     | 773 | PRO  |
| 1   | B     | 758 | MET  |
| 1   | B     | 843 | LEU  |
| 1   | A     | 755 | PHE  |
| 1   | B     | 542 | SER  |
| 1   | B     | 593 | GLU  |
| 1   | B     | 624 | CYS  |
| 1   | B     | 814 | PRO  |
| 1   | B     | 733 | GLY  |
| 1   | B     | 716 | ILE  |
| 1   | A     | 814 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |   |
|-----|-------|---------------|-----------|----------|-------------|---|
| 1   | A     | 279/289 (96%) | 239 (86%) | 40 (14%) | 3           | 6 |
| 1   | B     | 279/289 (96%) | 239 (86%) | 40 (14%) | 3           | 6 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles       |
|-----|-------|---------------|-----------|----------|-------------------|
| All | All   | 558/578 (96%) | 478 (86%) | 80 (14%) | <b>3</b> <b>6</b> |

All (80) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 543 | LEU  |
| 1   | A     | 558 | ASP  |
| 1   | A     | 559 | PHE  |
| 1   | A     | 569 | LEU  |
| 1   | A     | 585 | VAL  |
| 1   | A     | 586 | GLN  |
| 1   | A     | 589 | GLN  |
| 1   | A     | 591 | LYS  |
| 1   | A     | 601 | SER  |
| 1   | A     | 604 | LYS  |
| 1   | A     | 609 | ASN  |
| 1   | A     | 636 | ASN  |
| 1   | A     | 655 | LEU  |
| 1   | A     | 658 | ARG  |
| 1   | A     | 661 | ASN  |
| 1   | A     | 678 | HIS  |
| 1   | A     | 682 | GLU  |
| 1   | A     | 691 | MET  |
| 1   | A     | 698 | ASN  |
| 1   | A     | 710 | LYS  |
| 1   | A     | 713 | LEU  |
| 1   | A     | 718 | GLN  |
| 1   | A     | 727 | LEU  |
| 1   | A     | 747 | GLU  |
| 1   | A     | 752 | LYS  |
| 1   | A     | 758 | MET  |
| 1   | A     | 759 | LEU  |
| 1   | A     | 760 | MET  |
| 1   | A     | 765 | LEU  |
| 1   | A     | 775 | GLN  |
| 1   | A     | 782 | VAL  |
| 1   | A     | 795 | LYS  |
| 1   | A     | 797 | LEU  |
| 1   | A     | 798 | ASN  |
| 1   | A     | 818 | VAL  |
| 1   | A     | 828 | LEU  |
| 1   | A     | 833 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 838 | ASP  |
| 1   | A     | 850 | ARG  |
| 1   | A     | 858 | GLU  |
| 1   | B     | 543 | LEU  |
| 1   | B     | 558 | ASP  |
| 1   | B     | 559 | PHE  |
| 1   | B     | 569 | LEU  |
| 1   | B     | 580 | THR  |
| 1   | B     | 586 | GLN  |
| 1   | B     | 589 | GLN  |
| 1   | B     | 591 | LYS  |
| 1   | B     | 601 | SER  |
| 1   | B     | 604 | LYS  |
| 1   | B     | 609 | ASN  |
| 1   | B     | 636 | ASN  |
| 1   | B     | 655 | LEU  |
| 1   | B     | 658 | ARG  |
| 1   | B     | 661 | ASN  |
| 1   | B     | 678 | HIS  |
| 1   | B     | 682 | GLU  |
| 1   | B     | 691 | MET  |
