



## Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:56 PM UTC

PDB ID : 1WOK / pdb\_00001wok  
Title : Crystal structure of catalytic domain of human poly(ADP-ribose) polymerase complexed with a quinoxaline-type inhibitor  
Authors : Iwashita, A.; Hattori, K.; Yamamoto, H.; Ishida, J.; Kido, Y.; Kamijo, K.; Murano, K.; Miyake, H.; Kinoshita, T.; Warizaya, M.; Ohkubo, M.; Matsuoka, N.; Mutoh, S.  
Deposited on : 2004-08-20  
Resolution : 3.00 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:

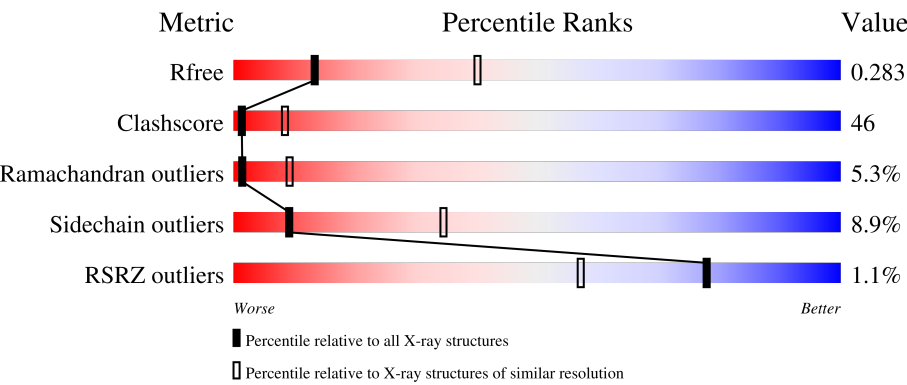
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| 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 i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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                      | 2672 (3.00-3.00)                                      |
| Clashscore            | 190562                      | 2977 (3.00-3.00)                                      |
| Ramachandran outliers | 187476                      | 2877 (3.00-3.00)                                      |
| Sidechain outliers    | 187428                      | 2880 (3.00-3.00)                                      |
| RSRZ outliers         | 180081                      | 2671 (3.00-3.00)                                      |

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     | 350    | <div><div>%</div><div><div></div><div>45%</div><div>45%</div><div>9%</div></div></div>               |
| 1   | B     | 350    | <div><div>%</div><div><div></div><div>40%</div><div>50%</div><div>10%</div></div></div>              |
| 1   | C     | 350    | <div><div></div><div><div></div><div>38%</div><div>50%</div><div>12%</div></div></div>               |
| 1   | D     | 350    | <div><div>3%</div><div><div></div><div>26%</div><div>59%</div><div>13%</div><div>.</div></div></div> |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | CNQ  | C     | 3   | -         | X        | -       | -                |

## 2 Entry composition [i](#)

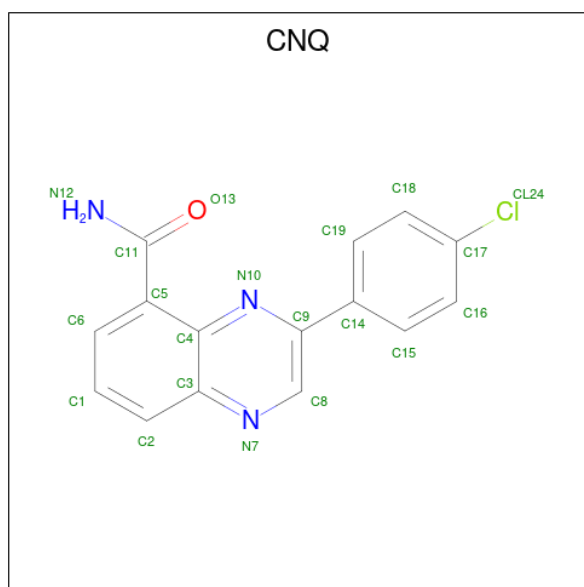
There are 2 unique types of molecules in this entry. The entry contains 11096 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Poly [ADP-ribose] polymerase-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 350      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2754  | 1752 | 465 | 526 | 11 |         |         |       |
| 1   | B     | 350      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2754  | 1752 | 465 | 526 | 11 |         |         |       |
| 1   | C     | 350      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2754  | 1752 | 465 | 526 | 11 |         |         |       |
| 1   | D     | 350      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2754  | 1752 | 465 | 526 | 11 |         |         |       |

- Molecule 2 is 3-(4-CHLOROPHENYL)QUINOXALINE-5-CARBOXAMIDE (CCD ID: CNQ) (formula: C<sub>15</sub>H<sub>10</sub>ClN<sub>3</sub>O).



| Mol | Chain | Residues | Atoms |    |    |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|-----|---------|---------|
| 2   | A     | 1        | Total | C  | Cl | N O | 0       | 0       |
|     |       |          | 20    | 15 | 1  | 3 1 |         |         |
| 2   | B     | 1        | Total | C  | Cl | N O | 0       | 0       |
|     |       |          | 20    | 15 | 1  | 3 1 |         |         |

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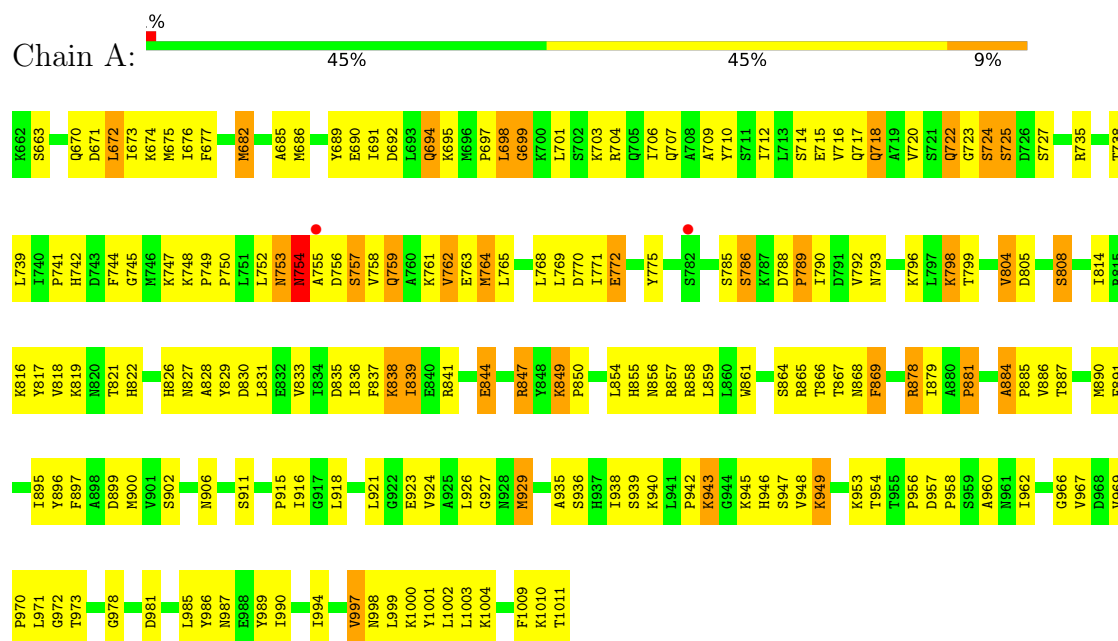
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| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 2   | C     | 1        | Total | C  | Cl | N | O | 0       | 0       |
|     |       |          | 20    | 15 | 1  | 3 | 1 |         |         |
| 2   | D     | 1        | Total | C  | Cl | N | O | 0       | 0       |
|     |       |          | 20    | 15 | 1  | 3 | 1 |         |         |

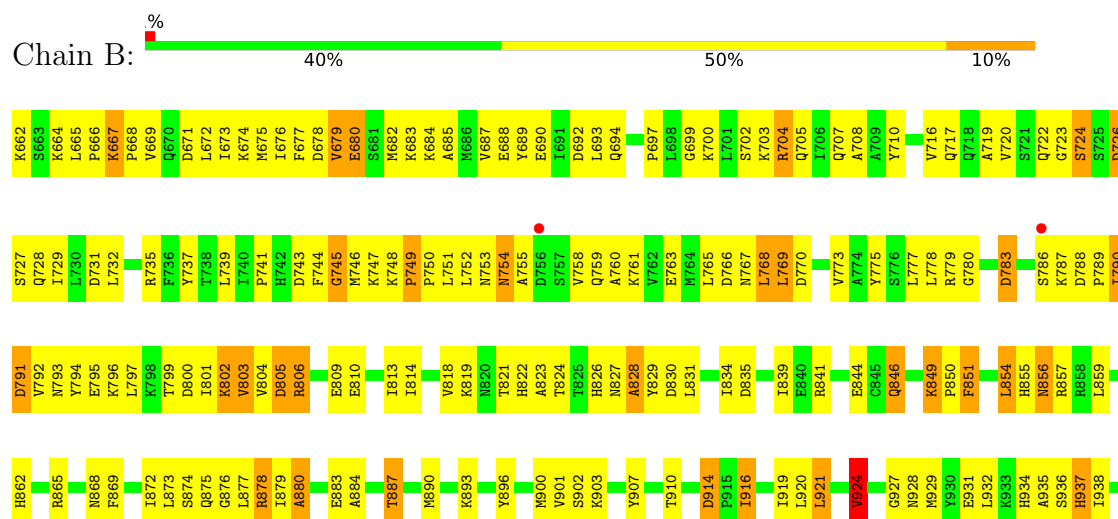
### 3 Residue-property plots

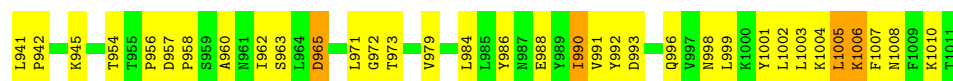
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Poly [ADP-ribose] polymerase-1



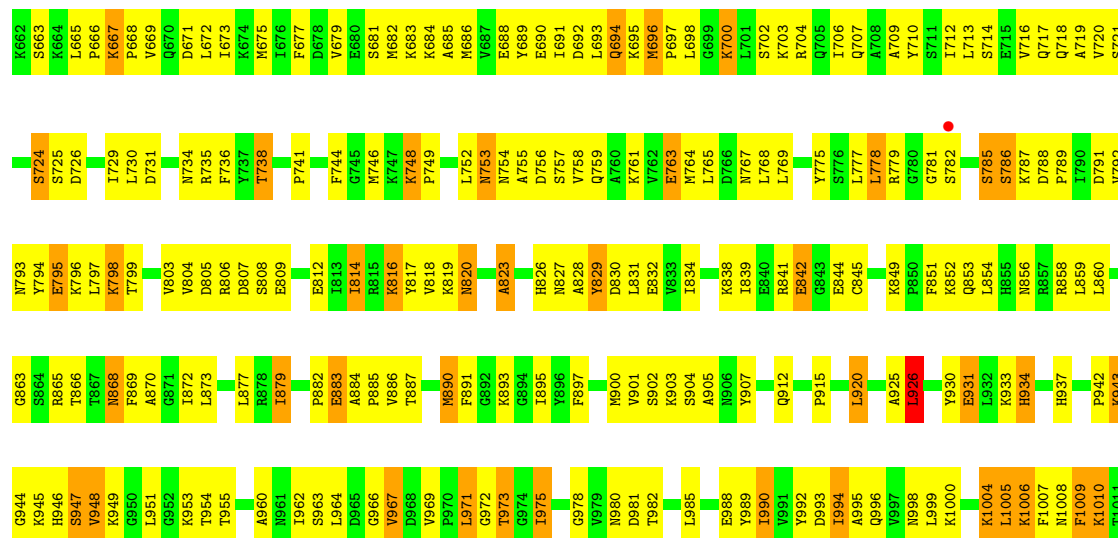
#### • Molecule 1: Poly [ADP-ribose] polymerase-1





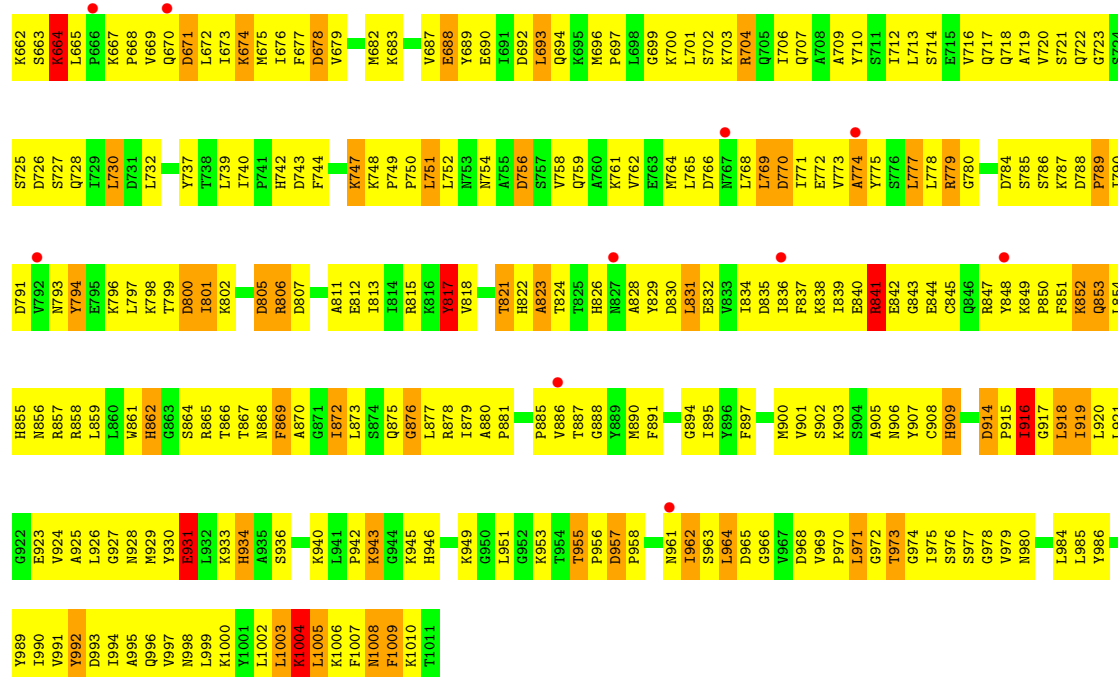
• Molecule 1: Poly [ADP-ribose] polymerase-1

Chain C: 38% 50% 12%



• Molecule 1: Poly [ADP-ribose] polymerase-1

Chain D: 3% 26% 59% 13%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 90.05Å 77.08Å 113.72Å<br>90.00° 117.43° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 29.25 – 3.00<br>29.25 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 93.4 (29.25-3.00)<br>94.0 (29.25-3.00)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 5.12 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | CNX 2002                                                    | Depositor        |
| R, $R_{free}$                                                           | 0.233 , 0.288<br>0.229 , 0.283                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1271 reflections (4.83%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 50.8                                                        | Xtriage          |
| Anisotropy                                                              | 0.259                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 60.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 11096                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 48.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.87% 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: CNQ

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     | 0.47         | 0/2806         | 1.00        | 15/3786 (0.4%)  |
| 1   | B     | 0.44         | 0/2806         | 0.98        | 12/3786 (0.3%)  |
| 1   | C     | 0.52         | 1/2806 (0.0%)  | 1.04        | 10/3786 (0.3%)  |
| 1   | D     | 0.38         | 0/2806         | 0.91        | 9/3786 (0.2%)   |
| All | All   | 0.46         | 1/11224 (0.0%) | 0.98        | 46/15144 (0.3%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | B     | 0                   | 1                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | C     | 948 | VAL  | CA-CB | 5.07 | 1.60        | 1.55     |

All (46) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | A     | 757  | SER  | N-CA-C | -8.34 | 103.08      | 113.18   |
| 1   | C     | 695  | LYS  | N-CA-C | -8.10 | 105.39      | 114.62   |
| 1   | C     | 926  | LEU  | N-CA-C | 7.94  | 119.94      | 111.28   |
| 1   | D     | 852  | LYS  | N-CA-C | -7.84 | 104.23      | 113.88   |
| 1   | A     | 884  | ALA  | CA-C-N | 7.78  | 128.92      | 120.13   |
| 1   | A     | 884  | ALA  | C-N-CA | 7.78  | 128.92      | 120.13   |
| 1   | C     | 1009 | PHE  | N-CA-C | 7.55  | 120.50      | 110.53   |
| 1   | A     | 869  | PHE  | N-CA-C | 7.52  | 120.54      | 111.82   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 914 | ASP  | CA-C-N  | 6.86  | 128.42      | 119.84   |
| 1   | B     | 914 | ASP  | C-N-CA  | 6.86  | 128.42      | 119.84   |
| 1   | C     | 748 | LYS  | CA-C-N  | 6.80  | 127.38      | 120.38   |
| 1   | C     | 748 | LYS  | C-N-CA  | 6.80  | 127.38      | 120.38   |
| 1   | C     | 868 | ASN  | N-CA-C  | -6.67 | 105.77      | 114.04   |
| 1   | C     | 890 | MET  | N-CA-C  | 6.39  | 119.06      | 111.33   |
| 1   | D     | 756 | ASP  | N-CA-C  | -6.26 | 104.54      | 111.36   |
| 1   | D     | 844 | GLU  | N-CA-C  | -6.23 | 105.77      | 113.19   |
| 1   | D     | 931 | GLU  | N-CA-C  | 6.19  | 118.80      | 108.96   |
| 1   | D     | 872 | ILE  | N-CA-C  | -5.98 | 105.23      | 113.00   |
| 1   | D     | 823 | ALA  | N-CA-C  | 5.87  | 117.87      | 110.24   |
| 1   | A     | 762 | VAL  | N-CA-C  | -5.83 | 104.83      | 110.42   |
| 1   | A     | 881 | PRO  | CA-C-N  | 5.80  | 125.17      | 118.85   |
| 1   | A     | 881 | PRO  | C-N-CA  | 5.80  | 125.17      | 118.85   |
| 1   | B     | 819 | LYS  | N-CA-C  | 5.72  | 117.52      | 111.28   |
| 1   | B     | 846 | GLN  | N-CA-C  | 5.69  | 117.48      | 111.28   |
| 1   | A     | 929 | MET  | N-CA-C  | 5.58  | 118.62      | 109.76   |
| 1   | B     | 708 | ALA  | N-CA-C  | -5.50 | 105.37      | 111.36   |
| 1   | A     | 899 | ASP  | N-CA-C  | -5.48 | 104.86      | 113.02   |
| 1   | B     | 924 | VAL  | N-CA-C  | 5.47  | 115.83      | 108.17   |
| 1   | B     | 880 | ALA  | CA-C-N  | -5.35 | 114.87      | 120.38   |
| 1   | B     | 880 | ALA  | C-N-CA  | -5.35 | 114.87      | 120.38   |
| 1   | B     | 680 | GLU  | N-CA-C  | 5.35  | 117.80      | 111.33   |
| 1   | A     | 997 | VAL  | N-CA-C  | 5.35  | 115.75      | 107.78   |
| 1   | D     | 957 | ASP  | CA-C-N  | 5.34  | 125.16      | 119.28   |
| 1   | D     | 957 | ASP  | C-N-CA  | 5.34  | 125.16      | 119.28   |
| 1   | C     | 920 | LEU  | N-CA-C  | 5.34  | 118.44      | 109.95   |
| 1   | A     | 849 | LYS  | CA-C-N  | 5.33  | 124.99      | 119.56   |
| 1   | A     | 849 | LYS  | C-N-CA  | 5.33  | 124.99      | 119.56   |
| 1   | C     | 724 | SER  | N-CA-C  | 5.26  | 115.33      | 108.07   |
| 1   | A     | 847 | ARG  | N-CA-C  | -5.23 | 106.73      | 113.01   |
| 1   | A     | 682 | MET  | N-CA-C  | -5.23 | 105.49      | 111.14   |
| 1   | C     | 763 | GLU  | N-CA-C  | -5.10 | 105.90      | 111.82   |
| 1   | B     | 990 | ILE  | CB-CA-C | -5.03 | 104.74      | 110.73   |
| 1   | B     | 887 | THR  | N-CA-C  | -5.02 | 106.99      | 112.72   |
| 1   | B     | 979 | VAL  | N-CA-C  | -5.01 | 101.27      | 108.89   |
| 1   | A     | 884 | ALA  | N-CA-C  | 5.01  | 116.00      | 109.64   |
| 1   | D     | 955 | THR  | N-CA-C  | 5.00  | 114.56      | 108.11   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | B     | 986 | TYR  | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2754  | 0        | 2795     | 189     | 0            |
| 1   | B     | 2754  | 0        | 2795     | 247     | 0            |
| 1   | C     | 2754  | 0        | 2795     | 228     | 0            |
| 1   | D     | 2754  | 0        | 2795     | 379     | 0            |
| 2   | A     | 20    | 0        | 10       | 1       | 0            |
| 2   | B     | 20    | 0        | 10       | 2       | 0            |
| 2   | C     | 20    | 0        | 10       | 2       | 0            |
| 2   | D     | 20    | 0        | 10       | 2       | 0            |
| All | All   | 11096 | 0        | 11220    | 1018    | 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 46.