| 1   | B     | 698 | ASN  |
| 1   | B     | 710 | LYS  |
| 1   | B     | 713 | LEU  |
| 1   | B     | 718 | GLN  |
| 1   | B     | 727 | LEU  |
| 1   | B     | 747 | GLU  |
| 1   | B     | 758 | MET  |
| 1   | B     | 759 | LEU  |
| 1   | B     | 760 | MET  |
| 1   | B     | 765 | LEU  |
| 1   | B     | 775 | GLN  |
| 1   | B     | 782 | VAL  |
| 1   | B     | 797 | LEU  |
| 1   | B     | 798 | ASN  |
| 1   | B     | 799 | ILE  |
| 1   | B     | 818 | VAL  |
| 1   | B     | 824 | ILE  |
| 1   | B     | 828 | LEU  |
| 1   | B     | 833 | THR  |
| 1   | B     | 838 | ASP  |
| 1   | B     | 850 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 858 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 583 | ASN  |
| 1   | A     | 586 | GLN  |
| 1   | A     | 587 | ASN  |
| 1   | A     | 592 | HIS  |
| 1   | A     | 605 | ASN  |
| 1   | A     | 609 | ASN  |
| 1   | A     | 617 | HIS  |
| 1   | A     | 620 | ASN  |
| 1   | A     | 635 | GLN  |
| 1   | A     | 636 | ASN  |
| 1   | A     | 662 | ASN  |
| 1   | A     | 685 | HIS  |
| 1   | A     | 698 | ASN  |
| 1   | A     | 699 | GLN  |
| 1   | A     | 718 | GLN  |
| 1   | A     | 743 | GLN  |
| 1   | A     | 751 | GLN  |
| 1   | A     | 834 | HIS  |
| 1   | A     | 849 | ASN  |
| 1   | A     | 851 | GLN  |
| 1   | B     | 583 | ASN  |
| 1   | B     | 586 | GLN  |
| 1   | B     | 587 | ASN  |
| 1   | B     | 592 | HIS  |
| 1   | B     | 605 | ASN  |
| 1   | B     | 609 | ASN  |
| 1   | B     | 613 | HIS  |
| 1   | B     | 617 | HIS  |
| 1   | B     | 620 | ASN  |
| 1   | B     | 635 | GLN  |
| 1   | B     | 636 | ASN  |
| 1   | B     | 662 | ASN  |
| 1   | B     | 685 | HIS  |
| 1   | B     | 698 | ASN  |
| 1   | B     | 699 | GLN  |
| 1   | B     | 743 | GLN  |
| 1   | B     | 751 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 798 | ASN  |
| 1   | B     | 834 | HIS  |
| 1   | B     | 849 | ASN  |
| 1   | B     | 851 | 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](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 4   | CIA  | A     | 1003 | -    | 34,34,34     | 4.65 | 23 (67%)    | 49,52,52    | 1.62 | 12 (24%)    |
| 4   | CIA  | B     | 2003 | -    | 34,34,34     | 4.39 | 23 (67%)    | 49,52,52    | 1.54 | 9 (18%)     |

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   | CIA  | A     | 1003 | -    | -       | 0/4/42/42 | 0/6/6/6 |
| 4   | CIA  | B     | 2003 | -    | -       | 0/4/42/42 | 0/6/6/6 |

All (46) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 4   | A     | 1003 | CIA  | C31-N15 | 8.53 | 1.42        | 1.34     |
| 4   | A     | 1003 | CIA  | C22-C13 | 8.47 | 1.63        | 1.52     |
| 4   | B     | 2003 | CIA  | C22-C13 | 7.80 | 1.62        | 1.52     |
| 4   | A     | 1003 | CIA  | C17-N12 | 7.60 | 1.42        | 1.35     |
| 4   | B     | 2003 | CIA  | C31-N15 | 7.41 | 1.41        | 1.34     |
| 4   | A     | 1003 | CIA  | C13-C8  | 7.14 | 1.60        | 1.50     |
| 4   | B     | 2003 | CIA  | C23-C22 | 6.88 | 1.49        | 1.39     |
| 4   | A     | 1003 | CIA  | C23-C22 | 6.84 | 1.49        | 1.39     |
| 4   | A     | 1003 | CIA  | C13-N12 | 6.79 | 1.58        | 1.47     |
| 4   | B     | 2003 | CIA  | C11-N12 | 6.68 | 1.57        | 1.47     |
| 4   | A     | 1003 | CIA  | C11-N12 | 6.60 | 1.57        | 1.47     |
| 4   | B     | 2003 | CIA  | C13-C8  | 6.48 | 1.59        | 1.50     |
| 4   | B     | 2003 | CIA  | C16-N15 | 6.27 | 1.51        | 1.45     |
| 4   | A     | 1003 | CIA  | C8-C7   | 6.24 | 1.44        | 1.36     |
| 4   | B     | 2003 | CIA  | C8-C7   | 6.17 | 1.44        | 1.36     |
| 4   | A     | 1003 | CIA  | C16-N15 | 5.81 | 1.51        | 1.45     |
| 4   | A     | 1003 | CIA  | C10-C7  | 5.72 | 1.57        | 1.50     |
| 4   | B     | 2003 | CIA  | C11-C31 | 5.61 | 1.62        | 1.51     |
| 4   | B     | 2003 | CIA  | C6-C5   | 5.53 | 1.48        | 1.41     |
| 4   | A     | 1003 | CIA  | C6-C5   | 5.52 | 1.48        | 1.41     |
| 4   | B     | 2003 | CIA  | C13-N12 | 5.41 | 1.56        | 1.47     |
| 4   | A     | 1003 | CIA  | C1-C6   | 5.41 | 1.48        | 1.39     |
| 4   | B     | 2003 | CIA  | C17-N12 | 5.33 | 1.40        | 1.35     |
| 4   | A     | 1003 | CIA  | C11-C31 | 5.29 | 1.61        | 1.51     |
| 4   | A     | 1003 | CIA  | C4-C5   | 5.06 | 1.47        | 1.39     |
| 4   | B     | 2003 | CIA  | C27-C22 | 5.01 | 1.47        | 1.39     |
| 4   | B     | 2003 | CIA  | C1-C6   | 4.75 | 1.47        | 1.39     |
| 4   | B     | 2003 | CIA  | C26-C25 | 4.66 | 1.49        | 1.39     |
| 4   | B     | 2003 | CIA  | C10-C7  | 4.62 | 1.56        | 1.50     |
| 4   | A     | 1003 | CIA  | C8-N9   | 4.47 | 1.43        | 1.38     |
| 4   | B     | 2003 | CIA  | C8-N9   | 4.39 | 1.43        | 1.38     |
| 4   | B     | 2003 | CIA  | C4-C5   | 4.39 | 1.46        | 1.39     |
| 4   | A     | 1003 | CIA  | C26-C25 | 4.28 | 1.48        | 1.39     |
| 4   | A     | 1003 | CIA  | C27-C22 | 4.07 | 1.45        | 1.39     |
| 4   | B     | 2003 | CIA  | C2-C3   | 3.67 | 1.46        | 1.38     |
| 4   | A     | 1003 | CIA  | C2-C1   | 3.48 | 1.44        | 1.38     |