All (1018) 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:C:879:ILE:HD13 | 1:C:879:ILE:H    | 1.19                     | 1.03              |
| 1:B:717:GLN:HE22 | 1:B:887:THR:HB   | 1.23                     | 1.00              |
| 1:B:697:PRO:HG2  | 1:B:700:LYS:HB2  | 1.40                     | 1.00              |
| 1:D:998:ASN:HD22 | 1:D:1000:LYS:HZ2 | 1.10                     | 0.99              |
| 1:B:920:LEU:HD21 | 1:B:999:LEU:HD13 | 1.43                     | 0.99              |
| 1:D:998:ASN:HD22 | 1:D:1000:LYS:NZ  | 1.59                     | 0.99              |
| 1:D:841:ARG:HB3  | 1:D:841:ARG:HH11 | 1.28                     | 0.98              |
| 1:D:962:ILE:HG12 | 1:D:971:LEU:HD11 | 1.46                     | 0.96              |
| 1:D:855:HIS:HA   | 1:D:857:ARG:HH12 | 1.29                     | 0.94              |
| 1:C:697:PRO:HG2  | 1:C:700:LYS:HB2  | 1.50                     | 0.93              |
| 1:D:839:ILE:HD13 | 1:D:1002:LEU:HB2 | 1.49                     | 0.92              |
| 1:D:964:LEU:HD22 | 1:D:965:ASP:H    | 1.32                     | 0.92              |
| 1:B:890:MET:HE2  | 1:B:935:ALA:HB2  | 1.52                     | 0.91              |
| 1:D:849:LYS:HA   | 1:D:852:LYS:HE2  | 1.52                     | 0.90              |
| 1:C:782:SER:HA   | 1:C:792:VAL:HG11 | 1.51                     | 0.90              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:703:LYS:HB3  | 1:C:704:ARG:NH1   | 1.87                     | 0.89              |
| 1:B:717:GLN:NE2  | 1:B:887:THR:HB    | 1.86                     | 0.89              |
| 1:C:754:ASN:HD22 | 1:C:757:SER:HB3   | 1.38                     | 0.88              |
| 1:D:798:LYS:HB3  | 1:D:842:GLU:HB2   | 1.56                     | 0.88              |
| 1:B:800:ASP:HB3  | 1:B:802:LYS:HE3   | 1.55                     | 0.87              |
| 1:D:841:ARG:HB3  | 1:D:841:ARG:NH1   | 1.90                     | 0.87              |
| 1:B:830:ASP:HB3  | 1:B:1008:ASN:HB2  | 1.57                     | 0.87              |
| 1:C:962:ILE:HG22 | 1:C:963:SER:H     | 1.39                     | 0.87              |
| 1:C:879:ILE:H    | 1:C:879:ILE:CD1   | 1.87                     | 0.87              |
| 1:B:878:ARG:HH11 | 1:B:878:ARG:HB3   | 1.38                     | 0.86              |
| 1:D:919:ILE:HD13 | 1:D:920:LEU:H     | 1.37                     | 0.86              |
| 1:D:706:ILE:HG23 | 1:D:765:LEU:HD22  | 1.59                     | 0.84              |
| 1:C:663:SER:HB2  | 1:C:791:ASP:OD1   | 1.77                     | 0.84              |
| 1:C:962:ILE:HG22 | 1:C:963:SER:N     | 1.91                     | 0.84              |
| 1:B:667:LYS:HB3  | 1:B:668:PRO:HD3   | 1.61                     | 0.83              |
| 1:D:930:TYR:HB2  | 1:D:945:LYS:HE2   | 1.60                     | 0.83              |
| 1:B:823:ALA:HB3  | 1:B:826:HIS:HD2   | 1.44                     | 0.82              |
| 1:B:679:VAL:HG23 | 1:B:680:GLU:H     | 1.44                     | 0.82              |
| 1:D:918:LEU:H    | 1:D:918:LEU:HD23  | 1.45                     | 0.81              |
| 1:D:665:LEU:H    | 1:D:665:LEU:HD22  | 1.43                     | 0.81              |
| 1:B:703:LYS:H    | 1:B:704:ARG:HH21  | 1.29                     | 0.80              |
| 1:A:865:ARG:HB2  | 1:A:868:ASN:HB2   | 1.64                     | 0.80              |
| 1:D:751:LEU:HD12 | 1:D:751:LEU:H     | 1.44                     | 0.80              |
| 1:A:839:ILE:HD13 | 1:A:839:ILE:H     | 1.48                     | 0.79              |
| 1:D:962:ILE:HG22 | 1:D:963:SER:H     | 1.47                     | 0.79              |
| 1:C:720:VAL:HG13 | 1:C:721:SER:H     | 1.47                     | 0.79              |
| 1:C:933:LYS:HB2  | 1:C:982:THR:HB    | 1.64                     | 0.79              |
| 1:D:770:ASP:OD1  | 1:D:868:ASN:HA    | 1.83                     | 0.78              |
| 1:B:920:LEU:HD13 | 1:B:1002:LEU:HD23 | 1.66                     | 0.78              |
| 1:C:962:ILE:CG2  | 1:C:963:SER:H     | 1.96                     | 0.78              |
| 1:D:919:ILE:CD1  | 1:D:920:LEU:H     | 1.97                     | 0.78              |
| 1:C:720:VAL:HG13 | 1:C:721:SER:N     | 2.00                     | 0.77              |
| 1:D:739:LEU:HD12 | 1:D:740:ILE:HG12  | 1.67                     | 0.77              |
| 1:C:679:VAL:HA   | 1:C:682:MET:HE3   | 1.67                     | 0.77              |
| 1:C:696:MET:HG3  | 1:C:741:PRO:HD2   | 1.66                     | 0.77              |
| 1:C:831:LEU:HD12 | 1:C:1005:LEU:HD22 | 1.66                     | 0.77              |
| 1:D:664:LYS:HD2  | 1:D:665:LEU:HD22  | 1.67                     | 0.76              |
| 1:D:920:LEU:HD23 | 1:D:921:LEU:N     | 2.00                     | 0.76              |
| 1:A:754:ASN:HD22 | 1:A:754:ASN:N     | 1.83                     | 0.76              |
| 1:D:975:ILE:HG13 | 1:D:976:SER:H     | 1.51                     | 0.76              |
| 1:C:704:ARG:HA   | 1:C:707:GLN:HE21  | 1.50                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:858:ARG:HD3  | 1:A:926:LEU:HD12 | 1.69                     | 0.75              |
| 1:D:865:ARG:HB2  | 1:D:868:ASN:OD1  | 1.86                     | 0.75              |
| 1:A:703:LYS:H    | 1:A:704:ARG:NH2  | 1.84                     | 0.75              |
| 1:D:1004:LYS:HB3 | 1:D:1004:LYS:HZ2 | 1.51                     | 0.75              |
| 1:D:841:ARG:NH2  | 1:D:875:GLN:HA   | 2.01                     | 0.75              |
| 1:A:717:GLN:O    | 1:A:720:VAL:HG12 | 1.88                     | 0.74              |
| 1:B:865:ARG:HB2  | 1:B:868:ASN:ND2  | 2.03                     | 0.74              |
| 1:C:689:TYR:CD1  | 1:C:764:MET:HG2  | 2.23                     | 0.73              |
| 1:D:799:THR:HG22 | 1:D:841:ARG:HA   | 1.68                     | 0.73              |
| 1:D:895:ILE:HD11 | 1:D:994:ILE:HD13 | 1.71                     | 0.73              |
| 1:B:777:LEU:HD11 | 1:B:796:LYS:HB3  | 1.71                     | 0.72              |
| 1:A:923:GLU:O    | 1:A:923:GLU:HG3  | 1.88                     | 0.72              |
| 1:A:878:ARG:HD2  | 1:A:994:ILE:HG21 | 1.71                     | 0.72              |
| 1:C:989:TYR:C    | 1:C:990:ILE:HD12 | 2.15                     | 0.72              |
| 1:B:901:VAL:HG13 | 1:B:902:SER:N    | 2.05                     | 0.72              |
| 1:D:696:MET:HE2  | 1:D:701:LEU:HD23 | 1.71                     | 0.71              |
| 1:B:991:VAL:HG11 | 1:B:996:GLN:HB2  | 1.72                     | 0.71              |
| 1:C:734:ASN:O    | 1:C:738:THR:HG22 | 1.90                     | 0.71              |
| 1:A:763:GLU:HA   | 2:A:1:CNQ:CL24   | 2.27                     | 0.71              |
| 1:C:931:GLU:HG3  | 1:C:951:LEU:HD21 | 1.72                     | 0.71              |
| 1:B:827:ASN:OD1  | 1:D:725:SER:HB3  | 1.91                     | 0.71              |
| 1:B:849:LYS:HB3  | 1:B:850:PRO:HD3  | 1.73                     | 0.70              |
| 1:C:704:ARG:HA   | 1:C:707:GLN:NE2  | 2.06                     | 0.70              |
| 1:D:806:ARG:HG2  | 1:D:807:ASP:OD1  | 1.90                     | 0.70              |
| 1:A:895:ILE:HD11 | 1:A:994:ILE:HG22 | 1.71                     | 0.70              |
| 1:A:943:LYS:N    | 1:A:943:LYS:HE2  | 2.05                     | 0.70              |
| 1:D:683:LYS:O    | 1:D:687:VAL:HG23 | 1.90                     | 0.70              |
| 1:D:676:ILE:HG23 | 1:D:870:ALA:HA   | 1.74                     | 0.70              |
| 1:D:710:TYR:HH   | 1:D:766:ASP:CG   | 2.00                     | 0.69              |
| 1:C:788:ASP:HB2  | 1:C:789:PRO:HD2  | 1.75                     | 0.69              |
| 1:D:770:ASP:CG   | 1:D:868:ASN:HA   | 2.17                     | 0.69              |
| 1:A:748:LYS:HG2  | 1:C:688:GLU:HB3  | 1.72                     | 0.69              |
| 1:C:706:ILE:HG23 | 1:C:765:LEU:HD22 | 1.72                     | 0.69              |
| 1:D:821:THR:O    | 1:D:901:VAL:HG12 | 1.91                     | 0.69              |
| 1:A:805:ASP:O    | 1:A:808:SER:HB3  | 1.93                     | 0.69              |
| 1:C:696:MET:CE   | 1:C:700:LYS:HB3  | 2.23                     | 0.69              |
| 1:C:895:ILE:O    | 1:C:990:ILE:HA   | 1.93                     | 0.69              |
| 1:C:788:ASP:HB2  | 1:C:789:PRO:CD   | 2.23                     | 0.69              |
| 1:D:841:ARG:HE   | 1:D:876:GLY:H    | 1.41                     | 0.68              |
| 1:B:765:LEU:HA   | 1:B:768:LEU:HD12 | 1.75                     | 0.68              |
| 1:D:744:PHE:HB3  | 1:D:747:LYS:HG3  | 1.75                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:746:MET:HA    | 1:C:746:MET:HE2   | 1.75                     | 0.68              |
| 1:C:816:LYS:HE2   | 1:C:820:ASN:CG    | 2.19                     | 0.68              |
| 1:C:903:LYS:NZ    | 1:C:988:GLU:HG3   | 2.09                     | 0.68              |
| 1:B:717:GLN:O     | 1:B:720:VAL:HG12  | 1.93                     | 0.68              |
| 1:C:943:LYS:HD3   | 1:C:944:GLY:H     | 1.59                     | 0.68              |
| 1:D:704:ARG:HA    | 1:D:707:GLN:NE2   | 2.08                     | 0.68              |
| 1:D:921:LEU:HD12  | 1:D:1003:LEU:HD11 | 1.74                     | 0.68              |
| 1:D:963:SER:O     | 1:D:964:LEU:HB2   | 1.91                     | 0.67              |
| 1:D:901:VAL:HG13  | 1:D:902:SER:N     | 2.09                     | 0.67              |
| 1:A:926:LEU:O     | 1:A:946:HIS:HB2   | 1.94                     | 0.67              |
| 1:C:826:HIS:HD2   | 1:C:902:SER:OG    | 1.76                     | 0.67              |
| 1:C:828:ALA:C     | 1:C:1010:LYS:HG2  | 2.20                     | 0.67              |
| 1:A:849:LYS:HB3   | 1:A:850:PRO:HD3   | 1.75                     | 0.67              |
| 1:D:662:LYS:O     | 1:D:787:LYS:HB3   | 1.95                     | 0.67              |
| 1:D:826:HIS:ND1   | 1:D:902:SER:HB2   | 2.09                     | 0.67              |
| 1:A:822:HIS:HA    | 1:A:902:SER:OG    | 1.95                     | 0.67              |
| 1:B:748:LYS:HB2   | 1:D:688:GLU:HG3   | 1.74                     | 0.67              |
| 1:B:1002:LEU:HD13 | 1:B:1003:LEU:N    | 2.10                     | 0.67              |
| 1:C:860:LEU:HB3   | 1:C:897:PHE:HB3   | 1.77                     | 0.67              |
| 1:D:664:LYS:HZ2   | 1:D:665:LEU:HD21  | 1.59                     | 0.67              |
| 1:D:864:SER:O     | 1:D:908:CYS:HA    | 1.95                     | 0.67              |
| 1:C:890:MET:HG2   | 1:C:891:PHE:CD2   | 2.30                     | 0.66              |
| 1:D:1006:LYS:HZ2  | 1:D:1008:ASN:H    | 1.40                     | 0.66              |
| 1:D:748:LYS:HD2   | 1:D:749:PRO:HD2   | 1.78                     | 0.66              |
| 1:C:667:LYS:HB3   | 1:C:668:PRO:HD3   | 1.76                     | 0.66              |
| 1:B:854:LEU:HD21  | 1:B:927:GLY:HA3   | 1.76                     | 0.66              |
| 1:B:856:ASN:HB3   | 1:B:927:GLY:H     | 1.61                     | 0.66              |
| 1:D:919:ILE:HG23  | 1:D:920:LEU:N     | 2.11                     | 0.66              |
| 1:B:841:ARG:HH12  | 1:B:874:SER:C     | 2.04                     | 0.66              |
| 1:D:692:ASP:C     | 1:D:694:GLN:H     | 2.04                     | 0.66              |
| 1:B:822:HIS:NE2   | 1:B:831:LEU:HD13  | 2.11                     | 0.65              |
| 1:B:956:PRO:HB3   | 1:B:972:GLY:O     | 1.96                     | 0.65              |
| 1:A:891:PHE:HB2   | 1:A:990:ILE:CD1   | 2.26                     | 0.65              |
| 1:D:856:ASN:OD1   | 1:D:929:MET:HE3   | 1.97                     | 0.65              |
| 1:B:799:THR:HG23  | 1:B:801:ILE:HD11  | 1.76                     | 0.65              |
| 1:C:704:ARG:H     | 1:C:704:ARG:NE    | 1.94                     | 0.65              |
| 1:C:797:LEU:HB3   | 1:C:799:THR:HG22  | 1.79                     | 0.65              |
| 1:D:859:LEU:HD23  | 1:D:923:GLU:HB3   | 1.78                     | 0.65              |
| 1:D:933:LYS:HD2   | 1:D:979:VAL:CG1   | 2.26                     | 0.65              |
| 1:A:826:HIS:HA    | 1:C:726:ASP:OD2   | 1.97                     | 0.65              |
| 1:B:854:LEU:CD2   | 1:B:927:GLY:HA3   | 2.25                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:878:ARG:HB3  | 1:B:878:ARG:NH1  | 2.10                     | 0.65              |
| 1:D:811:ALA:O    | 1:D:815:ARG:HG3  | 1.95                     | 0.65              |
| 1:D:702:SER:HA   | 1:D:772:GLU:HG3  | 1.79                     | 0.65              |
| 1:A:927:GLY:HA3  | 1:A:946:HIS:ND1  | 2.12                     | 0.65              |
| 1:D:998:ASN:ND2  | 1:D:1000:LYS:HZ2 | 1.90                     | 0.65              |
| 1:C:729:ILE:HG21 | 1:C:753:ASN:HD22 | 1.61                     | 0.65              |
| 1:D:868:ASN:O    | 1:D:870:ALA:N    | 2.30                     | 0.65              |
| 1:D:964:LEU:HD22 | 1:D:965:ASP:N    | 2.08                     | 0.65              |
| 1:B:745:GLY:O    | 1:B:746:MET:HE2  | 1.97                     | 0.65              |
| 1:D:855:HIS:HA   | 1:D:857:ARG:NH1  | 2.08                     | 0.65              |
| 1:D:875:GLN:O    | 1:D:876:GLY:O    | 2.16                     | 0.65              |
| 1:A:830:ASP:O    | 1:A:831:LEU:HD23 | 1.96                     | 0.64              |
| 1:D:835:ASP:HB3  | 1:D:837:PHE:CZ   | 2.33                     | 0.64              |
| 1:B:690:GLU:HG2  | 1:B:744:PHE:CE1  | 2.32                     | 0.64              |
| 1:C:729:ILE:HD12 | 1:C:729:ILE:H    | 1.61                     | 0.64              |
| 1:D:845:CYS:O    | 1:D:849:LYS:HG3  | 1.98                     | 0.64              |
| 1:C:890:MET:HG2  | 1:C:891:PHE:CE2  | 2.33                     | 0.64              |
| 1:A:916:ILE:H    | 1:A:916:ILE:HD12 | 1.63                     | 0.64              |
| 1:D:858:ARG:HA   | 1:D:968:ASP:H    | 1.63                     | 0.64              |
| 1:A:798:LYS:NZ   | 1:A:798:LYS:HB3  | 2.12                     | 0.64              |
| 1:B:761:LYS:HE2  | 1:B:761:LYS:HA   | 1.80                     | 0.64              |
| 1:B:823:ALA:HB3  | 1:B:826:HIS:CD2  | 2.30                     | 0.64              |
| 1:A:698:LEU:HD23 | 1:A:701:LEU:HD12 | 1.80                     | 0.63              |
| 1:B:702:SER:HB3  | 1:B:705:GLN:HB3  | 1.79                     | 0.63              |
| 1:B:813:ILE:HG22 | 1:B:814:ILE:N    | 2.12                     | 0.63              |
| 1:A:692:ASP:OD2  | 1:A:695:LYS:HD3  | 1.98                     | 0.63              |
| 1:D:670:GLN:C    | 1:D:672:LEU:H    | 2.05                     | 0.63              |
| 1:D:788:ASP:CG   | 1:D:789:PRO:HD2  | 2.23                     | 0.63              |
| 1:C:665:LEU:HD23 | 1:C:791:ASP:OD1  | 1.98                     | 0.63              |
| 1:D:861:TRP:O    | 1:D:862:HIS:HB2  | 1.96                     | 0.63              |
| 1:A:703:LYS:NZ   | 1:A:769:LEU:HD22 | 2.13                     | 0.63              |
| 1:A:839:ILE:HD12 | 1:A:1002:LEU:HB2 | 1.81                     | 0.63              |
| 1:B:916:ILE:HG22 | 1:B:1006:LYS:HA  | 1.80                     | 0.63              |
| 1:D:793:ASN:O    | 1:D:796:LYS:HG2  | 1.97                     | 0.63              |
| 1:D:1004:LYS:HD2 | 1:D:1004:LYS:C   | 2.23                     | 0.63              |
| 1:A:858:ARG:HD3  | 1:A:926:LEU:CD1  | 2.28                     | 0.63              |
| 1:B:887:THR:HG22 | 1:B:887:THR:O    | 1.96                     | 0.63              |
| 1:C:828:ALA:O    | 1:C:1010:LYS:HG2 | 1.98                     | 0.63              |
| 1:B:931:GLU:O    | 1:B:932:LEU:HD23 | 1.98                     | 0.63              |
| 1:C:841:ARG:HG2  | 1:C:841:ARG:HH11 | 1.63                     | 0.63              |
| 1:A:672:LEU:HD12 | 1:A:673:ILE:N    | 2.14                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:702:SER:HB2  | 1:C:704:ARG:NH2  | 2.14                     | 0.63              |
| 1:D:675:MET:HE2  | 1:D:866:THR:HG21 | 1.81                     | 0.63              |
| 1:B:703:LYS:N    | 1:B:704:ARG:HH21 | 1.96                     | 0.63              |
| 1:B:941:LEU:HD12 | 1:B:941:LEU:N    | 2.14                     | 0.63              |
| 1:D:764:MET:HE3  | 1:D:768:LEU:HD11 | 1.79                     | 0.63              |
| 1:D:989:TYR:C    | 1:D:990:ILE:HD12 | 2.23                     | 0.63              |
| 1:B:829:TYR:CE1  | 1:B:831:LEU:HD11 | 2.34                     | 0.62              |
| 1:B:1006:LYS:HB2 | 1:B:1006:LYS:NZ  | 2.14                     | 0.62              |
| 1:D:674:LYS:HD2  | 1:D:675:MET:N    | 2.13                     | 0.62              |
| 1:D:847:ARG:HD3  | 1:D:995:ALA:HA   | 1.80                     | 0.62              |
| 1:A:804:VAL:HB   | 1:A:836:ILE:HG22 | 1.80                     | 0.62              |
| 1:A:878:ARG:NH1  | 1:A:879:ILE:HG12 | 2.14                     | 0.62              |
| 1:D:918:LEU:HD23 | 1:D:918:LEU:N    | 2.14                     | 0.62              |
| 1:B:865:ARG:HH11 | 1:B:865:ARG:HG2  | 1.64                     | 0.62              |
| 1:B:993:ASP:HB3  | 1:B:996:GLN:HE21 | 1.64                     | 0.62              |
| 1:D:693:LEU:HD12 | 1:D:697:PRO:HA   | 1.82                     | 0.62              |
| 1:A:754:ASN:N    | 1:A:754:ASN:ND2  | 2.45                     | 0.62              |
| 1:D:868:ASN:C    | 1:D:870:ALA:H    | 2.08                     | 0.62              |
| 1:D:925:ALA:HB3  | 1:D:996:GLN:HG3  | 1.81                     | 0.62              |
| 1:B:907:TYR:CD1  | 2:B:2:CNQ:H15    | 2.35                     | 0.62              |
| 1:D:829:TYR:HA   | 1:D:1010:LYS:HE2 | 1.80                     | 0.62              |
| 1:C:920:LEU:HD13 | 1:C:999:LEU:HD22 | 1.81                     | 0.62              |
| 1:D:940:LYS:H    | 1:D:940:LYS:HD2  | 1.64                     | 0.62              |
| 1:D:778:LEU:C    | 1:D:780:GLY:H    | 2.07                     | 0.62              |
| 1:D:1004:LYS:HD2 | 1:D:1005:LEU:N   | 2.15                     | 0.62              |
| 1:B:697:PRO:HG2  | 1:B:700:LYS:CB   | 2.22                     | 0.61              |
| 1:D:852:LYS:C    | 1:D:854:LEU:H    | 2.08                     | 0.61              |
| 1:A:960:ALA:HB3  | 1:A:972:GLY:HA3  | 1.83                     | 0.61              |
| 1:B:770:ASP:HB3  | 1:B:868:ASN:HA   | 1.81                     | 0.61              |
| 1:C:752:LEU:HB3  | 1:C:758:VAL:HG12 | 1.82                     | 0.61              |
| 1:D:802:LYS:HB3  | 1:D:838:LYS:HB3  | 1.82                     | 0.61              |
| 1:D:720:VAL:HG13 | 1:D:721:SER:N    | 2.15                     | 0.61              |
| 1:D:671:ASP:O    | 1:D:674:LYS:HE2  | 1.99                     | 0.61              |
| 1:C:834:ILE:HD11 | 1:C:1006:LYS:CG  | 2.30                     | 0.61              |
| 1:D:751:LEU:HD12 | 1:D:751:LEU:N    | 2.15                     | 0.61              |
| 1:D:872:ILE:O    | 1:D:876:GLY:HA2  | 1.99                     | 0.61              |
| 1:C:834:ILE:HB   | 1:C:1004:LYS:O   | 2.01                     | 0.61              |
| 1:D:693:LEU:CD1  | 1:D:697:PRO:HA   | 2.31                     | 0.61              |
| 1:A:703:LYS:N    | 1:A:704:ARG:NH2  | 2.49                     | 0.61              |
| 1:B:862:HIS:NE2  | 1:B:877:LEU:HD21 | 2.15                     | 0.61              |
| 1:B:865:ARG:HB2  | 1:B:868:ASN:HD21 | 1.66                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:788:ASP:OD1  | 1:B:789:PRO:HD2   | 2.00                     | 0.61              |
| 1:A:694:GLN:HB3  | 1:A:695:LYS:HD2   | 1.83                     | 0.60              |
| 1:A:739:LEU:O    | 1:A:741:PRO:HD3   | 2.01                     | 0.60              |
| 1:A:891:PHE:HA   | 1:A:936:SER:O     | 2.01                     | 0.60              |
| 1:B:1002:LEU:C   | 1:B:1003:LEU:HD12 | 2.25                     | 0.60              |
| 1:D:821:THR:O    | 1:D:901:VAL:N     | 2.33                     | 0.60              |
| 1:A:866:THR:HG23 | 1:A:867:THR:N     | 2.15                     | 0.60              |
| 1:A:916:ILE:HD12 | 1:A:916:ILE:N     | 2.16                     | 0.60              |
| 1:A:929:MET:HG2  | 1:A:947:SER:OG    | 2.01                     | 0.60              |
| 1:B:729:ILE:HD13 | 1:B:753:ASN:HA    | 1.83                     | 0.60              |
| 1:B:868:ASN:O    | 1:B:872:ILE:HG13  | 2.00                     | 0.60              |
| 1:C:720:VAL:CG1  | 1:C:721:SER:H     | 2.14                     | 0.60              |
| 1:D:663:SER:HB2  | 1:D:790:ILE:HD11  | 1.83                     | 0.60              |
| 1:D:992:TYR:CD1  | 1:D:992:TYR:N     | 2.68                     | 0.60              |
| 1:C:865:ARG:O    | 1:C:868:ASN:HB2   | 2.02                     | 0.60              |
| 1:D:694:GLN:NE2  | 1:D:694:GLN:HA    | 2.15                     | 0.60              |
| 1:A:754:ASN:ND2  | 1:A:754:ASN:H     | 1.99                     | 0.60              |
| 1:C:683:LYS:HA   | 1:C:686:MET:HE3   | 1.82                     | 0.60              |
| 1:C:805:ASP:C    | 1:C:807:ASP:H     | 2.08                     | 0.60              |
| 1:D:806:ARG:H    | 1:D:806:ARG:HD2   | 1.64                     | 0.60              |
| 1:D:994:ILE:O    | 1:D:997:VAL:HG12  | 2.02                     | 0.60              |
| 1:D:1007:PHE:O   | 1:D:1008:ASN:C    | 2.43                     | 0.60              |
| 1:D:722:GLN:O    | 1:D:722:GLN:HG2   | 2.00                     | 0.60              |
| 1:A:670:GLN:O    | 1:A:674:LYS:HG2   | 2.02                     | 0.60              |
| 1:A:672:LEU:HD23 | 1:A:837:PHE:CE2   | 2.37                     | 0.60              |
| 1:B:692:ASP:HB2  | 1:B:743:ASP:HB2   | 1.84                     | 0.60              |
| 1:C:767:ASN:HD22 | 1:C:865:ARG:HE    | 1.50                     | 0.60              |
| 1:D:866:THR:HA   | 1:D:918:LEU:HD21  | 1.83                     | 0.60              |
| 1:C:849:LYS:O    | 1:C:849:LYS:HD3   | 2.01                     | 0.60              |
| 1:C:858:ARG:HG3  | 1:C:860:LEU:HD21  | 1.84                     | 0.60              |
| 1:D:678:ASP:O    | 1:D:682:MET:HG3   | 2.02                     | 0.60              |
| 1:A:677:PHE:CE2  | 1:A:793:ASN:HB3   | 2.37                     | 0.59              |
| 1:B:900:MET:CE   | 1:B:956:PRO:HG3   | 2.32                     | 0.59              |
| 1:D:831:LEU:HB3  | 1:D:1005:LEU:HD22 | 1.84                     | 0.59              |
| 1:D:862:HIS:HE2  | 1:D:877:LEU:HD22  | 1.65                     | 0.59              |
| 1:B:699:GLY:HA2  | 1:B:775:TYR:CE2   | 2.37                     | 0.59              |
| 1:C:816:LYS:HE3  | 1:C:816:LYS:HA    | 1.83                     | 0.59              |
| 1:B:748:LYS:HD3  | 1:B:749:PRO:N     | 2.17                     | 0.59              |
| 1:B:735:ARG:HH11 | 1:B:735:ARG:HG2   | 1.65                     | 0.59              |
| 1:B:830:ASP:HB2  | 1:B:1010:LYS:NZ   | 2.17                     | 0.59              |
| 1:D:836:ILE:HD12 | 1:D:836:ILE:N     | 2.17                     | 0.59              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:690:GLU:OE2   | 1:B:744:PHE:HA   | 2.03                     | 0.59              |
| 1:C:729:ILE:HD12  | 1:C:729:ILE:N    | 2.18                     | 0.59              |
| 1:D:671:ASP:HA    | 1:D:674:LYS:HZ3  | 1.68                     | 0.59              |
| 1:C:834:ILE:HD11  | 1:C:1006:LYS:HG2 | 1.84                     | 0.59              |
| 1:D:739:LEU:CD1   | 1:D:740:ILE:HG12 | 2.31                     | 0.59              |
| 1:D:747:LYS:HB2   | 1:D:747:LYS:NZ   | 2.18                     | 0.59              |
| 1:A:759:GLN:HA    | 1:A:762:VAL:HG23 | 1.85                     | 0.59              |
| 1:B:880:ALA:HB3   | 1:B:893:LYS:HG2  | 1.85                     | 0.59              |
| 1:B:829:TYR:CD1   | 1:B:831:LEU:HD11 | 2.37                     | 0.59              |
| 1:C:863:GLY:HA3   | 1:C:904:SER:O    | 2.03                     | 0.59              |
| 1:D:855:HIS:CA    | 1:D:857:ARG:HH12 | 2.11                     | 0.59              |
| 1:D:890:MET:SD    | 1:D:984:LEU:HD21 | 2.43                     | 0.59              |
| 1:A:735:ARG:O     | 1:A:738:THR:HG22 | 2.02                     | 0.58              |
| 1:D:831:LEU:N     | 1:D:831:LEU:HD22 | 2.17                     | 0.58              |
| 1:B:859:LEU:HD13  | 1:B:921:LEU:HD21 | 1.85                     | 0.58              |
| 1:B:878:ARG:HH12  | 1:B:879:ILE:HG12 | 1.67                     | 0.58              |
| 1:C:798:LYS:HD2   | 1:C:842:GLU:CD   | 2.28                     | 0.58              |
| 1:A:788:ASP:C     | 1:A:790:ILE:H    | 2.11                     | 0.58              |
| 1:B:855:HIS:O     | 1:B:927:GLY:HA2  | 2.03                     | 0.58              |
| 1:B:991:VAL:HG13  | 1:B:996:GLN:NE2  | 2.18                     | 0.58              |
| 1:C:689:TYR:O     | 1:C:690:GLU:HB2  | 2.03                     | 0.58              |
| 1:A:798:LYS:HB3   | 1:A:798:LYS:HZ3  | 1.64                     | 0.58              |
| 1:B:739:LEU:HD13  | 1:B:739:LEU:O    | 2.02                     | 0.58              |
| 1:B:859:LEU:HD22  | 1:B:921:LEU:HD23 | 1.86                     | 0.58              |
| 1:D:694:GLN:HA    | 1:D:694:GLN:HE21 | 1.68                     | 0.58              |
| 1:D:710:TYR:OH    | 1:D:766:ASP:CG   | 2.46                     | 0.58              |
| 1:A:1003:LEU:HD12 | 1:A:1003:LEU:N   | 2.18                     | 0.58              |
| 1:C:686:MET:HE3   | 1:C:693:LEU:HD21 | 1.85                     | 0.58              |
| 1:D:849:LYS:NZ    | 1:D:849:LYS:HB3  | 2.18                     | 0.58              |
| 1:A:754:ASN:CG    | 1:A:757:SER:HB3  | 2.28                     | 0.58              |
| 1:B:675:MET:HE1   | 1:B:1004:LYS:HE2 | 1.85                     | 0.58              |
| 1:C:706:ILE:CG2   | 1:C:765:LEU:HD22 | 2.34                     | 0.58              |
| 1:A:722:GLN:HE21  | 1:A:722:GLN:N    | 2.01                     | 0.58              |
| 1:A:742:HIS:NE2   | 1:A:764:MET:HE1  | 2.19                     | 0.58              |
| 1:D:667:LYS:HB3   | 1:D:668:PRO:HD3  | 1.84                     | 0.58              |
| 1:C:990:ILE:HD12  | 1:C:990:ILE:N    | 2.19                     | 0.58              |
| 1:A:735:ARG:HA    | 1:A:738:THR:HG22 | 1.85                     | 0.57              |
| 1:A:835:ASP:HB2   | 1:A:1004:LYS:HB3 | 1.85                     | 0.57              |
| 1:C:778:LEU:HD23  | 1:C:778:LEU:O    | 2.03                     | 0.57              |
| 1:C:943:LYS:HD3   | 1:C:944:GLY:N    | 2.18                     | 0.57              |
| 1:D:664:LYS:HZ2   | 1:D:665:LEU:HD11 | 1.68                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:664:LYS:HZ2  | 1:D:665:LEU:CD2   | 2.16                     | 0.57              |
| 1:D:709:ALA:HB1  | 1:D:765:LEU:HD11  | 1.86                     | 0.57              |
| 1:A:703:LYS:HZ3  | 1:A:769:LEU:HD22  | 1.68                     | 0.57              |
| 1:C:814:ILE:O    | 1:C:818:VAL:HG23  | 2.04                     | 0.57              |
| 1:D:799:THR:HG21 | 1:D:873:LEU:HB3   | 1.87                     | 0.57              |
| 1:B:739:LEU:HD13 | 1:B:739:LEU:C     | 2.29                     | 0.57              |
| 1:B:878:ARG:NH1  | 1:B:879:ILE:N     | 2.52                     | 0.57              |
| 1:C:759:GLN:HA   | 1:C:759:GLN:HE21  | 1.67                     | 0.57              |
| 1:A:735:ARG:C    | 1:A:738:THR:HG22  | 2.29                     | 0.57              |
| 1:B:702:SER:HB3  | 1:B:705:GLN:CB    | 2.35                     | 0.57              |
| 1:B:704:ARG:H    | 1:B:704:ARG:NE    | 2.02                     | 0.57              |
| 1:B:747:LYS:HG2  | 1:B:748:LYS:N     | 2.18                     | 0.57              |
| 1:B:830:ASP:HB3  | 1:B:1008:ASN:HD22 | 1.68                     | 0.57              |
| 1:C:879:ILE:HD13 | 1:C:879:ILE:N     | 2.03                     | 0.57              |
| 1:B:901:VAL:CG1  | 1:B:902:SER:N     | 2.67                     | 0.57              |
| 1:C:669:VAL:O    | 1:C:673:ILE:HG12  | 2.05                     | 0.57              |
| 1:C:946:HIS:O    | 1:C:947:SER:HB3   | 2.03                     | 0.57              |
| 1:A:707:GLN:O    | 1:A:710:TYR:HB2   | 2.04                     | 0.57              |
| 1:C:682:MET:HE1  | 1:C:778:LEU:HD13  | 1.86                     | 0.57              |
| 1:D:849:LYS:HB2  | 1:D:850:PRO:HD3   | 1.87                     | 0.57              |
| 1:A:938:ILE:HD12 | 1:A:948:VAL:HG21  | 1.87                     | 0.57              |
| 1:B:669:VAL:O    | 1:B:673:ILE:HG12  | 2.04                     | 0.57              |
| 1:B:878:ARG:NH1  | 1:B:879:ILE:H     | 2.03                     | 0.57              |
| 1:D:931:GLU:HA   | 1:D:949:LYS:O     | 2.05                     | 0.56              |
| 1:A:940:LYS:NZ   | 1:A:943:LYS:HE3   | 2.20                     | 0.56              |
| 1:C:679:VAL:O    | 1:C:682:MET:HB2   | 2.06                     | 0.56              |
| 1:C:754:ASN:HD22 | 1:C:757:SER:CB    | 2.13                     | 0.56              |
| 1:D:843:GLY:C    | 1:D:845:CYS:H     | 2.12                     | 0.56              |
| 1:D:1004:LYS:HB3 | 1:D:1004:LYS:NZ   | 2.18                     | 0.56              |
| 1:C:717:GLN:C    | 1:C:719:ALA:H     | 2.13                     | 0.56              |
| 1:A:709:ALA:HB2  | 1:A:739:LEU:HD23  | 1.88                     | 0.56              |
| 1:C:744:PHE:HD2  | 1:C:749:PRO:HG3   | 1.70                     | 0.56              |
| 1:D:917:GLY:H    | 1:D:1007:PHE:HE1  | 1.54                     | 0.56              |
| 1:B:720:VAL:HG21 | 1:B:755:ALA:HB2   | 1.88                     | 0.56              |
| 1:B:775:TYR:O    | 1:B:779:ARG:HG2   | 2.05                     | 0.56              |
| 1:D:712:ILE:O    | 1:D:716:VAL:HG23  | 2.04                     | 0.56              |
| 1:D:878:ARG:NH1  | 1:D:879:ILE:HG12  | 2.20                     | 0.56              |
| 1:D:854:LEU:HD23 | 1:D:946:HIS:ND1   | 2.20                     | 0.56              |
| 1:B:667:LYS:CB   | 1:B:668:PRO:HD3   | 2.35                     | 0.56              |
| 1:B:830:ASP:HB2  | 1:B:1010:LYS:HZ1  | 1.71                     | 0.56              |
| 1:C:754:ASN:O    | 1:C:756:ASP:N     | 2.36                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:861:TRP:CZ2   | 1:D:901:VAL:HB    | 2.41                     | 0.56              |
| 1:A:706:ILE:HG23  | 1:A:765:LEU:HG    | 1.88                     | 0.56              |
| 1:B:680:GLU:HA    | 1:B:683:LYS:HE2   | 1.88                     | 0.56              |
| 1:D:663:SER:CB    | 1:D:790:ILE:HD11  | 2.35                     | 0.56              |
| 1:D:689:TYR:CG    | 1:D:764:MET:HG3   | 2.41                     | 0.56              |
| 1:D:975:ILE:HG13  | 1:D:976:SER:N     | 2.21                     | 0.56              |
| 1:A:878:ARG:CZ    | 1:A:879:ILE:HG12  | 2.36                     | 0.56              |
| 1:B:799:THR:CG2   | 1:B:801:ILE:HD11  | 2.35                     | 0.56              |
| 1:C:988:GLU:HG2   | 2:C:3:CNQ:H2      | 1.87                     | 0.56              |
| 1:D:930:TYR:CB    | 1:D:945:LYS:HE2   | 2.35                     | 0.56              |
| 1:A:855:HIS:O     | 1:A:856:ASN:HB2   | 2.04                     | 0.55              |
| 1:B:777:LEU:HD13  | 1:B:777:LEU:C     | 2.31                     | 0.55              |
| 1:C:720:VAL:CG1   | 1:C:721:SER:N     | 2.69                     | 0.55              |
| 1:C:930:TYR:HB3   | 1:C:948:VAL:HG22  | 1.88                     | 0.55              |
| 1:B:920:LEU:CD1   | 1:B:1002:LEU:HD23 | 2.34                     | 0.55              |
| 1:D:703:LYS:HE2   | 1:D:707:GLN:OE1   | 2.07                     | 0.55              |
| 1:D:853:GLN:C     | 1:D:854:LEU:HD12  | 2.32                     | 0.55              |
| 1:C:707:GLN:O     | 1:C:710:TYR:HB2   | 2.07                     | 0.55              |
| 1:B:673:ILE:HD11  | 1:B:794:TYR:HD1   | 1.71                     | 0.55              |
| 1:D:864:SER:HB3   | 1:D:869:PHE:CE1   | 2.41                     | 0.55              |
| 1:C:663:SER:CB    | 1:C:791:ASP:OD1   | 2.54                     | 0.55              |
| 1:C:731:ASP:OD2   | 1:C:735:ARG:HD2   | 2.06                     | 0.55              |
| 1:D:963:SER:O     | 1:D:964:LEU:CB    | 2.54                     | 0.55              |
| 1:A:838:LYS:HD2   | 1:A:1001:TYR:CE1  | 2.42                     | 0.55              |
| 1:B:896:TYR:CE2   | 1:B:990:ILE:HG12  | 2.42                     | 0.55              |
| 1:B:942:PRO:O     | 1:B:945:LYS:HB2   | 2.07                     | 0.55              |
| 1:C:703:LYS:HB3   | 1:C:704:ARG:HH11  | 1.71                     | 0.55              |
| 1:C:731:ASP:OD2   | 1:C:731:ASP:C     | 2.49                     | 0.55              |
| 1:D:689:TYR:CD1   | 1:D:764:MET:HG3   | 2.41                     | 0.55              |
| 1:D:670:GLN:C     | 1:D:672:LEU:N     | 2.64                     | 0.55              |
| 1:D:887:THR:O     | 1:D:887:THR:HG22  | 2.07                     | 0.55              |
| 1:D:1003:LEU:HD12 | 1:D:1003:LEU:H    | 1.73                     | 0.55              |
| 1:A:748:LYS:HA    | 1:A:748:LYS:HE2   | 1.88                     | 0.54              |
| 1:B:869:PHE:CE2   | 1:B:1002:LEU:HD21 | 2.42                     | 0.54              |
| 1:D:709:ALA:CB    | 1:D:765:LEU:HD11  | 2.37                     | 0.54              |
| 1:A:718:GLN:O     | 1:A:722:GLN:HB2   | 2.07                     | 0.54              |
| 1:B:1005:LEU:HD12 | 1:B:1005:LEU:N    | 2.23                     | 0.54              |
| 1:B:790:ILE:HG22  | 1:B:791:ASP:N     | 2.23                     | 0.54              |
| 1:D:706:ILE:O     | 1:D:709:ALA:HB3   | 2.08                     | 0.54              |
| 1:D:714:SER:O     | 1:D:717:GLN:HG2   | 2.08                     | 0.54              |
| 1:A:752:LEU:HD11  | 1:A:761:LYS:NZ    | 2.22                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:792:VAL:O     | 1:A:796:LYS:HG3  | 2.07                     | 0.54              |
| 1:B:907:TYR:CE1   | 2:B:2:CNQ:H15    | 2.42                     | 0.54              |
| 1:B:859:LEU:HD13  | 1:B:921:LEU:CD2  | 2.37                     | 0.54              |
| 1:C:849:LYS:O     | 1:C:852:LYS:HB3  | 2.07                     | 0.54              |
| 1:D:891:PHE:HA    | 1:D:936:SER:O    | 2.07                     | 0.54              |
| 1:D:712:ILE:HG13  | 1:D:739:LEU:HD21 | 1.90                     | 0.54              |
| 1:B:818:VAL:O     | 1:B:901:VAL:HG11 | 2.07                     | 0.54              |
| 1:C:777:LEU:HD11  | 1:C:796:LYS:HB3  | 1.89                     | 0.54              |
| 1:A:735:ARG:HA    | 1:A:738:THR:CG2  | 2.38                     | 0.54              |
| 1:B:727:SER:OG    | 1:D:828:ALA:HA   | 2.07                     | 0.54              |
| 1:D:662:LYS:HA    | 1:D:788:ASP:H    | 1.72                     | 0.54              |
| 1:D:812:GLU:HA    | 1:D:815:ARG:HD2  | 1.89                     | 0.54              |
| 1:D:964:LEU:HD13  | 1:D:965:ASP:N    | 2.23                     | 0.54              |
| 1:D:770:ASP:OD2   | 1:D:868:ASN:O    | 2.26                     | 0.54              |
| 1:D:779:ARG:HA    | 1:D:779:ARG:NE   | 2.22                     | 0.54              |
| 1:D:879:ILE:O     | 1:D:880:ALA:C    | 2.51                     | 0.54              |
| 1:A:962:ILE:HG12  | 1:A:971:LEU:HD11 | 1.89                     | 0.53              |
| 1:B:717:GLN:C     | 1:B:720:VAL:HG12 | 2.33                     | 0.53              |
| 1:B:792:VAL:O     | 1:B:795:GLU:HG3  | 2.08                     | 0.53              |
| 1:C:905:ALA:C     | 1:C:907:TYR:H    | 2.15                     | 0.53              |
| 1:D:839:ILE:CD1   | 1:D:1002:LEU:HB2 | 2.30                     | 0.53              |
| 1:D:933:LYS:HD2   | 1:D:979:VAL:HG11 | 1.91                     | 0.53              |
| 1:B:865:ARG:HG2   | 1:B:865:ARG:NH1  | 2.23                     | 0.53              |
| 1:D:713:LEU:HD11  | 1:D:765:LEU:HD12 | 1.90                     | 0.53              |
| 1:D:856:ASN:HB3   | 1:D:926:LEU:HB2  | 1.90                     | 0.53              |
| 1:A:897:PHE:HB2   | 1:A:989:TYR:HB2  | 1.90                     | 0.53              |
| 1:D:992:TYR:N     | 1:D:992:TYR:HD1  | 2.06                     | 0.53              |
| 1:D:1003:LEU:HD12 | 1:D:1003:LEU:N   | 2.23                     | 0.53              |
| 1:C:778:LEU:HD23  | 1:C:778:LEU:C    | 2.33                     | 0.53              |
| 1:D:852:LYS:O     | 1:D:854:LEU:N    | 2.41                     | 0.53              |
| 1:A:724:SER:O     | 1:A:725:SER:HB3  | 2.08                     | 0.53              |
| 1:B:739:LEU:O     | 1:B:741:PRO:HD3  | 2.09                     | 0.53              |
| 1:C:702:SER:HB2   | 1:C:704:ARG:HH21 | 1.71                     | 0.53              |
| 1:D:720:VAL:HG13  | 1:D:721:SER:H    | 1.73                     | 0.53              |
| 1:A:718:GLN:C     | 1:A:718:GLN:NE2  | 2.67                     | 0.53              |
| 1:A:994:ILE:O     | 1:A:997:VAL:HG12 | 2.08                     | 0.53              |
| 1:C:716:VAL:O     | 1:C:720:VAL:HG12 | 2.09                     | 0.53              |
| 1:C:903:LYS:HZ3   | 1:C:988:GLU:HG3  | 1.73                     | 0.53              |
| 1:D:664:LYS:HD2   | 1:D:665:LEU:H    | 1.73                     | 0.53              |
| 1:D:692:ASP:O     | 1:D:694:GLN:N    | 2.42                     | 0.53              |
| 1:D:794:TYR:HD2   | 1:D:794:TYR:O    | 1.92                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:879:ILE:CG2  | 1:D:894:GLY:HA2  | 2.39                     | 0.53              |
| 1:A:753:ASN:C    | 1:A:755:ALA:H    | 2.17                     | 0.52              |
| 1:C:960:ALA:HB3  | 1:C:972:GLY:HA3  | 1.90                     | 0.52              |
| 1:D:832:GLU:O    | 1:D:834:ILE:HG12 | 2.09                     | 0.52              |
| 1:B:667:LYS:HE3  | 1:B:671:ASP:OD2  | 2.10                     | 0.52              |
| 1:A:938:ILE:CD1  | 1:A:948:VAL:HG21 | 2.39                     | 0.52              |
| 1:B:765:LEU:HD23 | 1:B:768:LEU:HD12 | 1.90                     | 0.52              |
| 1:B:862:HIS:CD2  | 1:B:877:LEU:HD21 | 2.44                     | 0.52              |
| 1:C:900:MET:O    | 1:C:901:VAL:C    | 2.53                     | 0.52              |
| 1:D:933:LYS:HD2  | 1:D:979:VAL:HG13 | 1.92                     | 0.52              |
| 1:A:698:LEU:HD23 | 1:A:701:LEU:CD1  | 2.39                     | 0.52              |
| 1:D:662:LYS:N    | 1:D:787:LYS:HG3  | 2.24                     | 0.52              |
| 1:A:709:ALA:HB3  | 1:A:765:LEU:HD21 | 1.91                     | 0.52              |
| 1:C:677:PHE:CE2  | 1:C:793:ASN:HB3  | 2.44                     | 0.52              |
| 1:C:829:TYR:HD1  | 1:C:829:TYR:O    | 1.92                     | 0.52              |
| 1:D:777:LEU:HD13 | 1:D:777:LEU:C    | 2.34                     | 0.52              |
| 1:D:878:ARG:CZ   | 1:D:879:ILE:HG12 | 2.40                     | 0.52              |
| 1:D:964:LEU:C    | 1:D:966:GLY:H    | 2.15                     | 0.52              |
| 1:A:772:GLU:OE1  | 1:A:772:GLU:C    | 2.53                     | 0.52              |
| 1:B:849:LYS:HZ2  | 1:B:849:LYS:HA   | 1.74                     | 0.52              |
| 1:D:797:LEU:HB3  | 1:D:799:THR:OG1  | 2.10                     | 0.52              |
| 1:A:710:TYR:CE2  | 1:A:881:PRO:HG3  | 2.45                     | 0.52              |
| 1:A:718:GLN:C    | 1:A:718:GLN:HE21 | 2.18                     | 0.52              |
| 1:C:729:ILE:H    | 1:C:729:ILE:CD1  | 2.23                     | 0.52              |
| 1:C:953:LYS:HE3  | 1:C:980:ASN:HB2  | 1.92                     | 0.52              |
| 1:B:679:VAL:HG23 | 1:B:680:GLU:N    | 2.21                     | 0.52              |
| 1:D:671:ASP:HA   | 1:D:674:LYS:NZ   | 2.25                     | 0.52              |
| 1:D:805:ASP:OD2  | 1:D:805:ASP:N    | 2.43                     | 0.52              |
| 1:A:788:ASP:OD1  | 1:A:790:ILE:HG12 | 2.10                     | 0.51              |
| 1:A:911:SER:CB   | 1:C:748:LYS:HE3  | 2.40                     | 0.51              |
| 1:A:962:ILE:CG1  | 1:A:971:LEU:HD11 | 2.40                     | 0.51              |
| 1:B:671:ASP:HA   | 1:B:674:LYS:HD3  | 1.91                     | 0.51              |
| 1:A:703:LYS:HG3  | 1:A:707:GLN:NE2  | 2.25                     | 0.51              |
| 1:D:854:LEU:HD12 | 1:D:854:LEU:N    | 2.25                     | 0.51              |
| 1:A:857:ARG:HA   | 1:A:924:VAL:O    | 2.10                     | 0.51              |
| 1:D:861:TRP:O    | 1:D:862:HIS:CB   | 2.58                     | 0.51              |
| 1:A:686:MET:O    | 1:A:691:ILE:HB   | 2.10                     | 0.51              |
| 1:A:742:HIS:CE1  | 1:A:764:MET:HE1  | 2.45                     | 0.51              |
| 1:D:679:VAL:HA   | 1:D:682:MET:SD   | 2.50                     | 0.51              |
| 1:D:919:ILE:HG22 | 1:D:1003:LEU:HB2 | 1.93                     | 0.51              |
| 1:A:682:MET:O    | 1:A:685:ALA:HB3  | 2.09                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:697:PRO:O    | 1:A:698:LEU:C    | 2.53                     | 0.51              |
| 1:D:674:LYS:HE2  | 1:D:675:MET:HG3  | 1.92                     | 0.51              |
| 1:D:815:ARG:HB3  | 1:D:815:ARG:NH1  | 2.24                     | 0.51              |
| 1:B:901:VAL:CG1  | 1:B:902:SER:H    | 2.24                     | 0.51              |
| 1:A:896:TYR:CE2  | 1:A:990:ILE:HD11 | 2.46                     | 0.51              |
| 1:D:858:ARG:HB3  | 1:D:968:ASP:HB3  | 1.92                     | 0.51              |
| 1:D:924:VAL:HG23 | 1:D:926:LEU:HG   | 1.91                     | 0.51              |
| 1:A:788:ASP:O    | 1:A:790:ILE:N    | 2.44                     | 0.51              |
| 1:B:826:HIS:HA   | 1:D:726:ASP:OD2  | 2.10                     | 0.51              |
| 1:C:767:ASN:ND2  | 1:C:865:ARG:HE   | 2.08                     | 0.51              |
| 1:D:829:TYR:CA   | 1:D:1010:LYS:HE2 | 2.40                     | 0.51              |
| 1:D:990:ILE:HG22 | 1:D:992:TYR:CE1  | 2.45                     | 0.51              |
| 1:A:789:PRO:HA   | 1:A:792:VAL:CG2  | 2.41                     | 0.51              |
| 1:B:821:THR:O    | 1:B:901:VAL:HG12 | 2.10                     | 0.51              |
| 1:C:823:ALA:HB3  | 1:C:826:HIS:CD2  | 2.46                     | 0.51              |
| 1:D:862:HIS:HA   | 2:D:4:CNQ:O13    | 2.10                     | 0.51              |
| 1:D:901:VAL:CG1  | 1:D:902:SER:N    | 2.74                     | 0.51              |
| 1:D:1003:LEU:O   | 1:D:1004:LYS:HB2 | 2.11                     | 0.51              |
| 1:A:796:LYS:O    | 1:A:798:LYS:HG2  | 2.11                     | 0.51              |
| 1:B:737:TYR:OH   | 1:B:750:PRO:HG2  | 2.11                     | 0.51              |
| 1:B:830:ASP:C    | 1:B:831:LEU:HD12 | 2.35                     | 0.51              |
| 1:C:933:LYS:HG2  | 1:C:934:HIS:ND1  | 2.25                     | 0.51              |
| 1:A:788:ASP:OD1  | 1:A:789:PRO:HD2  | 2.12                     | 0.50              |
| 1:B:702:SER:OG   | 1:B:704:ARG:NH2  | 2.45                     | 0.50              |
| 1:B:827:ASN:CG   | 1:D:725:SER:HB3  | 2.36                     | 0.50              |
| 1:C:1007:PHE:HB2 | 1:C:1009:PHE:CE1 | 2.46                     | 0.50              |
| 1:D:665:LEU:H    | 1:D:665:LEU:CD2  | 2.20                     | 0.50              |
| 1:D:692:ASP:C    | 1:D:694:GLN:N    | 2.69                     | 0.50              |
| 1:D:775:TYR:O    | 1:D:778:LEU:N    | 2.42                     | 0.50              |
| 1:D:842:GLU:O    | 1:D:842:GLU:HG3  | 2.11                     | 0.50              |
| 1:A:714:SER:CB   | 1:A:885:PRO:HB3  | 2.42                     | 0.50              |
| 1:A:788:ASP:C    | 1:A:790:ILE:N    | 2.69                     | 0.50              |
| 1:B:685:ALA:O    | 1:B:688:GLU:HG2  | 2.11                     | 0.50              |
| 1:D:662:LYS:HB3  | 1:D:788:ASP:HB2  | 1.94                     | 0.50              |
| 1:A:838:LYS:HD2  | 1:A:1001:TYR:HE1 | 1.76                     | 0.50              |
| 1:A:890:MET:HE2  | 1:A:935:ALA:HB2  | 1.92                     | 0.50              |
| 1:A:998:ASN:HD22 | 1:A:1000:LYS:HE2 | 1.76                     | 0.50              |
| 1:D:794:TYR:C    | 1:D:794:TYR:CD2  | 2.90                     | 0.50              |
| 1:D:862:HIS:ND1  | 2:D:4:CNQ:N12    | 2.59                     | 0.50              |
| 1:D:901:VAL:HG13 | 1:D:902:SER:H    | 1.74                     | 0.50              |
| 1:D:964:LEU:C    | 1:D:966:GLY:N    | 2.69                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:981:ASP:OD1  | 1:A:981:ASP:N     | 2.43                     | 0.50              |
| 1:B:793:ASN:HA   | 1:B:796:LYS:HD2   | 1.94                     | 0.50              |
| 1:C:759:GLN:HA   | 1:C:759:GLN:NE2   | 2.26                     | 0.50              |