| 4   | B     | 2003 | CIA  | C26-C27 | 3.40 | 1.44        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 4   | A     | 1003 | CIA  | C26-C27 | 3.33 | 1.44        | 1.38     |
| 4   | A     | 1003 | CIA  | C2-C3   | 3.31 | 1.45        | 1.38     |
| 4   | B     | 2003 | CIA  | C2-C1   | 3.15 | 1.44        | 1.38     |
| 4   | B     | 2003 | CIA  | C3-C4   | 2.86 | 1.43        | 1.38     |
| 4   | A     | 1003 | CIA  | C3-C4   | 2.81 | 1.43        | 1.38     |
| 4   | A     | 1003 | CIA  | O32-C31 | 2.72 | 1.27        | 1.22     |
| 4   | B     | 2003 | CIA  | C16-C17 | 2.39 | 1.55        | 1.51     |
| 4   | B     | 2003 | CIA  | O32-C31 | 2.16 | 1.26        | 1.22     |
| 4   | A     | 1003 | CIA  | C10-C11 | 2.08 | 1.57        | 1.53     |

All (21) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | B     | 2003 | CIA  | C5-N9-C8    | -5.09 | 104.13      | 108.53   |
| 4   | A     | 1003 | CIA  | C5-N9-C8    | -4.14 | 104.95      | 108.53   |
| 4   | B     | 2003 | CIA  | C13-C8-C7   | -4.08 | 121.21      | 125.50   |
| 4   | A     | 1003 | CIA  | C13-C8-C7   | -3.41 | 121.91      | 125.50   |
| 4   | A     | 1003 | CIA  | C6-C7-C8    | -3.00 | 104.86      | 106.90   |
| 4   | A     | 1003 | CIA  | C10-C7-C6   | 2.94  | 134.86      | 130.85   |
| 4   | A     | 1003 | CIA  | C18-N15-C31 | 2.85  | 122.42      | 119.42   |
| 4   | A     | 1003 | CIA  | C22-C13-C8  | -2.64 | 104.73      | 111.61   |
| 4   | B     | 2003 | CIA  | C7-C8-N9    | 2.51  | 112.46      | 110.22   |
| 4   | A     | 1003 | CIA  | C22-C13-N12 | 2.48  | 114.77      | 111.90   |
| 4   | A     | 1003 | CIA  | O20-C17-N12 | 2.46  | 125.57      | 122.36   |
| 4   | A     | 1003 | CIA  | C7-C8-N9    | 2.44  | 112.40      | 110.22   |
| 4   | B     | 2003 | CIA  | C6-C5-N9    | 2.42  | 110.95      | 108.23   |
| 4   | B     | 2003 | CIA  | C4-C5-C6    | -2.39 | 119.88      | 122.19   |
| 4   | B     | 2003 | CIA  | C18-N15-C31 | 2.38  | 121.93      | 119.42   |
| 4   | B     | 2003 | CIA  | C13-C8-N9   | 2.36  | 126.33      | 123.78   |
| 4   | B     | 2003 | CIA  | C6-C7-C8    | -2.31 | 105.33      | 106.90   |
| 4   | B     | 2003 | CIA  | C10-C7-C6   | 2.30  | 133.98      | 130.85   |
| 4   | A     | 1003 | CIA  | C6-C5-N9    | 2.14  | 110.64      | 108.23   |
| 4   | A     | 1003 | CIA  | C10-C11-N12 | 2.04  | 113.96      | 111.05   |
| 4   | A     | 1003 | CIA  | C4-C5-C6    | -2.02 | 120.23      | 122.19   |

There are no chirality outliers.

There are no torsion outliers.

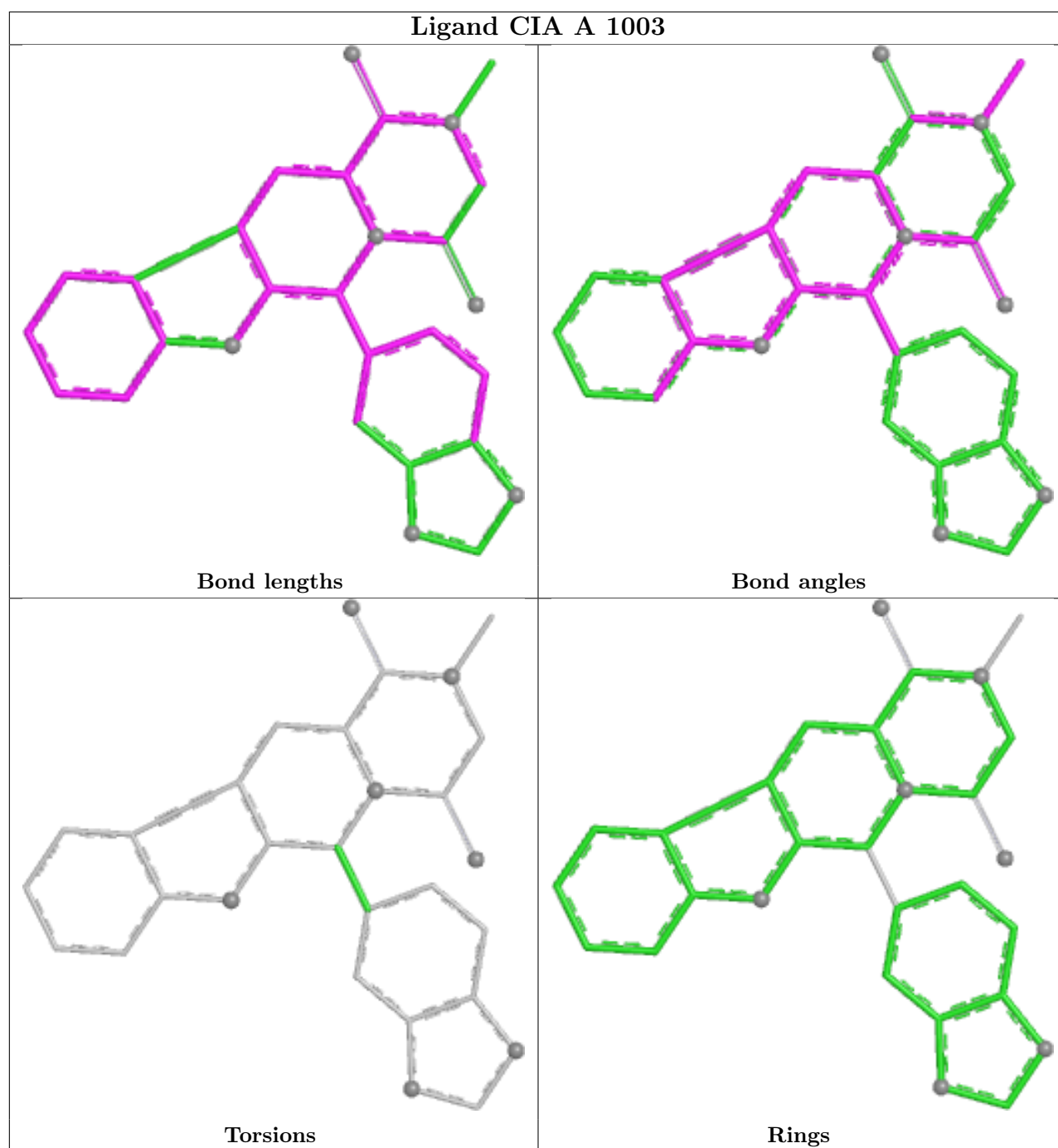
There are no ring outliers.