| 1:C:985:LEU:HD22 | 1:C:985:LEU:N     | 2.27                     | 0.50              |
| 1:D:886:VAL:C    | 1:D:888:GLY:H     | 2.20                     | 0.50              |
| 1:B:841:ARG:NH1  | 1:B:873:LEU:O     | 2.45                     | 0.50              |
| 1:D:726:ASP:O    | 1:D:730:LEU:HB2   | 2.12                     | 0.50              |
| 1:B:1004:LYS:C   | 1:B:1005:LEU:HD12 | 2.37                     | 0.50              |
| 1:D:701:LEU:O    | 1:D:702:SER:HB3   | 2.12                     | 0.50              |
| 1:D:713:LEU:CD1  | 1:D:765:LEU:HD12  | 2.42                     | 0.50              |
| 1:D:955:THR:CG2  | 1:D:977:SER:HB3   | 2.42                     | 0.50              |
| 1:C:1007:PHE:HD1 | 1:C:1007:PHE:H    | 1.60                     | 0.50              |
| 1:D:664:LYS:HZ2  | 1:D:665:LEU:CD1   | 2.25                     | 0.50              |
| 1:D:664:LYS:NZ   | 1:D:665:LEU:HD11  | 2.26                     | 0.50              |
| 1:A:861:TRP:CZ3  | 1:A:921:LEU:HG    | 2.47                     | 0.49              |
| 1:D:790:ILE:HG13 | 1:D:791:ASP:N     | 2.26                     | 0.49              |
| 1:D:865:ARG:HH21 | 1:D:909:HIS:CE1   | 2.30                     | 0.49              |
| 1:B:702:SER:OG   | 1:B:704:ARG:CZ    | 2.60                     | 0.49              |
| 1:B:703:LYS:H    | 1:B:704:ARG:NH2   | 2.05                     | 0.49              |
| 1:B:748:LYS:HD3  | 1:B:748:LYS:C     | 2.36                     | 0.49              |
| 1:D:919:ILE:HD13 | 1:D:920:LEU:N     | 2.16                     | 0.49              |
| 1:D:759:GLN:HE21 | 1:D:759:GLN:HA    | 1.78                     | 0.49              |
| 1:A:844:GLU:OE1  | 1:A:999:LEU:N     | 2.45                     | 0.49              |
| 1:D:669:VAL:O    | 1:D:673:ILE:HG12  | 2.11                     | 0.49              |
| 1:D:797:LEU:O    | 1:D:799:THR:HG23  | 2.13                     | 0.49              |
| 1:A:924:VAL:HG23 | 1:A:926:LEU:HG    | 1.94                     | 0.49              |
| 1:B:901:VAL:HG13 | 1:B:902:SER:H     | 1.73                     | 0.49              |
| 1:C:785:SER:O    | 1:C:786:SER:C     | 2.54                     | 0.49              |
| 1:A:844:GLU:HA   | 1:A:847:ARG:HG2   | 1.93                     | 0.49              |
| 1:B:683:LYS:O    | 1:B:687:VAL:HG23  | 2.12                     | 0.49              |
| 1:B:775:TYR:O    | 1:B:778:LEU:HB3   | 2.12                     | 0.49              |
| 1:C:782:SER:CA   | 1:C:792:VAL:HG11  | 2.34                     | 0.49              |
| 1:D:754:ASN:O    | 1:D:756:ASP:N     | 2.39                     | 0.49              |
| 1:D:835:ASP:HB3  | 1:D:837:PHE:CE2   | 2.47                     | 0.49              |
| 1:D:920:LEU:HD23 | 1:D:920:LEU:C     | 2.36                     | 0.49              |
| 1:A:866:THR:CG2  | 1:A:867:THR:N     | 2.76                     | 0.49              |
| 1:B:726:ASP:C    | 1:D:828:ALA:HB2   | 2.37                     | 0.49              |
| 1:B:786:SER:O    | 1:B:787:LYS:HD2   | 2.12                     | 0.49              |
| 1:C:782:SER:HA   | 1:C:792:VAL:CG1   | 2.34                     | 0.49              |
| 1:C:882:PRO:O    | 1:C:884:ALA:N     | 2.46                     | 0.49              |
| 1:D:854:LEU:HD23 | 1:D:927:GLY:HA3   | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:854:LEU:HB3  | 1:D:927:GLY:HA2  | 1.94                     | 0.49              |
| 1:D:933:LYS:HG2  | 1:D:951:LEU:HB2  | 1.94                     | 0.49              |
| 1:D:682:MET:CE   | 1:D:774:ALA:HB3  | 2.43                     | 0.49              |
| 1:D:737:TYR:OH   | 1:D:750:PRO:HG2  | 2.13                     | 0.49              |
| 1:D:841:ARG:HH11 | 1:D:841:ARG:CB   | 2.11                     | 0.49              |
| 1:D:841:ARG:HE   | 1:D:876:GLY:N    | 2.08                     | 0.49              |
| 1:B:752:LEU:HB3  | 1:B:758:VAL:HG12 | 1.95                     | 0.49              |
| 1:B:839:ILE:HD11 | 1:B:920:LEU:HD11 | 1.94                     | 0.49              |
| 1:B:958:PRO:C    | 1:B:960:ALA:H    | 2.21                     | 0.49              |
| 1:D:768:LEU:O    | 1:D:769:LEU:C    | 2.56                     | 0.49              |
| 1:A:715:GLU:OE2  | 1:A:735:ARG:NH2  | 2.46                     | 0.48              |
| 1:B:822:HIS:CD2  | 1:B:831:LEU:HD22 | 2.48                     | 0.48              |
| 1:C:703:LYS:HG2  | 1:C:707:GLN:CD   | 2.38                     | 0.48              |
| 1:C:869:PHE:O    | 1:C:870:ALA:C    | 2.56                     | 0.48              |
| 1:D:778:LEU:O    | 1:D:780:GLY:N    | 2.46                     | 0.48              |
| 1:D:838:LYS:HE2  | 1:D:840:GLU:OE2  | 2.13                     | 0.48              |
| 1:B:823:ALA:O    | 1:B:826:HIS:HB2  | 2.13                     | 0.48              |
| 1:B:827:ASN:O    | 1:B:828:ALA:HB2  | 2.14                     | 0.48              |
| 1:A:827:ASN:HD21 | 1:C:725:SER:HB2  | 1.77                     | 0.48              |
| 1:B:666:PRO:O    | 1:B:667:LYS:C    | 2.56                     | 0.48              |
| 1:B:717:GLN:HA   | 1:B:720:VAL:HG12 | 1.95                     | 0.48              |
| 1:B:890:MET:HG3  | 1:B:935:ALA:CB   | 2.44                     | 0.48              |
| 1:C:681:SER:HA   | 1:C:684:LYS:HG3  | 1.94                     | 0.48              |
| 1:D:786:SER:C    | 1:D:787:LYS:HD2  | 2.37                     | 0.48              |
| 1:A:663:SER:HB3  | 1:A:670:GLN:CD   | 2.39                     | 0.48              |
| 1:A:826:HIS:ND1  | 1:A:902:SER:CB   | 2.76                     | 0.48              |
| 1:B:687:VAL:HG22 | 1:B:693:LEU:HD23 | 1.96                     | 0.48              |
| 1:B:719:ALA:HB1  | 1:B:724:SER:OG   | 2.13                     | 0.48              |
| 1:C:816:LYS:HE2  | 1:C:820:ASN:ND2  | 2.26                     | 0.48              |
| 1:C:872:ILE:HG23 | 1:C:877:LEU:HD23 | 1.94                     | 0.48              |
| 1:B:722:GLN:HA   | 1:B:722:GLN:OE1  | 2.14                     | 0.48              |
| 1:C:901:VAL:HG13 | 1:C:902:SER:N    | 2.28                     | 0.48              |
| 1:D:905:ALA:C    | 1:D:907:TYR:H    | 2.21                     | 0.48              |
| 1:C:697:PRO:CG   | 1:C:700:LYS:HB2  | 2.34                     | 0.48              |
| 1:C:851:PHE:C    | 1:C:853:GLN:N    | 2.69                     | 0.48              |
| 1:D:765:LEU:HD23 | 1:D:768:LEU:HD12 | 1.95                     | 0.48              |
| 1:D:855:HIS:O    | 1:D:856:ASN:HB2  | 2.14                     | 0.48              |
| 1:B:707:GLN:HB3  | 1:B:883:GLU:HG2  | 1.95                     | 0.48              |
| 1:C:666:PRO:O    | 1:C:667:LYS:C    | 2.57                     | 0.48              |
| 1:C:744:PHE:CD2  | 1:C:749:PRO:HG3  | 2.49                     | 0.48              |
| 1:C:856:ASN:HD21 | 1:C:858:ARG:HH11 | 1.61                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:706:ILE:CD1  | 1:A:768:LEU:HB3   | 2.44                     | 0.48              |
| 1:B:887:THR:HG23 | 1:B:937:HIS:CD2   | 2.48                     | 0.48              |
| 1:D:662:LYS:CA   | 1:D:788:ASP:H     | 2.26                     | 0.48              |
| 1:D:813:ILE:HD12 | 1:D:813:ILE:N     | 2.28                     | 0.48              |
| 1:D:849:LYS:HB3  | 1:D:849:LYS:HZ3   | 1.78                     | 0.48              |
| 1:A:744:PHE:O    | 1:A:747:LYS:HG2   | 2.13                     | 0.48              |
| 1:A:942:PRO:O    | 1:A:945:LYS:HG2   | 2.14                     | 0.47              |
| 1:B:824:THR:C    | 1:B:826:HIS:N     | 2.72                     | 0.47              |
| 1:B:869:PHE:HE2  | 1:B:1002:LEU:HD21 | 1.79                     | 0.47              |
| 1:C:832:GLU:O    | 1:C:834:ILE:HD12  | 2.13                     | 0.47              |
| 1:D:841:ARG:HH21 | 1:D:875:GLN:HA    | 1.77                     | 0.47              |
| 1:D:903:LYS:O    | 1:D:906:ASN:HB2   | 2.14                     | 0.47              |
| 1:B:801:ILE:N    | 1:B:801:ILE:HD13  | 2.29                     | 0.47              |
| 1:B:839:ILE:HD13 | 1:B:1002:LEU:HB2  | 1.95                     | 0.47              |
| 1:C:763:GLU:HA   | 2:C:3:CNQ:CL24    | 2.51                     | 0.47              |
| 1:D:670:GLN:O    | 1:D:672:LEU:N     | 2.46                     | 0.47              |
| 1:D:696:MET:HE2  | 1:D:701:LEU:CD2   | 2.42                     | 0.47              |
| 1:D:964:LEU:HD13 | 1:D:965:ASP:CB    | 2.44                     | 0.47              |
| 1:A:735:ARG:CA   | 1:A:738:THR:HG22  | 2.45                     | 0.47              |
| 1:B:827:ASN:HD21 | 1:D:725:SER:CB    | 2.27                     | 0.47              |
| 1:B:827:ASN:HD21 | 1:D:725:SER:HB3   | 1.79                     | 0.47              |
| 1:B:857:ARG:HA   | 1:B:924:VAL:O     | 2.14                     | 0.47              |
| 1:D:702:SER:CA   | 1:D:772:GLU:HG3   | 2.43                     | 0.47              |
| 1:D:703:LYS:HG2  | 1:D:707:GLN:OE1   | 2.14                     | 0.47              |
| 1:D:759:GLN:HA   | 1:D:759:GLN:NE2   | 2.29                     | 0.47              |
| 1:D:868:ASN:C    | 1:D:870:ALA:N     | 2.72                     | 0.47              |
| 1:A:826:HIS:ND1  | 1:A:902:SER:HB2   | 2.29                     | 0.47              |
| 1:B:827:ASN:ND2  | 1:D:725:SER:HB3   | 2.29                     | 0.47              |
| 1:C:829:TYR:CD1  | 1:C:829:TYR:C     | 2.92                     | 0.47              |
| 1:D:975:ILE:CG1  | 1:D:976:SER:H     | 2.26                     | 0.47              |
| 1:A:723:GLY:O    | 1:A:724:SER:HB3   | 2.13                     | 0.47              |
| 1:A:759:GLN:HA   | 1:A:759:GLN:HE21  | 1.79                     | 0.47              |
| 1:B:672:LEU:O    | 1:B:676:ILE:HG12  | 2.14                     | 0.47              |
| 1:B:788:ASP:CG   | 1:B:789:PRO:HD2   | 2.40                     | 0.47              |
| 1:C:777:LEU:HD13 | 1:C:796:LYS:HD3   | 1.96                     | 0.47              |
| 1:D:843:GLY:C    | 1:D:845:CYS:N     | 2.70                     | 0.47              |
| 1:A:703:LYS:HB3  | 1:A:704:ARG:NH1   | 2.30                     | 0.47              |
| 1:B:689:TYR:O    | 1:B:690:GLU:HB3   | 2.15                     | 0.47              |
| 1:B:872:ILE:O    | 1:B:876:GLY:N     | 2.45                     | 0.47              |
| 1:B:941:LEU:N    | 1:B:941:LEU:CD1   | 2.77                     | 0.47              |
| 1:C:714:SER:HA   | 1:C:885:PRO:HB3   | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:879:ILE:CD1  | 1:C:879:ILE:N    | 2.65                     | 0.47              |
| 1:D:831:LEU:N    | 1:D:831:LEU:CD2  | 2.77                     | 0.47              |
| 1:D:862:HIS:NE2  | 1:D:877:LEU:HD22 | 2.29                     | 0.47              |
| 1:A:706:ILE:HD12 | 1:A:769:LEU:HD23 | 1.97                     | 0.47              |
| 1:B:688:GLU:HA   | 1:D:747:LYS:HA   | 1.96                     | 0.47              |
| 1:B:777:LEU:HD11 | 1:B:796:LYS:CB   | 2.44                     | 0.47              |
| 1:C:869:PHE:HA   | 1:C:872:ILE:HD12 | 1.97                     | 0.47              |
| 1:D:915:PRO:HB3  | 1:D:1009:PHE:CE1 | 2.50                     | 0.47              |
| 1:D:931:GLU:HB3  | 1:D:949:LYS:HB3  | 1.97                     | 0.47              |
| 1:D:991:VAL:C    | 1:D:992:TYR:CD1  | 2.92                     | 0.47              |
| 1:D:1009:PHE:O   | 1:D:1010:LYS:HD3 | 2.14                     | 0.47              |
| 1:B:834:ILE:HB   | 1:B:1004:LYS:HG2 | 1.97                     | 0.47              |
| 1:B:856:ASN:HB3  | 1:B:927:GLY:N    | 2.27                     | 0.47              |
| 1:C:942:PRO:O    | 1:C:945:LYS:HB2  | 2.14                     | 0.47              |
| 1:D:794:TYR:O    | 1:D:797:LEU:HB2  | 2.14                     | 0.47              |
| 1:D:821:THR:C    | 1:D:901:VAL:HG12 | 2.39                     | 0.47              |
| 1:D:831:LEU:HD12 | 1:D:1005:LEU:CD1 | 2.45                     | 0.47              |
| 1:B:763:GLU:O    | 1:B:766:ASP:HB2  | 2.15                     | 0.47              |
| 1:B:797:LEU:CB   | 1:B:799:THR:HG22 | 2.45                     | 0.47              |
| 1:B:803:VAL:HG12 | 1:B:804:VAL:N    | 2.29                     | 0.47              |
| 1:D:849:LYS:O    | 1:D:852:LYS:HG3  | 2.15                     | 0.47              |
| 1:A:826:HIS:CE1  | 1:A:906:ASN:HD21 | 2.33                     | 0.47              |
| 1:A:841:ARG:HG2  | 1:A:841:ARG:HH11 | 1.80                     | 0.47              |
| 1:B:690:GLU:OE1  | 1:D:747:LYS:HE2  | 2.15                     | 0.47              |
| 1:B:759:GLN:O    | 1:B:763:GLU:HG2  | 2.15                     | 0.47              |
| 1:B:846:GLN:NE2  | 1:B:846:GLN:HA   | 2.30                     | 0.47              |
| 1:D:768:LEU:O    | 1:D:771:ILE:N    | 2.47                     | 0.47              |
| 1:C:816:LYS:C    | 1:C:816:LYS:HD3  | 2.40                     | 0.46              |
| 1:C:851:PHE:C    | 1:C:853:GLN:H    | 2.23                     | 0.46              |
| 1:D:762:VAL:O    | 1:D:766:ASP:OD1  | 2.33                     | 0.46              |
| 1:A:758:VAL:O    | 1:A:762:VAL:HG23 | 2.15                     | 0.46              |
| 1:A:911:SER:HB3  | 1:C:748:LYS:HE3  | 1.97                     | 0.46              |
| 1:C:797:LEU:HB3  | 1:C:799:THR:CG2  | 2.45                     | 0.46              |
| 1:D:754:ASN:C    | 1:D:756:ASP:H    | 2.21                     | 0.46              |
| 1:D:778:LEU:C    | 1:D:780:GLY:N    | 2.73                     | 0.46              |
| 1:D:798:LYS:HB3  | 1:D:842:GLU:CB   | 2.38                     | 0.46              |
| 1:D:915:PRO:O    | 1:D:916:ILE:HG23 | 2.15                     | 0.46              |
| 1:D:985:LEU:HD23 | 1:D:986:TYR:CE2  | 2.49                     | 0.46              |
| 1:A:671:ASP:O    | 1:A:674:LYS:HG3  | 2.15                     | 0.46              |
| 1:A:754:ASN:C    | 1:A:756:ASP:H    | 2.23                     | 0.46              |
| 1:C:912:GLN:O    | 1:C:915:PRO:HD3  | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:955:THR:O    | 1:C:975:ILE:N    | 2.46                     | 0.46              |
| 1:D:714:SER:C    | 1:D:716:VAL:H    | 2.23                     | 0.46              |
| 1:D:972:GLY:O    | 1:D:973:THR:C    | 2.57                     | 0.46              |
| 1:C:734:ASN:O    | 1:C:735:ARG:C    | 2.59                     | 0.46              |
| 1:D:702:SER:O    | 1:D:706:ILE:HG13 | 2.15                     | 0.46              |
| 1:D:822:HIS:CD2  | 1:D:831:LEU:HD23 | 2.50                     | 0.46              |
| 1:D:1007:PHE:O   | 1:D:1009:PHE:N   | 2.48                     | 0.46              |
| 1:D:664:LYS:HD2  | 1:D:665:LEU:N    | 2.30                     | 0.46              |
| 1:B:851:PHE:CD1  | 1:B:996:GLN:HG2  | 2.51                     | 0.46              |
| 1:B:934:HIS:ND1  | 1:B:934:HIS:N    | 2.64                     | 0.46              |
| 1:A:701:LEU:HD21 | 1:A:768:LEU:HD22 | 1.98                     | 0.46              |
| 1:A:839:ILE:HD13 | 1:A:839:ILE:N    | 2.24                     | 0.46              |
| 1:A:869:PHE:CE1  | 1:A:918:LEU:HB2  | 2.51                     | 0.46              |
| 1:B:720:VAL:HG11 | 1:B:755:ALA:HB2  | 1.98                     | 0.46              |
| 1:C:859:LEU:HB2  | 1:C:969:VAL:HG22 | 1.97                     | 0.46              |
| 1:C:873:LEU:HD23 | 1:C:873:LEU:HA   | 1.73                     | 0.46              |
| 1:C:1007:PHE:CD1 | 1:C:1007:PHE:N   | 2.84                     | 0.46              |
| 1:D:861:TRP:CE3  | 1:D:921:LEU:HD21 | 2.50                     | 0.46              |
| 1:A:953:LYS:HD2  | 1:A:985:LEU:HD12 | 1.98                     | 0.46              |
| 1:B:887:THR:HG23 | 1:B:937:HIS:NE2  | 2.30                     | 0.46              |
| 1:C:683:LYS:HA   | 1:C:686:MET:CE   | 2.45                     | 0.46              |
| 1:D:677:PHE:CE2  | 1:D:793:ASN:HB3  | 2.51                     | 0.46              |
| 1:D:876:GLY:O    | 1:D:877:LEU:C    | 2.57                     | 0.46              |
| 1:A:858:ARG:HA   | 1:A:967:VAL:HG13 | 1.98                     | 0.46              |
| 1:A:866:THR:C    | 1:A:868:ASN:H    | 2.23                     | 0.46              |
| 1:C:830:ASP:O    | 1:C:1008:ASN:ND2 | 2.42                     | 0.46              |
| 1:C:953:LYS:HD3  | 1:C:980:ASN:HB3  | 1.98                     | 0.46              |
| 1:D:662:LYS:O    | 1:D:788:ASP:N    | 2.47                     | 0.46              |
| 1:D:905:ALA:C    | 1:D:907:TYR:N    | 2.72                     | 0.46              |
| 1:D:920:LEU:HD21 | 1:D:999:LEU:HD22 | 1.97                     | 0.46              |
| 1:B:748:LYS:CB   | 1:D:688:GLU:HG3  | 2.42                     | 0.46              |
| 1:B:958:PRO:C    | 1:B:960:ALA:N    | 2.73                     | 0.46              |
| 1:C:829:TYR:HD1  | 1:C:829:TYR:C    | 2.24                     | 0.46              |
| 1:D:670:GLN:OE1  | 1:D:790:ILE:HD12 | 2.16                     | 0.46              |
| 1:A:821:THR:HB   | 1:A:900:MET:HA   | 1.99                     | 0.45              |
| 1:B:957:ASP:OD2  | 1:B:957:ASP:C    | 2.59                     | 0.45              |
| 1:C:744:PHE:CE2  | 1:C:749:PRO:HB3  | 2.51                     | 0.45              |
| 1:C:882:PRO:C    | 1:C:884:ALA:H    | 2.24                     | 0.45              |
| 1:C:975:ILE:HD12 | 1:C:975:ILE:HA   | 1.74                     | 0.45              |
| 1:D:730:LEU:HD23 | 1:D:730:LEU:HA   | 1.78                     | 0.45              |
| 1:B:677:PHE:CD2  | 1:B:793:ASN:HB3  | 2.50                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:722:GLN:O    | 1:B:723:GLY:C    | 2.58                     | 0.45              |
| 1:B:806:ARG:NH1  | 1:B:806:ARG:HB2  | 2.32                     | 0.45              |
| 1:B:859:LEU:HD22 | 1:B:921:LEU:CD2  | 2.46                     | 0.45              |
| 1:B:880:ALA:HB3  | 1:B:893:LYS:CG   | 2.46                     | 0.45              |
| 1:C:779:ARG:O    | 1:C:779:ARG:HG3  | 2.16                     | 0.45              |
| 1:C:829:TYR:HA   | 1:C:1010:LYS:HD3 | 1.97                     | 0.45              |
| 1:D:662:LYS:C    | 1:D:787:LYS:HB3  | 2.42                     | 0.45              |
| 1:D:699:GLY:HA2  | 1:D:775:TYR:CE2  | 2.50                     | 0.45              |
| 1:D:801:ILE:O    | 1:D:801:ILE:HG22 | 2.16                     | 0.45              |
| 1:D:822:HIS:HD2  | 1:D:831:LEU:HD23 | 1.81                     | 0.45              |
| 1:D:823:ALA:HB2  | 1:D:900:MET:HE3  | 1.98                     | 0.45              |
| 1:D:832:GLU:HB3  | 1:D:1006:LYS:HG2 | 1.98                     | 0.45              |
| 1:D:861:TRP:HA   | 1:D:921:LEU:HD23 | 1.98                     | 0.45              |
| 1:D:964:LEU:HD13 | 1:D:965:ASP:HB2  | 1.97                     | 0.45              |
| 1:A:878:ARG:NH2  | 1:A:879:ILE:O    | 2.49                     | 0.45              |
| 1:B:824:THR:C    | 1:B:826:HIS:H    | 2.24                     | 0.45              |
| 1:C:691:ILE:HG22 | 1:C:692:ASP:N    | 2.31                     | 0.45              |
| 1:C:712:ILE:HG21 | 1:C:736:PHE:HB2  | 1.98                     | 0.45              |
| 1:C:962:ILE:HB   | 1:C:971:LEU:HD11 | 1.99                     | 0.45              |
| 1:D:662:LYS:O    | 1:D:788:ASP:HB3  | 2.16                     | 0.45              |
| 1:D:728:GLN:OE1  | 1:D:728:GLN:N    | 2.49                     | 0.45              |
| 1:D:853:GLN:O    | 1:D:853:GLN:HG3  | 2.17                     | 0.45              |
| 1:D:879:ILE:HG21 | 1:D:894:GLY:HA2  | 1.99                     | 0.45              |
| 1:A:818:VAL:HG12 | 1:A:819:LYS:N    | 2.31                     | 0.45              |
| 1:C:887:THR:HG22 | 1:C:937:HIS:CD2  | 2.52                     | 0.45              |
| 1:D:670:GLN:HE22 | 1:D:790:ILE:CD1  | 2.29                     | 0.45              |
| 1:D:762:VAL:CG2  | 1:D:885:PRO:HG3  | 2.46                     | 0.45              |
| 1:D:817:TYR:CE1  | 1:D:821:THR:HG21 | 2.51                     | 0.45              |
| 1:A:1011:THR:HB  | 1:C:730:LEU:HD11 | 1.99                     | 0.45              |
| 1:C:826:HIS:HD2  | 1:C:902:SER:CB   | 2.30                     | 0.45              |
| 1:C:844:GLU:OE1  | 1:C:998:ASN:HA   | 2.17                     | 0.45              |
| 1:A:816:LYS:HE3  | 1:A:816:LYS:HB2  | 1.77                     | 0.45              |
| 1:B:677:PHE:CE2  | 1:B:793:ASN:HB3  | 2.52                     | 0.45              |
| 1:B:731:ASP:O    | 1:B:735:ARG:HG3  | 2.17                     | 0.45              |
| 1:B:749:PRO:HA   | 1:B:750:PRO:HD2  | 1.81                     | 0.45              |
| 1:D:663:SER:OG   | 1:D:790:ILE:HD11 | 2.16                     | 0.45              |
| 1:C:697:PRO:O    | 1:C:698:LEU:C    | 2.59                     | 0.45              |
| 1:C:709:ALA:O    | 1:C:713:LEU:HD23 | 2.17                     | 0.45              |
| 1:C:854:LEU:HD23 | 1:C:925:ALA:HB1  | 1.98                     | 0.45              |
| 1:D:677:PHE:CD1  | 1:D:778:LEU:HD22 | 2.52                     | 0.45              |
| 1:D:790:ILE:HG13 | 1:D:791:ASP:OD1  | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:684:LYS:HD3  | 1:B:684:LYS:C    | 2.42                     | 0.45              |
| 1:B:777:LEU:HD13 | 1:B:777:LEU:O    | 2.17                     | 0.45              |
| 1:C:704:ARG:N    | 1:C:704:ARG:CD   | 2.79                     | 0.45              |
| 1:D:717:GLN:CG   | 1:D:718:GLN:N    | 2.80                     | 0.45              |
| 1:D:806:ARG:HD2  | 1:D:806:ARG:N    | 2.29                     | 0.45              |
| 1:D:998:ASN:HD22 | 1:D:1000:LYS:HZ1 | 1.57                     | 0.45              |
| 1:C:808:SER:O    | 1:C:809:GLU:C    | 2.60                     | 0.45              |
| 1:D:858:ARG:HH21 | 1:D:970:PRO:CG   | 2.29                     | 0.45              |
| 1:A:942:PRO:HB2  | 1:A:945:LYS:HG3  | 1.98                     | 0.45              |
| 1:A:943:LYS:HE2  | 1:A:943:LYS:CA   | 2.46                     | 0.45              |
| 1:B:765:LEU:O    | 1:B:766:ASP:C    | 2.59                     | 0.45              |
| 1:B:854:LEU:HD22 | 1:B:855:HIS:O    | 2.16                     | 0.45              |
| 1:C:686:MET:O    | 1:C:689:TYR:HB2  | 2.17                     | 0.45              |
| 1:C:761:LYS:HA   | 1:C:761:LYS:HD3  | 1.73                     | 0.45              |
| 1:C:943:LYS:C    | 1:C:945:LYS:H    | 2.25                     | 0.45              |
| 1:A:704:ARG:CZ   | 1:A:704:ARG:H    | 2.30                     | 0.44              |
| 1:B:903:LYS:NZ   | 1:B:988:GLU:HG2  | 2.32                     | 0.44              |
| 1:D:777:LEU:HD22 | 1:D:777:LEU:O    | 2.18                     | 0.44              |
| 1:D:848:TYR:O    | 1:D:848:TYR:CG   | 2.69                     | 0.44              |
| 1:D:914:ASP:N    | 1:D:915:PRO:CD   | 2.80                     | 0.44              |
| 1:A:695:LYS:HD2  | 1:A:695:LYS:N    | 2.33                     | 0.44              |
| 1:A:828:ALA:O    | 1:A:829:TYR:HB3  | 2.16                     | 0.44              |
| 1:A:858:ARG:O    | 1:A:923:GLU:HA   | 2.17                     | 0.44              |
| 1:C:696:MET:CG   | 1:C:741:PRO:HD2  | 2.41                     | 0.44              |
| 1:C:866:THR:C    | 1:C:868:ASN:H    | 2.25                     | 0.44              |
| 1:C:868:ASN:O    | 1:C:872:ILE:HG13 | 2.18                     | 0.44              |
| 1:D:717:GLN:HE22 | 1:D:886:VAL:HG23 | 1.82                     | 0.44              |
| 1:A:674:LYS:HG3  | 1:A:675:MET:N    | 2.33                     | 0.44              |
| 1:B:743:ASP:C    | 1:B:745:GLY:H    | 2.24                     | 0.44              |
| 1:B:910:THR:HB   | 1:B:914:ASP:O    | 2.16                     | 0.44              |
| 1:C:954:THR:HG22 | 1:C:955:THR:N    | 2.31                     | 0.44              |
| 1:C:993:ASP:HB3  | 1:C:996:GLN:HE21 | 1.82                     | 0.44              |
| 1:D:676:ILE:CG2  | 1:D:870:ALA:HA   | 2.43                     | 0.44              |
| 1:D:895:ILE:HD11 | 1:D:994:ILE:CD1  | 2.45                     | 0.44              |
| 1:A:1010:LYS:HD2 | 1:A:1010:LYS:N   | 2.33                     | 0.44              |
| 1:B:920:LEU:HD21 | 1:B:999:LEU:CD1  | 2.28                     | 0.44              |
| 1:C:841:ARG:HG2  | 1:C:841:ARG:NH1  | 2.32                     | 0.44              |
| 1:C:994:ILE:HD13 | 1:C:994:ILE:N    | 2.32                     | 0.44              |
| 1:D:775:TYR:CZ   | 1:D:779:ARG:HD2  | 2.52                     | 0.44              |
| 1:D:779:ARG:HA   | 1:D:779:ARG:HE   | 1.81                     | 0.44              |
| 1:B:662:LYS:HE2  | 1:B:788:ASP:OD2  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:793:ASN:O    | 1:C:796:LYS:HB2   | 2.18                     | 0.44              |
| 1:C:826:HIS:CD2  | 1:C:902:SER:OG    | 2.65                     | 0.44              |
| 1:A:759:GLN:O    | 1:A:763:GLU:HG3   | 2.18                     | 0.44              |
| 1:A:866:THR:C    | 1:A:868:ASN:N     | 2.74                     | 0.44              |
| 1:B:1006:LYS:HB2 | 1:B:1006:LYS:HZ3  | 1.83                     | 0.44              |
| 1:C:754:ASN:ND2  | 1:C:757:SER:HB3   | 2.20                     | 0.44              |
| 1:D:682:MET:HE1  | 1:D:774:ALA:HB3   | 2.00                     | 0.44              |
| 1:D:901:VAL:CG1  | 1:D:902:SER:H     | 2.29                     | 0.44              |
| 1:A:828:ALA:CB   | 1:C:726:ASP:HB3   | 2.48                     | 0.44              |
| 1:B:684:LYS:HD3  | 1:B:684:LYS:O     | 2.17                     | 0.44              |
| 1:B:689:TYR:HE2  | 1:B:767:ASN:ND2   | 2.15                     | 0.44              |
| 1:B:856:ASN:HD21 | 1:B:929:MET:HE2   | 1.83                     | 0.44              |
| 1:C:966:GLY:O    | 1:C:967:VAL:C     | 2.59                     | 0.44              |
| 1:A:699:GLY:HA2  | 1:A:775:TYR:CE2   | 2.53                     | 0.44              |
| 1:A:828:ALA:HB2  | 1:C:726:ASP:HB3   | 2.00                     | 0.44              |
| 1:A:938:ILE:HG22 | 1:A:939:SER:N     | 2.32                     | 0.44              |
| 1:B:801:ILE:HD12 | 1:B:839:ILE:HG22  | 1.99                     | 0.44              |
| 1:B:821:THR:C    | 1:B:901:VAL:HG12  | 2.43                     | 0.44              |
| 1:C:805:ASP:C    | 1:C:807:ASP:N     | 2.74                     | 0.44              |
| 1:D:675:MET:HE2  | 1:D:866:THR:CG2   | 2.46                     | 0.44              |
| 1:D:699:GLY:HA2  | 1:D:775:TYR:HE2   | 1.83                     | 0.44              |
| 1:D:926:LEU:HB3  | 1:D:929:MET:HE2   | 1.99                     | 0.44              |
| 1:A:759:GLN:HA   | 1:A:762:VAL:CG2   | 2.46                     | 0.43              |
| 1:A:915:PRO:HG2  | 1:A:916:ILE:HD12  | 2.00                     | 0.43              |
| 1:B:1007:PHE:CD1 | 1:B:1007:PHE:N    | 2.85                     | 0.43              |
| 1:A:672:LEU:HD12 | 1:A:673:ILE:HD13  | 2.00                     | 0.43              |
| 1:A:814:ILE:CG2  | 1:A:1003:LEU:HD21 | 2.48                     | 0.43              |
| 1:A:864:SER:OG   | 1:A:865:ARG:N     | 2.51                     | 0.43              |
| 1:B:665:LEU:HB3  | 1:B:669:VAL:HB    | 2.00                     | 0.43              |
| 1:B:902:SER:O    | 1:B:903:LYS:C     | 2.61                     | 0.43              |
| 1:C:972:GLY:O    | 1:C:973:THR:C     | 2.59                     | 0.43              |
| 1:C:1006:LYS:HE2 | 1:C:1006:LYS:HB2  | 1.70                     | 0.43              |
| 1:D:778:LEU:HD13 | 1:D:793:ASN:OD1   | 2.19                     | 0.43              |
| 1:A:759:GLN:HE21 | 1:A:759:GLN:CA    | 2.31                     | 0.43              |
| 1:B:890:MET:HG3  | 1:B:935:ALA:HB1   | 1.99                     | 0.43              |
| 1:D:716:VAL:HG22 | 1:D:732:LEU:HD13  | 1.99                     | 0.43              |
| 1:C:694:GLN:HA   | 1:C:694:GLN:HE21  | 1.82                     | 0.43              |
| 1:C:1009:PHE:C   | 1:C:1010:LYS:HD2  | 2.44                     | 0.43              |
| 1:D:943:LYS:HA   | 1:D:943:LYS:HZ3   | 1.84                     | 0.43              |
| 1:A:949:LYS:HE2  | 1:A:987:ASN:CG    | 2.43                     | 0.43              |
| 1:A:978:GLY:HA3  | 1:D:942:PRO:HA    | 2.00                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:834:ILE:HD13 | 1:B:834:ILE:HA    | 1.83                     | 0.43              |
| 1:D:856:ASN:OD1  | 1:D:927:GLY:O     | 2.36                     | 0.43              |
| 1:D:918:LEU:HB3  | 1:D:1004:LYS:HG2  | 1.99                     | 0.43              |
| 1:D:928:ASN:O    | 1:D:945:LYS:HE3   | 2.18                     | 0.43              |
| 1:A:881:PRO:HG2  | 1:A:884:ALA:HB2   | 1.99                     | 0.43              |
| 1:B:872:ILE:O    | 1:B:876:GLY:HA2   | 2.19                     | 0.43              |
| 1:B:938:ILE:C    | 1:B:938:ILE:HD12  | 2.44                     | 0.43              |
| 1:C:754:ASN:O    | 1:C:755:ALA:HB3   | 2.19                     | 0.43              |
| 1:D:717:GLN:HG3  | 1:D:718:GLN:N     | 2.33                     | 0.43              |
| 1:D:849:LYS:CA   | 1:D:852:LYS:HE2   | 2.36                     | 0.43              |
| 1:D:861:TRP:CE2  | 1:D:901:VAL:HB    | 2.54                     | 0.43              |
| 1:D:878:ARG:NH2  | 1:D:879:ILE:O     | 2.52                     | 0.43              |
| 1:A:785:SER:O    | 1:A:786:SER:HB2   | 2.18                     | 0.43              |
| 1:B:664:LYS:HE3  | 1:B:791:ASP:OD1   | 2.19                     | 0.43              |
| 1:C:675:MET:HE1  | 1:C:1004:LYS:NZ   | 2.33                     | 0.43              |
| 1:C:794:TYR:O    | 1:C:797:LEU:N     | 2.49                     | 0.43              |
| 1:D:674:LYS:CE   | 1:D:675:MET:HG3   | 2.48                     | 0.43              |
| 1:D:793:ASN:O    | 1:D:794:TYR:C     | 2.62                     | 0.43              |
| 1:A:833:VAL:O    | 1:A:833:VAL:HG12  | 2.18                     | 0.43              |
| 1:B:673:ILE:O    | 1:B:677:PHE:HB2   | 2.18                     | 0.43              |
| 1:A:804:VAL:O    | 1:A:804:VAL:HG12  | 2.18                     | 0.43              |
| 1:B:689:TYR:HE2  | 1:B:767:ASN:HD22  | 1.65                     | 0.43              |
| 1:D:839:ILE:HD13 | 1:D:1002:LEU:HD12 | 2.01                     | 0.43              |
| 1:D:953:LYS:HE2  | 1:D:953:LYS:HB2   | 1.82                     | 0.43              |
| 1:D:973:THR:HG23 | 1:D:973:THR:O     | 2.18                     | 0.43              |
| 1:B:710:TYR:CD1  | 1:B:765:LEU:HD12  | 2.53                     | 0.43              |
| 1:B:775:TYR:CE2  | 1:B:779:ARG:HD2   | 2.54                     | 0.43              |
| 1:D:752:LEU:HD21 | 1:D:761:LYS:HE3   | 2.01                     | 0.43              |
| 1:D:866:THR:HG23 | 1:D:918:LEU:HD21  | 2.01                     | 0.43              |
| 1:A:857:ARG:HH21 | 1:A:966:GLY:HA3   | 1.84                     | 0.42              |
| 1:B:878:ARG:HH22 | 1:B:879:ILE:HG12  | 1.84                     | 0.42              |
| 1:B:879:ILE:HG13 | 1:B:880:ALA:O     | 2.19                     | 0.42              |
| 1:B:963:SER:O    | 1:B:965:ASP:N     | 2.50                     | 0.42              |
| 1:C:717:GLN:C    | 1:C:719:ALA:N     | 2.76                     | 0.42              |
| 1:C:992:TYR:CD1  | 1:C:992:TYR:N     | 2.87                     | 0.42              |
| 1:D:895:ILE:HG22 | 1:D:897:PHE:CE1   | 2.54                     | 0.42              |
| 1:B:849:LYS:HA   | 1:B:849:LYS:NZ    | 2.34                     | 0.42              |
| 1:C:905:ALA:C    | 1:C:907:TYR:N     | 2.75                     | 0.42              |
| 1:D:865:ARG:NE   | 1:D:909:HIS:HB2   | 2.34                     | 0.42              |
| 1:D:1006:LYS:NZ  | 1:D:1006:LYS:HB2  | 2.32                     | 0.42              |
| 1:B:704:ARG:H    | 1:B:704:ARG:HE    | 1.66                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:829:TYR:CD1   | 1:B:831:LEU:CD1   | 3.03                     | 0.42              |
| 1:B:844:GLU:CD    | 1:B:998:ASN:HA    | 2.44                     | 0.42              |
| 1:C:672:LEU:O     | 1:C:675:MET:HB3   | 2.19                     | 0.42              |
| 1:C:852:LYS:O     | 1:C:852:LYS:HG3   | 2.16                     | 0.42              |
| 1:C:926:LEU:HD23  | 1:C:947:SER:OG    | 2.19                     | 0.42              |
| 1:C:971:LEU:HD12  | 1:C:971:LEU:H     | 1.85                     | 0.42              |
| 1:B:748:LYS:HD3   | 1:B:749:PRO:CD    | 2.50                     | 0.42              |
| 1:B:809:GLU:O     | 1:B:810:GLU:C     | 2.61                     | 0.42              |
| 1:C:805:ASP:O     | 1:C:807:ASP:N     | 2.50                     | 0.42              |
| 1:D:849:LYS:C     | 1:D:851:PHE:N     | 2.77                     | 0.42              |
| 1:D:869:PHE:HA    | 1:D:872:ILE:HD12  | 2.02                     | 0.42              |
| 1:A:753:ASN:C     | 1:A:755:ALA:N     | 2.77                     | 0.42              |
| 1:A:886:VAL:HG23  | 1:A:887:THR:N     | 2.35                     | 0.42              |
| 1:A:969:VAL:HA    | 1:A:970:PRO:HD3   | 1.69                     | 0.42              |
| 1:B:729:ILE:HG22  | 1:B:751:LEU:HD11  | 2.00                     | 0.42              |
| 1:B:942:PRO:HA    | 1:C:978:GLY:HA3   | 2.01                     | 0.42              |
| 1:C:667:LYS:CB    | 1:C:668:PRO:HD3   | 2.46                     | 0.42              |
| 1:C:792:VAL:O     | 1:C:795:GLU:HG3   | 2.20                     | 0.42              |
| 1:C:860:LEU:CB    | 1:C:897:PHE:HB3   | 2.48                     | 0.42              |
| 1:D:990:ILE:HD12  | 1:D:990:ILE:N     | 2.35                     | 0.42              |
| 1:A:1009:PHE:C    | 1:A:1010:LYS:HD2  | 2.44                     | 0.42              |
| 1:B:797:LEU:HB3   | 1:B:799:THR:HG22  | 2.02                     | 0.42              |
| 1:D:696:MET:HE1   | 1:D:700:LYS:O     | 2.20                     | 0.42              |
| 1:D:728:GLN:O     | 1:D:732:LEU:HG    | 2.20                     | 0.42              |
| 1:B:775:TYR:HE2   | 1:B:779:ARG:HH11  | 1.68                     | 0.42              |
| 1:B:1002:LEU:HD22 | 1:B:1002:LEU:HA   | 1.74                     | 0.42              |
| 1:C:838:LYS:HB2   | 1:C:838:LYS:HE3   | 1.80                     | 0.42              |
| 1:C:851:PHE:HE2   | 1:C:995:ALA:HB3   | 1.84                     | 0.42              |
| 1:D:716:VAL:O     | 1:D:719:ALA:HB3   | 2.20                     | 0.42              |
| 1:D:801:ILE:O     | 1:D:802:LYS:C     | 2.63                     | 0.42              |
| 1:A:817:TYR:CE1   | 1:A:821:THR:HG21  | 2.54                     | 0.42              |
| 1:B:678:ASP:O     | 1:B:682:MET:HE3   | 2.20                     | 0.42              |
| 1:B:830:ASP:CB    | 1:B:1008:ASN:HD22 | 2.33                     | 0.42              |
| 1:C:686:MET:CE    | 1:C:698:LEU:HG    | 2.50                     | 0.42              |
| 1:D:786:SER:O     | 1:D:787:LYS:HD2   | 2.20                     | 0.42              |
| 1:D:993:ASP:O     | 1:D:996:GLN:HB3   | 2.20                     | 0.42              |
| 1:D:1009:PHE:C    | 1:D:1010:LYS:HD3  | 2.45                     | 0.42              |
| 1:B:692:ASP:HB2   | 1:B:743:ASP:CB    | 2.49                     | 0.42              |
| 1:C:685:ALA:O     | 1:C:686:MET:C     | 2.63                     | 0.42              |
| 1:A:706:ILE:HD13  | 1:A:768:LEU:HB3   | 2.02                     | 0.42              |
| 1:A:712:ILE:O     | 1:A:715:GLU:HB2   | 2.20                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:770:ASP:O     | 1:A:771:ILE:C    | 2.63                     | 0.42              |
| 1:A:956:PRO:O     | 1:A:957:ASP:C    | 2.63                     | 0.42              |
| 1:B:744:PHE:CZ    | 1:B:750:PRO:HD2  | 2.55                     | 0.42              |
| 1:C:671:ASP:O     | 1:C:675:MET:HB2  | 2.20                     | 0.42              |
| 1:C:710:TYR:HB3   | 1:C:883:GLU:O    | 2.20                     | 0.42              |
| 1:C:803:VAL:HG12  | 1:C:804:VAL:N    | 2.35                     | 0.42              |
| 1:D:676:ILE:HG23  | 1:D:870:ALA:CA   | 2.45                     | 0.42              |
| 1:D:829:TYR:CD1   | 1:D:830:ASP:N    | 2.87                     | 0.42              |
| 1:D:957:ASP:HA    | 1:D:958:PRO:HD2  | 1.88                     | 0.42              |
| 1:C:882:PRO:O     | 1:C:893:LYS:HE3  | 2.20                     | 0.41              |
| 1:D:1002:LEU:HD23 | 1:D:1003:LEU:O   | 2.20                     | 0.41              |
| 1:A:749:PRO:HA    | 1:A:750:PRO:HD2  | 1.87                     | 0.41              |
| 1:A:752:LEU:HD11  | 1:A:761:LYS:HZ3  | 1.85                     | 0.41              |
| 1:B:662:LYS:O     | 1:B:787:LYS:HG3  | 2.19                     | 0.41              |
| 1:B:710:TYR:HB3   | 1:B:884:ALA:HA   | 2.02                     | 0.41              |
| 1:C:725:SER:O     | 1:C:726:ASP:C    | 2.61                     | 0.41              |
| 1:C:839:ILE:HG12  | 1:C:1000:LYS:O   | 2.20                     | 0.41              |
| 1:D:663:SER:OG    | 1:D:664:LYS:N    | 2.53                     | 0.41              |
| 1:D:826:HIS:CD2   | 1:D:826:HIS:N    | 2.88                     | 0.41              |
| 1:B:760:ALA:HA    | 1:B:763:GLU:HG3  | 2.01                     | 0.41              |
| 1:C:933:LYS:HB2   | 1:C:982:THR:CB   | 2.43                     | 0.41              |
| 1:D:677:PHE:HE1   | 1:D:777:LEU:HD12 | 1.85                     | 0.41              |
| 1:D:841:ARG:NE    | 1:D:876:GLY:H    | 2.11                     | 0.41              |
| 1:D:972:GLY:O     | 1:D:974:GLY:N    | 2.53                     | 0.41              |
| 1:D:1002:LEU:HD23 | 1:D:1002:LEU:C   | 2.45                     | 0.41              |
| 1:A:716:VAL:O     | 1:A:720:VAL:HB   | 2.21                     | 0.41              |
| 1:A:829:TYR:CD1   | 1:A:829:TYR:C    | 2.98                     | 0.41              |
| 1:A:957:ASP:HA    | 1:A:958:PRO:HD2  | 1.91                     | 0.41              |
| 1:B:690:GLU:O     | 1:B:690:GLU:HG3  | 2.21                     | 0.41              |
| 1:B:921:LEU:HB3   | 1:B:1001:TYR:HB2 | 2.02                     | 0.41              |
| 1:C:717:GLN:O     | 1:C:719:ALA:N    | 2.46                     | 0.41              |
| 1:C:887:THR:HA    | 1:C:937:HIS:CE1  | 2.56                     | 0.41              |
| 1:D:664:LYS:NZ    | 1:D:665:LEU:HD21 | 2.33                     | 0.41              |
| 1:D:720:VAL:CG1   | 1:D:721:SER:N    | 2.83                     | 0.41              |
| 1:D:765:LEU:HA    | 1:D:768:LEU:HD12 | 2.02                     | 0.41              |
| 1:D:879:ILE:HG22  | 1:D:894:GLY:C    | 2.45                     | 0.41              |
| 1:B:759:GLN:C     | 1:B:761:LYS:N    | 2.78                     | 0.41              |
| 1:B:991:VAL:CG1   | 1:B:992:TYR:N    | 2.84                     | 0.41              |
| 1:C:698:LEU:HD22  | 1:C:775:TYR:CD1  | 2.56                     | 0.41              |
| 1:A:753:ASN:O     | 1:A:755:ALA:N    | 2.54                     | 0.41              |
| 1:B:903:LYS:NZ    | 1:B:988:GLU:CG   | 2.83                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:827:ASN:OD1  | 1:B:827:ASN:O    | 2.39                     | 0.41              |
| 1:C:724:SER:HB3  | 1:C:725:SER:H    | 1.66                     | 0.41              |
| 1:C:768:LEU:HD23 | 1:C:768:LEU:HA   | 1.88                     | 0.41              |
| 1:C:863:GLY:N    | 1:C:904:SER:HB2  | 2.35                     | 0.41              |
| 1:D:677:PHE:O    | 1:D:679:VAL:N    | 2.54                     | 0.41              |
| 1:D:800:ASP:O    | 1:D:802:LYS:N    | 2.45                     | 0.41              |
| 1:D:918:LEU:N    | 1:D:918:LEU:CD2  | 2.84                     | 0.41              |
| 1:A:804:VAL:HB   | 1:A:836:ILE:CG2  | 2.48                     | 0.41              |
| 1:B:728:GLN:O    | 1:B:732:LEU:HB2  | 2.21                     | 0.41              |
| 1:C:903:LYS:HZ1  | 1:C:988:GLU:HG3  | 1.81                     | 0.41              |
| 1:D:920:LEU:HD11 | 1:D:999:LEU:HD13 | 2.02                     | 0.41              |
| 1:A:727:SER:HB3  | 1:C:827:ASN:ND2  | 2.35                     | 0.41              |
| 1:A:878:ARG:NH1  | 1:A:879:ILE:CG1  | 2.84                     | 0.41              |
| 1:A:878:ARG:CD   | 1:A:994:ILE:HG21 | 2.47                     | 0.41              |
| 1:A:938:ILE:CG2  | 1:A:939:SER:N    | 2.84                     | 0.41              |
| 1:A:942:PRO:HA   | 1:D:978:GLY:HA3  | 2.03                     | 0.41              |
| 1:B:665:LEU:O    | 1:B:666:PRO:C    | 2.61                     | 0.41              |
| 1:B:739:LEU:C    | 1:B:739:LEU:CD1  | 2.94                     | 0.41              |
| 1:B:805:ASP:O    | 1:B:806:ARG:C    | 2.64                     | 0.41              |
| 1:C:755:ALA:O    | 1:C:759:GLN:HB2  | 2.19                     | 0.41              |
| 1:C:787:LYS:HD2  | 1:C:787:LYS:N    | 2.36                     | 0.41              |
| 1:D:727:SER:HB3  | 1:D:728:GLN:OE1  | 2.20                     | 0.41              |
| 1:D:765:LEU:HD23 | 1:D:765:LEU:HA   | 1.84                     | 0.41              |
| 1:D:811:ALA:O    | 1:D:812:GLU:C    | 2.64                     | 0.41              |
| 1:A:689:TYR:O    | 1:A:690:GLU:HB2  | 2.21                     | 0.41              |
| 1:A:714:SER:HB3  | 1:A:885:PRO:HB3  | 2.02                     | 0.41              |
| 1:B:735:ARG:HG2  | 1:B:735:ARG:NH1  | 2.35                     | 0.41              |
| 1:B:769:LEU:O    | 1:B:773:VAL:HG23 | 2.21                     | 0.41              |
| 1:B:839:ILE:CD1  | 1:B:920:LEU:HD11 | 2.50                     | 0.41              |
| 1:B:872:ILE:O    | 1:B:876:GLY:CA   | 2.69                     | 0.41              |
| 1:C:812:GLU:O    | 1:C:816:LYS:HB2  | 2.21                     | 0.41              |
| 1:C:817:TYR:OH   | 1:C:859:LEU:O    | 2.39                     | 0.41              |
| 1:D:934:HIS:ND1  | 1:D:934:HIS:N    | 2.68                     | 0.41              |
| 1:D:953:LYS:NZ   | 1:D:980:ASN:HA   | 2.37                     | 0.41              |
| 1:D:956:PRO:HB3  | 1:D:970:PRO:O    | 2.21                     | 0.41              |
| 1:C:704:ARG:H    | 1:C:704:ARG:CZ   | 2.33                     | 0.40              |
| 1:D:692:ASP:HA   | 1:D:743:ASP:HB2  | 2.03                     | 0.40              |
| 1:D:754:ASN:C    | 1:D:756:ASP:N    | 2.80                     | 0.40              |
| 1:A:686:MET:HE3  | 1:A:686:MET:HB3  | 1.88                     | 0.40              |
| 1:A:748:LYS:CG   | 1:C:688:GLU:HB3  | 2.46                     | 0.40              |
| 1:B:802:LYS:N    | 1:B:802:LYS:HE2  | 2.37                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:748:LYS:HA   | 1:D:749:PRO:HD3  | 1.91                     | 0.40              |
| 1:D:847:ARG:NH1  | 1:D:994:ILE:HG22 | 2.37                     | 0.40              |
| 1:D:849:LYS:HG2  | 1:D:852:LYS:HE2  | 2.03                     | 0.40              |
| 1:D:866:THR:HG23 | 1:D:918:LEU:CD2  | 2.52                     | 0.40              |
| 1:D:953:LYS:O    | 1:D:953:LYS:HG3  | 2.22                     | 0.40              |
| 1:A:985:LEU:HD23 | 1:A:986:TYR:HE2  | 1.86                     | 0.40              |
| 1:B:677:PHE:CZ   | 1:B:777:LEU:HD12 | 2.56                     | 0.40              |
| 1:B:792:VAL:HG12 | 1:B:796:LYS:HE3  | 2.03                     | 0.40              |
| 1:B:856:ASN:ND2  | 1:B:929:MET:HE2  | 2.36                     | 0.40              |
| 1:C:754:ASN:ND2  | 1:C:757:SER:CB   | 2.83                     | 0.40              |
| 1:C:849:LYS:HD3  | 1:C:849:LYS:C    | 2.46                     | 0.40              |
| 1:D:665:LEU:HB3  | 1:D:669:VAL:HB   | 2.03                     | 0.40              |
| 1:D:794:TYR:HD2  | 1:D:794:TYR:C    | 2.28                     | 0.40              |
| 1:D:969:VAL:HG23 | 1:D:969:VAL:O    | 2.21                     | 0.40              |
| 1:B:753:ASN:CG   | 1:B:754:ASN:N    | 2.80                     | 0.40              |
| 1:C:803:VAL:CG1  | 1:C:804:VAL:N    | 2.85                     | 0.40              |
| 1:A:857:ARG:O    | 1:A:967:VAL:HA   | 2.21                     | 0.40              |
| 1:D:815:ARG:CB   | 1:D:815:ARG:HH11 | 2.35                     | 0.40              |
| 1:D:924:VAL:HG12 | 1:D:997:VAL:HG23 | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 348/350 (99%)   | 294 (84%)  | 44 (13%)  | 10 (3%)  | 3           | 20 |
| 1   | B     | 348/350 (99%)   | 275 (79%)  | 56 (16%)  | 17 (5%)  | 1           | 10 |
| 1   | C     | 348/350 (99%)   | 279 (80%)  | 55 (16%)  | 14 (4%)  | 2           | 14 |
| 1   | D     | 348/350 (99%)   | 254 (73%)  | 61 (18%)  | 33 (10%) | 0           | 2  |
| All | All   | 1392/1400 (99%) | 1102 (79%) | 216 (16%) | 74 (5%)  | 1           | 9  |

All (74) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 724  | SER  |
| 1   | A     | 786  | SER  |
| 1   | B     | 724  | SER  |
| 1   | B     | 828  | ALA  |
| 1   | B     | 965  | ASP  |
| 1   | C     | 753  | ASN  |
| 1   | C     | 785  | SER  |
| 1   | C     | 786  | SER  |
| 1   | C     | 883  | GLU  |
| 1   | D     | 693  | LEU  |
| 1   | D     | 841  | ARG  |
| 1   | D     | 862  | HIS  |
| 1   | D     | 869  | PHE  |
| 1   | D     | 876  | GLY  |
| 1   | D     | 964  | LEU  |
| 1   | D     | 1008 | ASN  |
| 1   | A     | 725  | SER  |
| 1   | A     | 753  | ASN  |
| 1   | B     | 783  | ASP  |
| 1   | B     | 790  | ILE  |
| 1   | C     | 781  | GLY  |
| 1   | C     | 806  | ARG  |
| 1   | C     | 947  | SER  |
| 1   | C     | 981  | ASP  |
| 1   | D     | 678  | ASP  |
| 1   | D     | 784  | ASP  |
| 1   | D     | 785  | SER  |
| 1   | D     | 800  | ASP  |
| 1   | D     | 853  | GLN  |
| 1   | D     | 916  | ILE  |
| 1   | D     | 962  | ILE  |
| 1   | D     | 1004 | LYS  |
| 1   | A     | 745  | GLY  |
| 1   | A     | 754  | ASN  |
| 1   | B     | 667  | LYS  |
| 1   | B     | 768  | LEU  |
| 1   | B     | 806  | ARG  |
| 1   | C     | 718  | GLN  |
| 1   | C     | 823  | ALA  |
| 1   | C     | 842  | GLU  |
| 1   | D     | 671  | ASP  |
| 1   | D     | 779  | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 801  | ILE  |
| 1   | D     | 817  | TYR  |
| 1   | D     | 909  | HIS  |
| 1   | D     | 973  | THR  |
| 1   | D     | 1003 | LEU  |
| 1   | D     | 1009 | PHE  |
| 1   | B     | 745  | GLY  |
| 1   | B     | 803  | VAL  |
| 1   | D     | 664  | LYS  |
| 1   | D     | 774  | ALA  |
| 1   | D     | 961  | ASN  |
| 1   | A     | 698  | LEU  |
| 1   | B     | 754  | ASN  |
| 1   | B     | 780  | GLY  |
| 1   | B     | 851  | PHE  |
| 1   | B     | 937  | HIS  |
| 1   | C     | 931  | GLU  |
| 1   | C     | 967  | VAL  |
| 1   | D     | 769  | LEU  |
| 1   | D     | 821  | THR  |
| 1   | A     | 789  | PRO  |
| 1   | B     | 679  | VAL  |
| 1   | B     | 749  | PRO  |
| 1   | B     | 805  | ASP  |
| 1   | C     | 778  | LEU  |
| 1   | D     | 914  | ASP  |
| 1   | D     | 881  | PRO  |
| 1   | A     | 699  | GLY  |
| 1   | D     | 818  | VAL  |
| 1   | D     | 773  | VAL  |
| 1   | A     | 676  | ILE  |
| 1   | D     | 723  | GLY  |