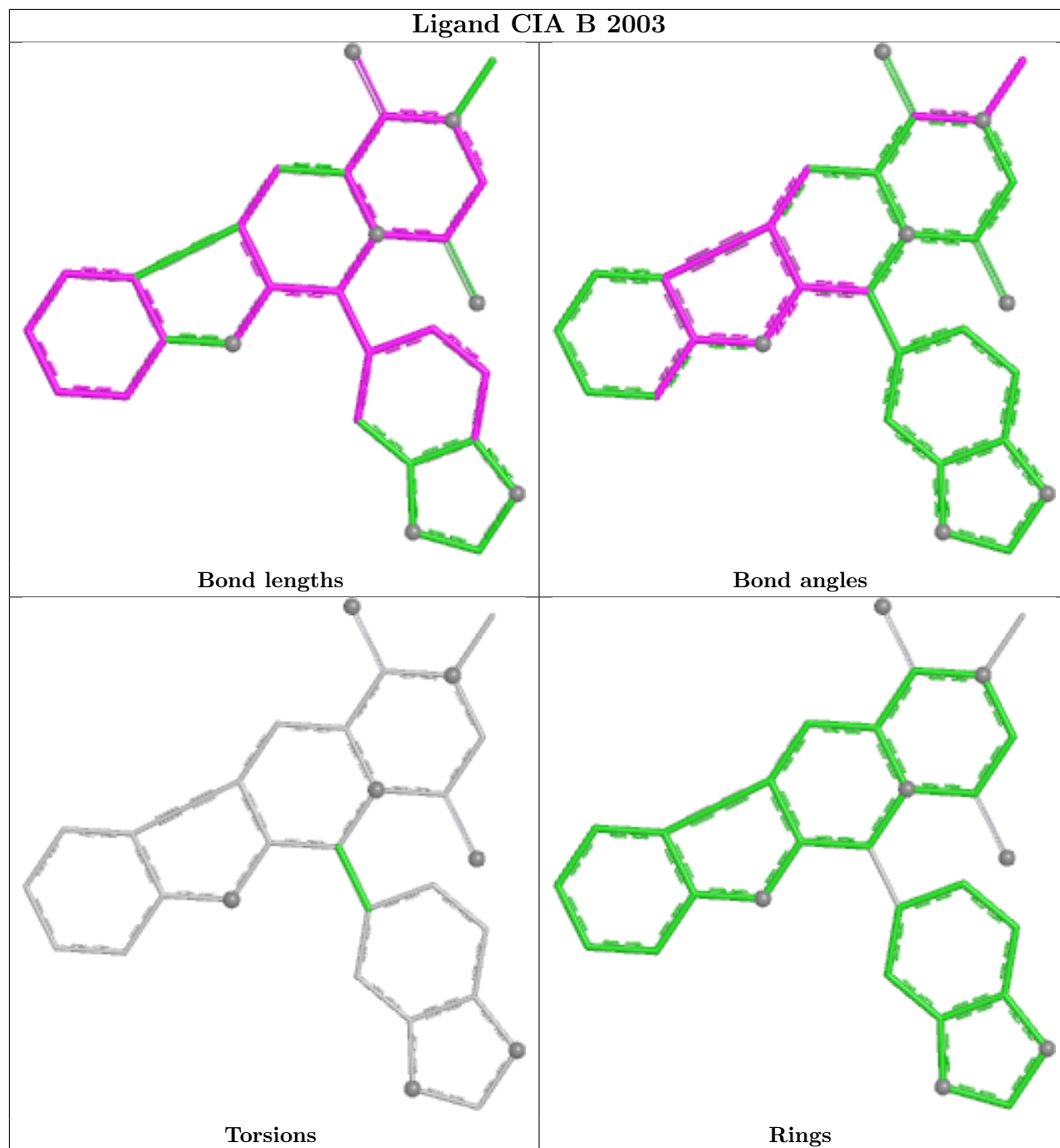
2 monomers are involved in 9 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | A     | 1003 | CIA  | 8       | 0            |
| 4   | B     | 2003 | CIA  | 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 1   | A     | 313/324 (96%) | 0.36   | 6 (1%) 66 59  | 13, 47, 78, 104       | 0     |
| 1   | B     | 313/324 (96%) | 0.43   | 10 (3%) 50 40 | 10, 47, 83, 97        | 0     |
| All | All   | 626/648 (96%) | 0.40   | 16 (2%) 57 48 | 10, 47, 81, 104       | 0     |

All (16) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 859 | GLN  | 3.8  |
| 1   | A     | 542 | SER  | 3.4  |
| 1   | A     | 692 | ILE  | 2.9  |
| 1   | B     | 800 | GLU  | 2.7  |
| 1   | A     | 801 | PRO  | 2.5  |