### 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     | 308/308 (100%)   | 286 (93%)  | 22 (7%)  | 13          | 43 |
| 1   | B     | 308/308 (100%)   | 281 (91%)  | 27 (9%)  | 9           | 35 |
| 1   | C     | 308/308 (100%)   | 278 (90%)  | 30 (10%) | 8           | 30 |
| 1   | D     | 308/308 (100%)   | 277 (90%)  | 31 (10%) | 7           | 29 |
| All | All   | 1232/1232 (100%) | 1122 (91%) | 110 (9%) | 9           | 34 |

All (110) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 672 | LEU  |
| 1   | A     | 694 | GLN  |
| 1   | A     | 718 | GLN  |
| 1   | A     | 722 | GLN  |
| 1   | A     | 754 | ASN  |
| 1   | A     | 759 | GLN  |
| 1   | A     | 764 | MET  |
| 1   | A     | 772 | GLU  |
| 1   | A     | 798 | LYS  |
| 1   | A     | 799 | THR  |
| 1   | A     | 804 | VAL  |
| 1   | A     | 808 | SER  |
| 1   | A     | 838 | LYS  |
| 1   | A     | 839 | ILE  |
| 1   | A     | 844 | GLU  |
| 1   | A     | 854 | LEU  |
| 1   | A     | 859 | LEU  |
| 1   | A     | 878 | ARG  |
| 1   | A     | 943 | LYS  |
| 1   | A     | 949 | LYS  |
| 1   | A     | 954 | THR  |
| 1   | A     | 973 | THR  |
| 1   | B     | 694 | GLN  |
| 1   | B     | 704 | ARG  |
| 1   | B     | 716 | VAL  |
| 1   | B     | 726 | ASP  |
| 1   | B     | 769 | LEU  |
| 1   | B     | 783 | ASP  |
| 1   | B     | 791 | ASP  |
| 1   | B     | 802 | LYS  |
| 1   | B     | 835 | ASP  |
| 1   | B     | 849 | LYS  |
| 1   | B     | 854 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 856  | ASN  |
| 1   | B     | 875  | GLN  |
| 1   | B     | 878  | ARG  |
| 1   | B     | 916  | ILE  |
| 1   | B     | 919  | ILE  |
| 1   | B     | 921  | LEU  |
| 1   | B     | 924  | VAL  |
| 1   | B     | 928  | ASN  |
| 1   | B     | 936  | SER  |
| 1   | B     | 954  | THR  |
| 1   | B     | 962  | ILE  |
| 1   | B     | 971  | LEU  |
| 1   | B     | 973  | THR  |
| 1   | B     | 984  | LEU  |
| 1   | B     | 1005 | LEU  |
| 1   | B     | 1006 | LYS  |
| 1   | C     | 667  | LYS  |
| 1   | C     | 694  | GLN  |
| 1   | C     | 696  | MET  |
| 1   | C     | 700  | LYS  |
| 1   | C     | 738  | THR  |
| 1   | C     | 769  | LEU  |
| 1   | C     | 795  | GLU  |
| 1   | C     | 798  | LYS  |
| 1   | C     | 814  | ILE  |
| 1   | C     | 816  | LYS  |
| 1   | C     | 819  | LYS  |
| 1   | C     | 820  | ASN  |
| 1   | C     | 829  | TYR  |
| 1   | C     | 845  | CYS  |
| 1   | C     | 879  | ILE  |
| 1   | C     | 886  | VAL  |
| 1   | C     | 926  | LEU  |
| 1   | C     | 934  | HIS  |
| 1   | C     | 943  | LYS  |
| 1   | C     | 949  | LYS  |
| 1   | C     | 964  | LEU  |
| 1   | C     | 971  | LEU  |
| 1   | C     | 973  | THR  |
| 1   | C     | 975  | ILE  |
| 1   | C     | 990  | ILE  |
| 1   | C     | 994  | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1004 | LYS  |
| 1   | C     | 1005 | LEU  |
| 1   | C     | 1006 | LYS  |
| 1   | C     | 1010 | LYS  |
| 1   | D     | 664  | LYS  |
| 1   | D     | 674  | LYS  |
| 1   | D     | 688  | GLU  |
| 1   | D     | 690  | GLU  |
| 1   | D     | 704  | ARG  |
| 1   | D     | 730  | LEU  |
| 1   | D     | 742  | HIS  |
| 1   | D     | 747  | LYS  |
| 1   | D     | 751  | LEU  |
| 1   | D     | 758  | VAL  |
| 1   | D     | 770  | ASP  |
| 1   | D     | 777  | LEU  |
| 1   | D     | 789  | PRO  |
| 1   | D     | 794  | TYR  |
| 1   | D     | 805  | ASP  |
| 1   | D     | 806  | ARG  |
| 1   | D     | 817  | TYR  |
| 1   | D     | 824  | THR  |
| 1   | D     | 831  | LEU  |
| 1   | D     | 841  | ARG  |
| 1   | D     | 867  | THR  |
| 1   | D     | 916  | ILE  |
| 1   | D     | 918  | LEU  |
| 1   | D     | 919  | ILE  |
| 1   | D     | 931  | GLU  |
| 1   | D     | 934  | HIS  |
| 1   | D     | 943  | LYS  |
| 1   | D     | 971  | LEU  |
| 1   | D     | 992  | TYR  |
| 1   | D     | 1004 | LYS  |
| 1   | D     | 1005 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 694 | GLN  |
| 1   | A     | 707 | GLN  |
| 1   | A     | 722 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 754  | ASN  |
| 1   | A     | 759  | GLN  |
| 1   | A     | 767  | ASN  |
| 1   | A     | 793  | ASN  |
| 1   | A     | 875  | GLN  |
| 1   | A     | 906  | ASN  |
| 1   | A     | 909  | HIS  |
| 1   | A     | 961  | ASN  |
| 1   | A     | 980  | ASN  |
| 1   | A     | 996  | GLN  |
| 1   | A     | 1008 | ASN  |
| 1   | B     | 707  | GLN  |
| 1   | B     | 717  | GLN  |
| 1   | B     | 718  | GLN  |
| 1   | B     | 793  | ASN  |
| 1   | B     | 826  | HIS  |
| 1   | B     | 846  | GLN  |
| 1   | B     | 853  | GLN  |
| 1   | B     | 856  | ASN  |
| 1   | B     | 909  | HIS  |
| 1   | B     | 961  | ASN  |
| 1   | B     | 996  | GLN  |
| 1   | C     | 670  | GLN  |
| 1   | C     | 694  | GLN  |
| 1   | C     | 707  | GLN  |
| 1   | C     | 722  | GLN  |
| 1   | C     | 734  | ASN  |
| 1   | C     | 754  | ASN  |
| 1   | C     | 759  | GLN  |
| 1   | C     | 767  | ASN  |
| 1   | C     | 820  | ASN  |
| 1   | C     | 826  | HIS  |
| 1   | C     | 856  | ASN  |
| 1   | C     | 987  | ASN  |
| 1   | C     | 996  | GLN  |
| 1   | D     | 694  | GLN  |
| 1   | D     | 717  | GLN  |
| 1   | D     | 759  | GLN  |
| 1   | D     | 767  | ASN  |
| 1   | D     | 856  | ASN  |
| 1   | D     | 928  | ASN  |
| 1   | D     | 961  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 980 | ASN  |
| 1   | D     | 998 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 2   | CNQ  | A     | 1   | -    | 22,22,22     | 2.08 | 9 (40%)     | 31,31,31    | 2.36 | 11 (35%)    |
| 2   | CNQ  | B     | 2   | -    | 22,22,22     | 2.05 | 9 (40%)     | 31,31,31    | 2.46 | 8 (25%)     |
| 2   | CNQ  | D     | 4   | -    | 22,22,22     | 1.96 | 9 (40%)     | 31,31,31    | 2.37 | 9 (29%)     |
| 2   | CNQ  | C     | 3   | -    | 22,22,22     | 2.11 | 10 (45%)    | 31,31,31    | 2.53 | 12 (38%)    |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 2   | CNQ  | A     | 1   | -    | -       | 5/8/8/8  | 0/3/3/3 |
| 2   | CNQ  | B     | 2   | -    | -       | 4/8/8/8  | 0/3/3/3 |
| 2   | CNQ  | D     | 4   | -    | -       | 5/8/8/8  | 0/3/3/3 |
| 2   | CNQ  | C     | 3   | -    | -       | 6/8/8/8  | 0/3/3/3 |

All (37) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | C     | 3   | CNQ  | C9-N10  | 4.75 | 1.40        | 1.33     |
| 2   | A     | 1   | CNQ  | C9-N10  | 4.68 | 1.40        | 1.33     |
| 2   | D     | 4   | CNQ  | C9-N10  | 4.61 | 1.39        | 1.33     |
| 2   | B     | 2   | CNQ  | C9-N10  | 4.55 | 1.39        | 1.33     |
| 2   | C     | 3   | CNQ  | C8-N7   | 3.55 | 1.37        | 1.31     |
| 2   | A     | 1   | CNQ  | C6-C5   | 3.28 | 1.44        | 1.38     |
| 2   | B     | 2   | CNQ  | C8-N7   | 3.18 | 1.37        | 1.31     |
| 2   | C     | 3   | CNQ  | C6-C5   | 3.10 | 1.44        | 1.38     |
| 2   | A     | 1   | CNQ  | C8-N7   | 3.07 | 1.36        | 1.31     |
| 2   | D     | 4   | CNQ  | C8-N7   | 3.06 | 1.36        | 1.31     |
| 2   | C     | 3   | CNQ  | C1-C6   | 3.05 | 1.44        | 1.38     |
| 2   | B     | 2   | CNQ  | C6-C5   | 2.95 | 1.43        | 1.38     |
| 2   | B     | 2   | CNQ  | C19-C18 | 2.87 | 1.43        | 1.38     |
| 2   | C     | 3   | CNQ  | C4-C3   | 2.77 | 1.47        | 1.42     |
| 2   | A     | 1   | CNQ  | C1-C6   | 2.63 | 1.43        | 1.38     |
| 2   | B     | 2   | CNQ  | C4-C3   | 2.61 | 1.47        | 1.42     |
| 2   | C     | 3   | CNQ  | C19-C18 | 2.61 | 1.43        | 1.38     |
| 2   | D     | 4   | CNQ  | C6-C5   | 2.57 | 1.43        | 1.38     |
| 2   | A     | 1   | CNQ  | C1-C2   | 2.56 | 1.42        | 1.36     |
| 2   | A     | 1   | CNQ  | C4-C3   | 2.53 | 1.47        | 1.42     |
| 2   | C     | 3   | CNQ  | C18-C17 | 2.52 | 1.42        | 1.38     |
| 2   | B     | 2   | CNQ  | C1-C2   | 2.47 | 1.41        | 1.36     |
| 2   | B     | 2   | CNQ  | C1-C6   | 2.45 | 1.43        | 1.38     |
| 2   | D     | 4   | CNQ  | C19-C18 | 2.44 | 1.42        | 1.38     |
| 2   | D     | 4   | CNQ  | C4-C3   | 2.39 | 1.46        | 1.42     |
| 2   | C     | 3   | CNQ  | C1-C2   | 2.38 | 1.41        | 1.36     |
| 2   | D     | 4   | CNQ  | C1-C2   | 2.36 | 1.41        | 1.36     |
| 2   | B     | 2   | CNQ  | C18-C17 | 2.33 | 1.42        | 1.38     |
| 2   | D     | 4   | CNQ  | C1-C6   | 2.29 | 1.42        | 1.38     |
| 2   | A     | 1   | CNQ  | C19-C18 | 2.28 | 1.42        | 1.38     |
| 2   | D     | 4   | CNQ  | C18-C17 | 2.23 | 1.42        | 1.38     |
| 2   | B     | 2   | CNQ  | C16-C15 | 2.21 | 1.42        | 1.38     |
| 2   | A     | 1   | CNQ  | C16-C17 | 2.11 | 1.41        | 1.38     |
| 2   | A     | 1   | CNQ  | C16-C15 | 2.08 | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | C     | 3   | CNQ  | C16-C17 | 2.05 | 1.41        | 1.38     |
| 2   | D     | 4   | CNQ  | C16-C17 | 2.05 | 1.41        | 1.38     |
| 2   | C     | 3   | CNQ  | C16-C15 | 2.01 | 1.42        | 1.38     |