| 1   | B     | 721 | LEU  | 2.5  |
| 1   | B     | 540 | LEU  | 2.4  |
| 1   | B     | 645 | ALA  | 2.3  |
| 1   | A     | 663 | SER  | 2.3  |
| 1   | B     | 815 | SER  | 2.3  |
| 1   | B     | 778 | ILE  | 2.2  |
| 1   | B     | 813 | ILE  | 2.2  |
| 1   | B     | 596 | CYS  | 2.2  |
| 1   | B     | 611 | ALA  | 2.2  |
| 1   | B     | 660 | VAL  | 2.1  |
| 1   | A     | 776 | GLN  | 2.1  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

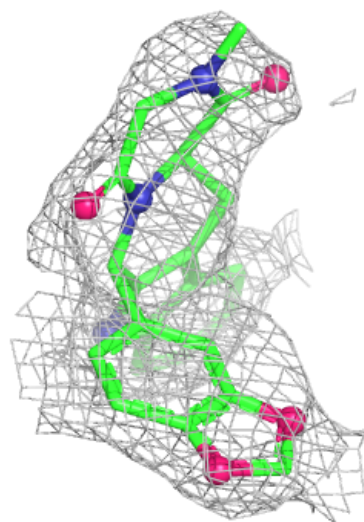
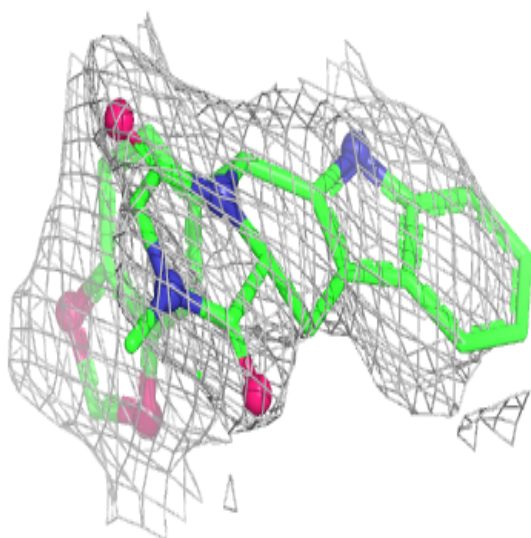
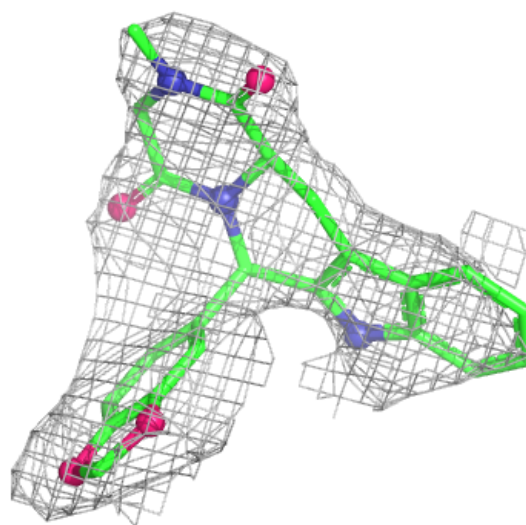
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | MG   | A     | 1002 | 1/1   | 0.86 | 0.20 | 36,36,36,36                 | 0     |