All (40) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | C     | 3   | CNQ  | O13-C11-C5  | 6.57  | 127.98      | 120.23   |
| 2   | B     | 2   | CNQ  | O13-C11-C5  | 5.89  | 127.18      | 120.23   |
| 2   | C     | 3   | CNQ  | C9-N10-C4   | 5.81  | 122.60      | 118.28   |
| 2   | B     | 2   | CNQ  | C9-N10-C4   | 5.76  | 122.56      | 118.28   |
| 2   | A     | 1   | CNQ  | O13-C11-C5  | 5.58  | 126.81      | 120.23   |
| 2   | D     | 4   | CNQ  | C9-N10-C4   | 5.58  | 122.43      | 118.28   |
| 2   | B     | 2   | CNQ  | C5-C4-N10   | 5.54  | 123.93      | 119.56   |
| 2   | D     | 4   | CNQ  | C5-C4-N10   | 5.33  | 123.76      | 119.56   |
| 2   | A     | 1   | CNQ  | C9-N10-C4   | 5.31  | 122.23      | 118.28   |
| 2   | D     | 4   | CNQ  | O13-C11-C5  | 5.19  | 126.35      | 120.23   |
| 2   | A     | 1   | CNQ  | C5-C4-N10   | 4.91  | 123.43      | 119.56   |
| 2   | C     | 3   | CNQ  | C9-C8-N7    | -4.49 | 120.25      | 123.62   |
| 2   | D     | 4   | CNQ  | C9-C8-N7    | -4.43 | 120.30      | 123.62   |
| 2   | C     | 3   | CNQ  | C5-C4-N10   | 4.41  | 123.04      | 119.56   |
| 2   | A     | 1   | CNQ  | C8-N7-C3    | 4.38  | 122.03      | 116.96   |
| 2   | B     | 2   | CNQ  | C3-C4-N10   | -4.19 | 116.93      | 121.41   |
| 2   | D     | 4   | CNQ  | C8-N7-C3    | 4.16  | 121.77      | 116.96   |
| 2   | C     | 3   | CNQ  | C8-N7-C3    | 4.12  | 121.72      | 116.96   |
| 2   | B     | 2   | CNQ  | C8-N7-C3    | 4.09  | 121.70      | 116.96   |
| 2   | A     | 1   | CNQ  | C9-C8-N7    | -4.04 | 120.59      | 123.62   |
| 2   | D     | 4   | CNQ  | C3-C4-N10   | -4.03 | 117.10      | 121.41   |
| 2   | B     | 2   | CNQ  | C9-C8-N7    | -3.84 | 120.75      | 123.62   |
| 2   | C     | 3   | CNQ  | C3-C4-N10   | -3.83 | 117.31      | 121.41   |
| 2   | A     | 1   | CNQ  | C3-C4-N10   | -3.79 | 117.35      | 121.41   |
| 2   | B     | 2   | CNQ  | O13-C11-N12 | -3.76 | 117.19      | 122.62   |
| 2   | C     | 3   | CNQ  | O13-C11-N12 | -3.22 | 117.97      | 122.62   |
| 2   | D     | 4   | CNQ  | O13-C11-N12 | -3.00 | 118.28      | 122.62   |
| 2   | A     | 1   | CNQ  | O13-C11-N12 | -2.94 | 118.37      | 122.62   |
| 2   | C     | 3   | CNQ  | C5-C11-N12  | -2.72 | 114.06      | 118.27   |
| 2   | B     | 2   | CNQ  | C8-C9-N10   | -2.69 | 118.68      | 120.78   |
| 2   | A     | 1   | CNQ  | C8-C9-N10   | -2.60 | 118.75      | 120.78   |
| 2   | C     | 3   | CNQ  | C4-C5-C11   | -2.43 | 122.64      | 125.16   |
| 2   | C     | 3   | CNQ  | C8-C9-N10   | -2.37 | 118.93      | 120.78   |
| 2   | C     | 3   | CNQ  | C8-C9-C14   | 2.35  | 125.23      | 122.10   |
| 2   | C     | 3   | CNQ  | C15-C14-C9  | -2.33 | 117.59      | 121.28   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | A     | 1   | CNQ  | C4-C5-C11  | -2.32 | 122.76      | 125.16   |
| 2   | D     | 4   | CNQ  | C15-C14-C9 | -2.23 | 117.75      | 121.28   |
| 2   | A     | 1   | CNQ  | C5-C11-N12 | -2.23 | 114.81      | 118.27   |
| 2   | D     | 4   | CNQ  | C8-C9-N10  | -2.23 | 119.04      | 120.78   |
| 2   | A     | 1   | CNQ  | C8-C9-C14  | 2.09  | 124.88      | 122.10   |

There are no chirality outliers.