| 2   | ZN   | A     | 1001 | 1/1   | 0.89 | 0.22 | 105,105,105,105             | 0     |
| 4   | CIA  | B     | 2003 | 29/29 | 0.90 | 0.12 | 9,49,77,105                 | 0     |
| 2   | ZN   | B     | 2001 | 1/1   | 0.92 | 0.20 | 105,105,105,105             | 0     |
| 4   | CIA  | A     | 1003 | 29/29 | 0.93 | 0.10 | 15,59,81,83                 | 0     |
| 3   | MG   | B     | 2002 | 1/1   | 0.97 | 0.13 | 15,15,15,15                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

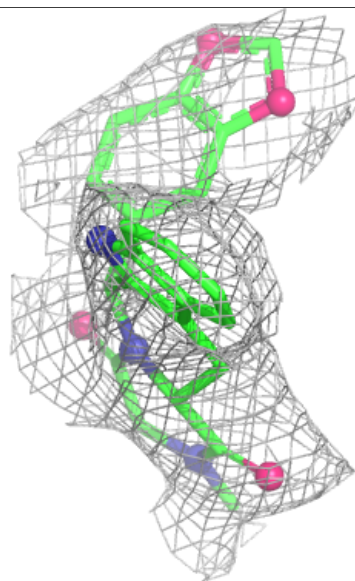
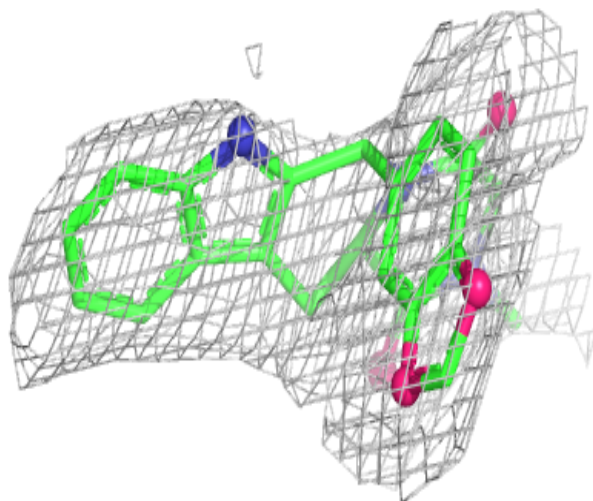
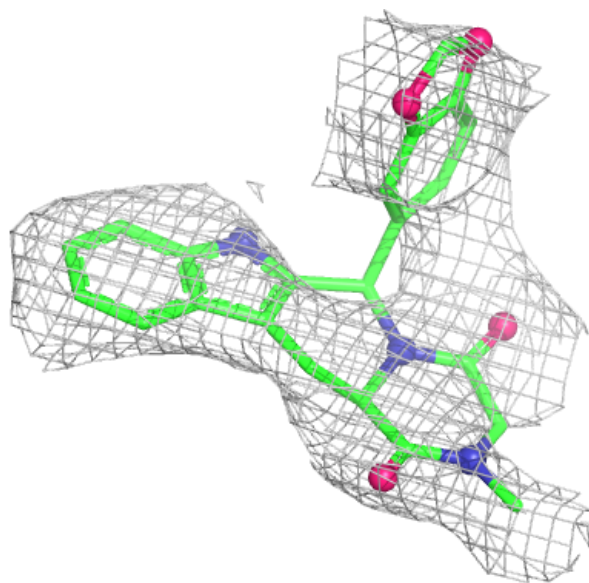
**Electron density around CIA B 2003:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CIA A 1003:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.