All (20) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | B     | 2   | CNQ  | C15-C14-C9-C8  |
| 2   | B     | 2   | CNQ  | C19-C14-C9-C8  |
| 2   | B     | 2   | CNQ  | C15-C14-C9-N10 |
| 2   | B     | 2   | CNQ  | C19-C14-C9-N10 |
| 2   | A     | 1   | CNQ  | N12-C11-C5-C4  |
| 2   | C     | 3   | CNQ  | N12-C11-C5-C4  |
| 2   | C     | 3   | CNQ  | O13-C11-C5-C4  |
| 2   | D     | 4   | CNQ  | N12-C11-C5-C4  |
| 2   | D     | 4   | CNQ  | O13-C11-C5-C4  |
| 2   | C     | 3   | CNQ  | C19-C14-C9-C8  |
| 2   | A     | 1   | CNQ  | C15-C14-C9-C8  |
| 2   | D     | 4   | CNQ  | C19-C14-C9-C8  |
| 2   | A     | 1   | CNQ  | O13-C11-C5-C4  |
| 2   | C     | 3   | CNQ  | C15-C14-C9-C8  |
| 2   | C     | 3   | CNQ  | C15-C14-C9-N10 |
| 2   | C     | 3   | CNQ  | C19-C14-C9-N10 |
| 2   | D     | 4   | CNQ  | C15-C14-C9-C8  |
| 2   | D     | 4   | CNQ  | C15-C14-C9-N10 |
| 2   | A     | 1   | CNQ  | C19-C14-C9-N10 |
| 2   | A     | 1   | CNQ  | C19-C14-C9-C8  |

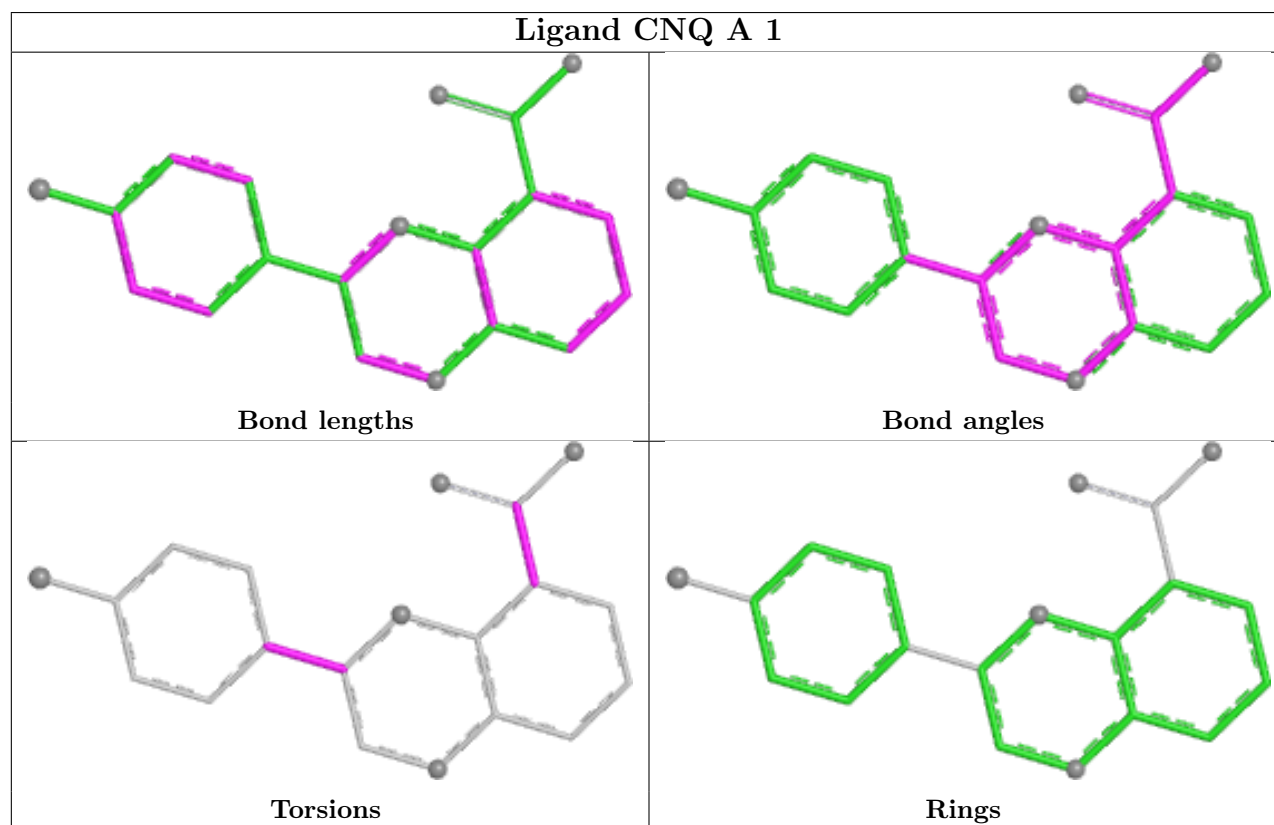
There are no ring outliers.

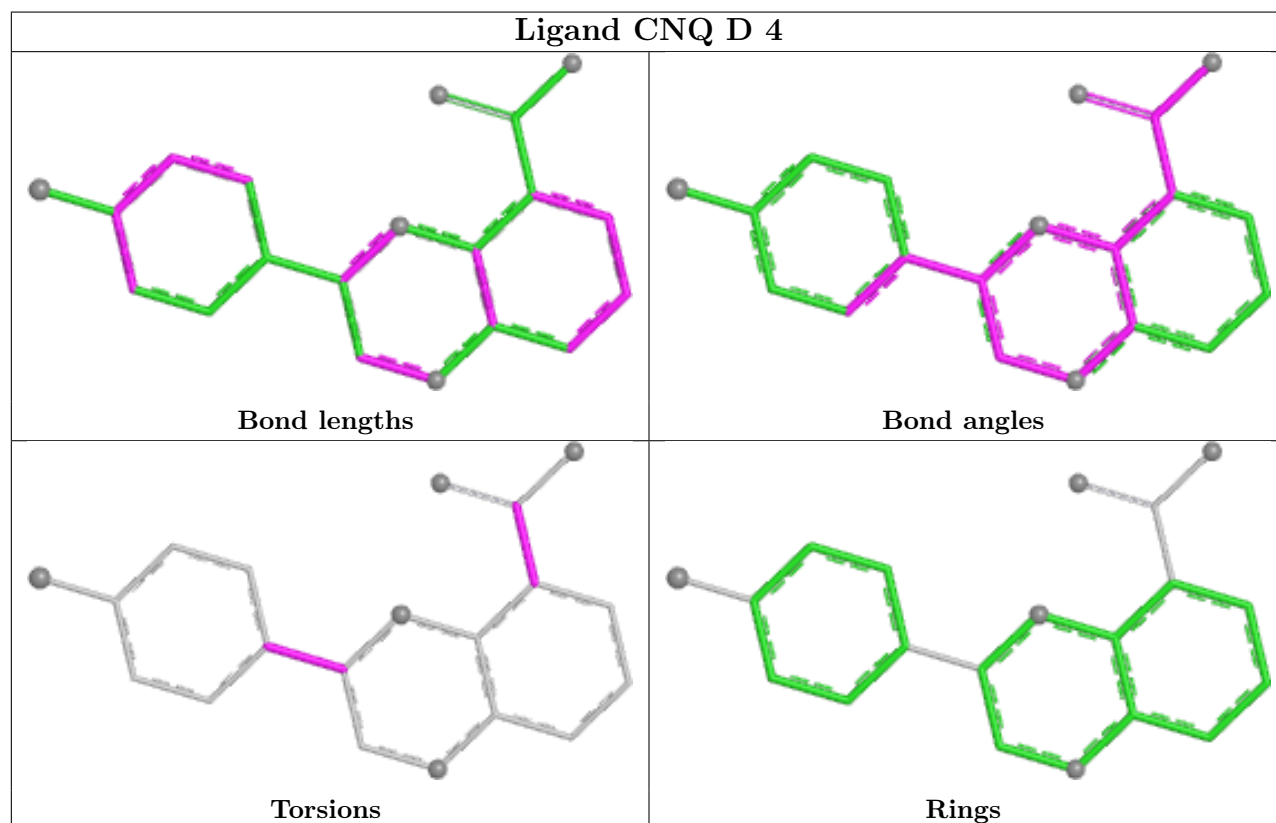
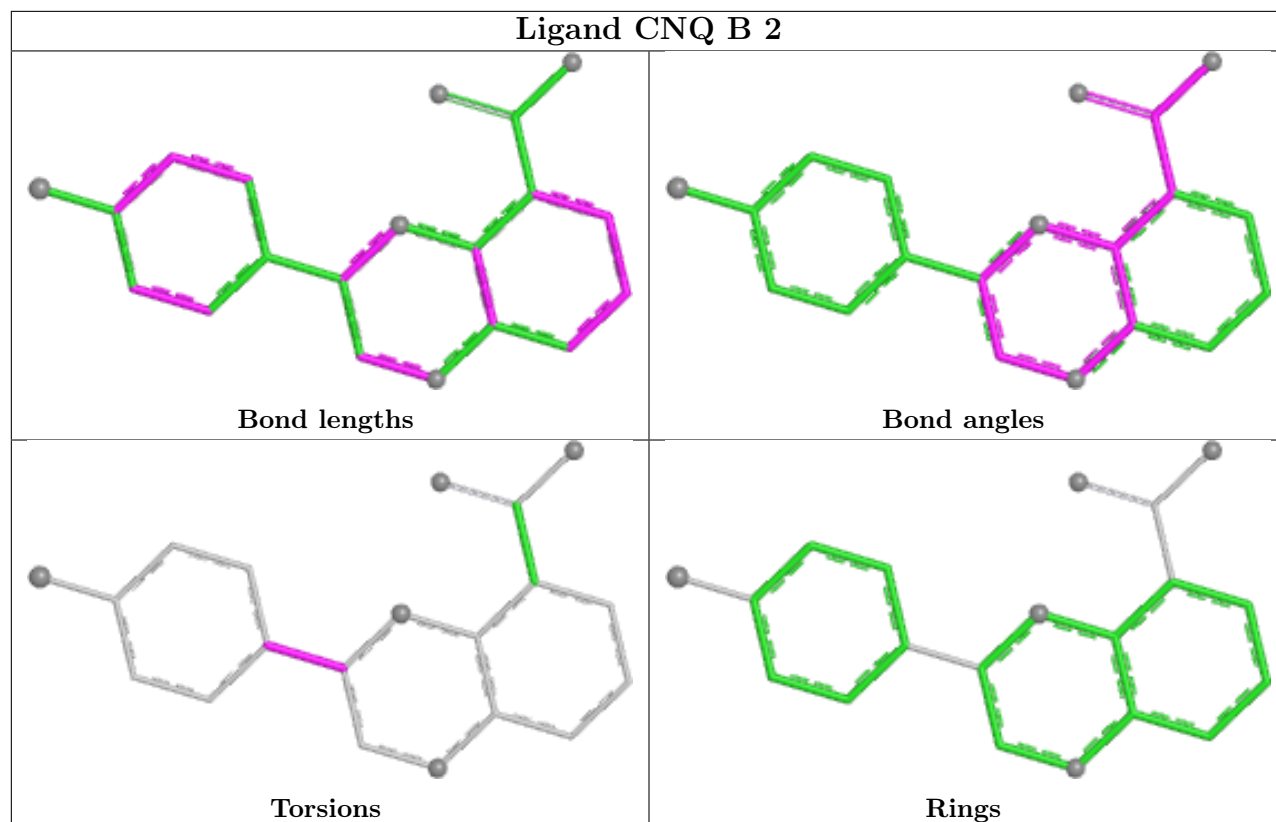
4 monomers are involved in 7 short contacts:

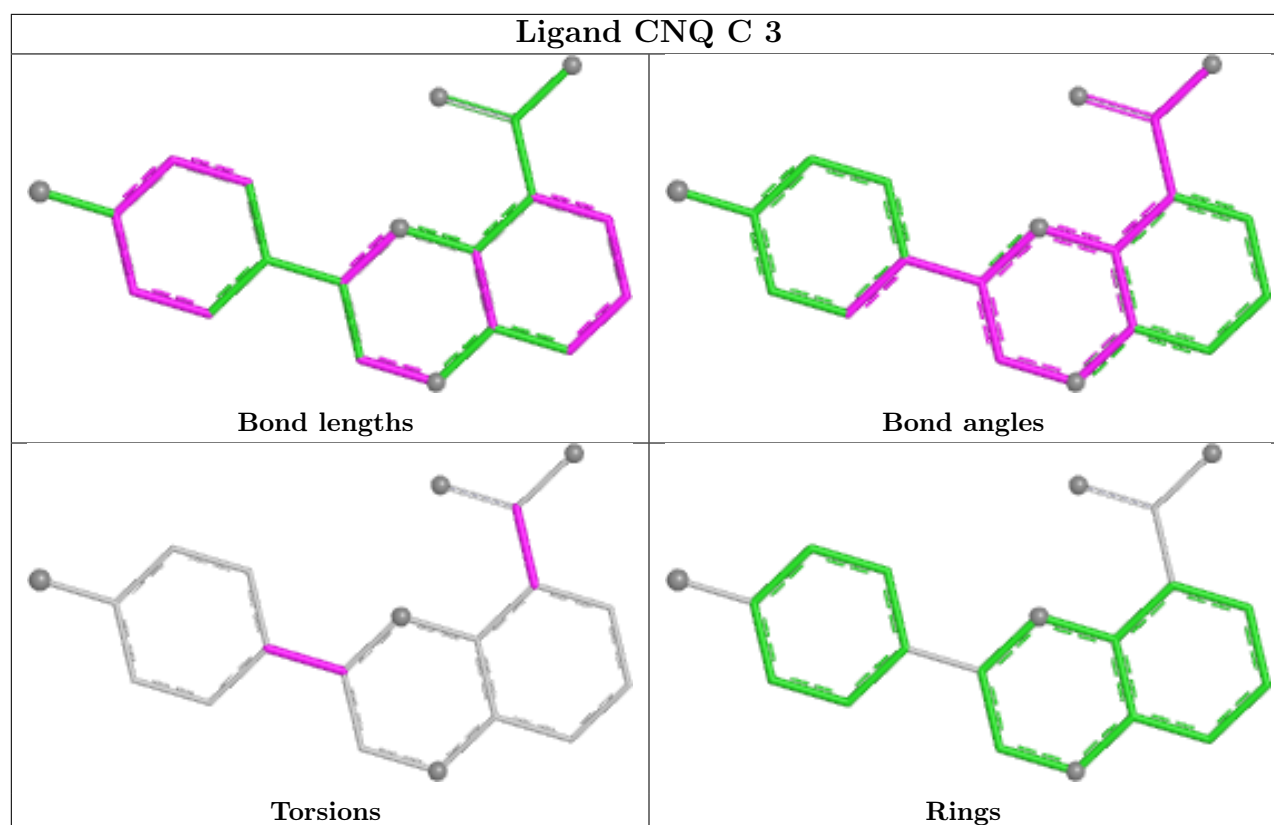
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | A     | 1   | CNQ  | 1       | 0            |
| 2   | B     | 2   | CNQ  | 2       | 0            |
| 2   | D     | 4   | CNQ  | 2       | 0            |
| 2   | C     | 3   | CNQ  | 2       | 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     | 350/350 (100%)   | -0.36  | 2 (0%) 85 69  | 10, 34, 85, 147       | 0     |
| 1   | B     | 350/350 (100%)   | -0.21  | 2 (0%) 85 69  | 9, 42, 102, 124       | 0     |
| 1   | C     | 350/350 (100%)   | -0.42  | 1 (0%) 90 79  | 9, 30, 77, 129        | 0     |
| 1   | D     | 350/350 (100%)   | 0.30   | 10 (2%) 53 31 | 15, 71, 126, 145      | 0     |
| All | All   | 1400/1400 (100%) | -0.17  | 15 (1%) 78 57 | 9, 41, 111, 147       | 0     |

All (15) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 756 | ASP  | 3.2  |
| 1   | D     | 836 | ILE  | 2.9  |
| 1   | A     | 782 | SER  | 2.6  |
| 1   | D     | 666 | PRO  | 2.5  |
| 1   | A     | 755 | ALA  | 2.3  |
| 1   | D     | 827 | ASN  | 2.3  |
| 1   | D     | 767 | ASN  | 2.3  |
| 1   | D     | 792 | VAL  | 2.2  |
| 1   | B     | 786 | SER  | 2.2  |
| 1   | D     | 848 | TYR  | 2.1  |
| 1   | D     | 670 | GLN  | 2.1  |
| 1   | C     | 782 | SER  | 2.1  |
| 1   | D     | 961 | ASN  | 2.1  |
| 1   | D     | 774 | ALA  | 2.0  |
| 1   | D     | 886 | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

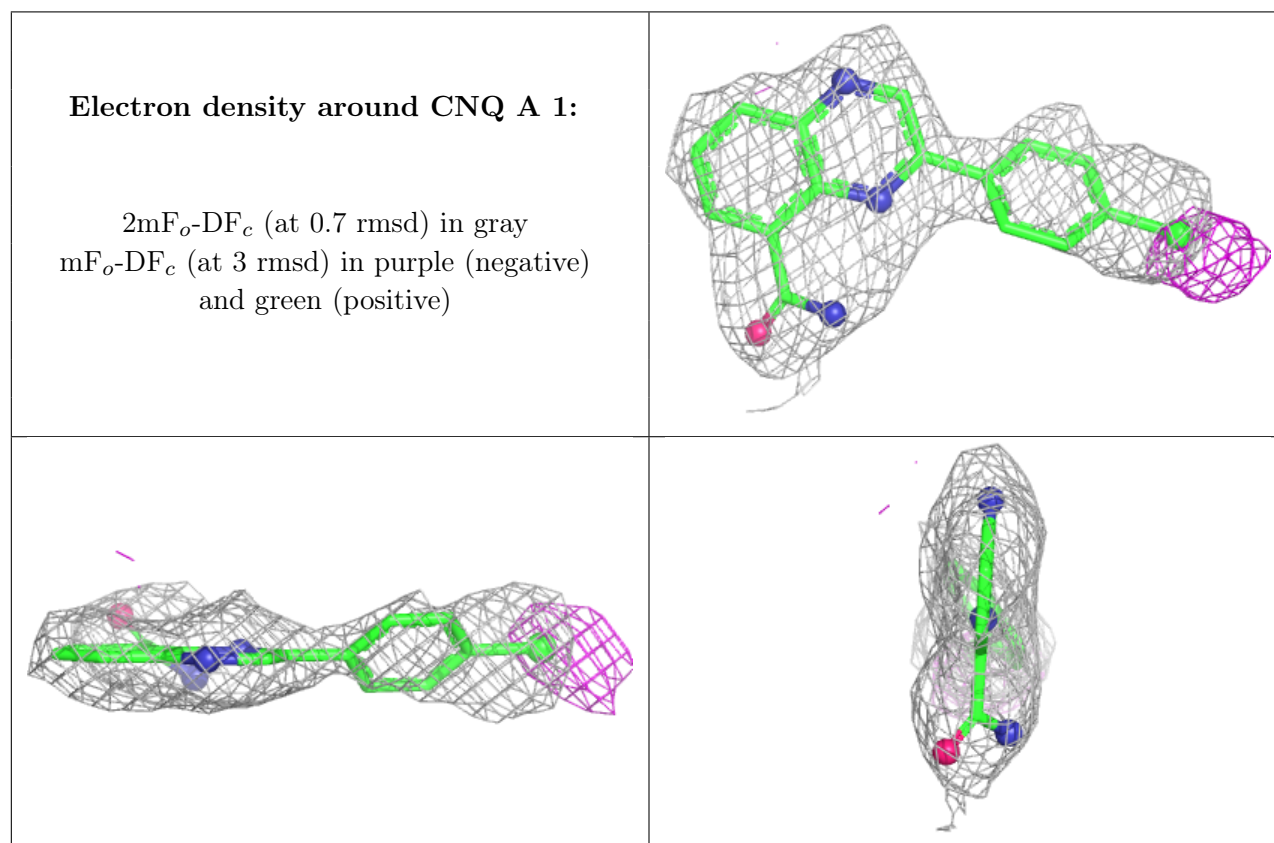
There are no oligosaccharides in this entry.

## 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.

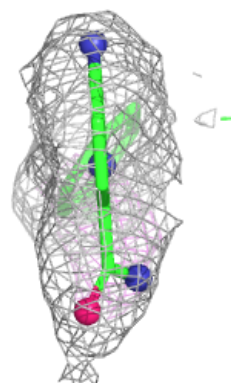
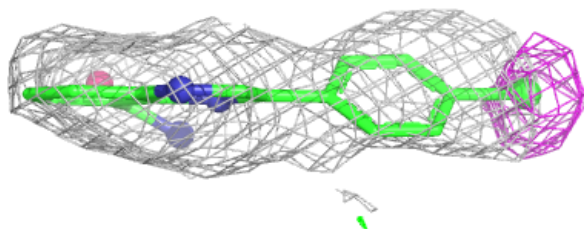
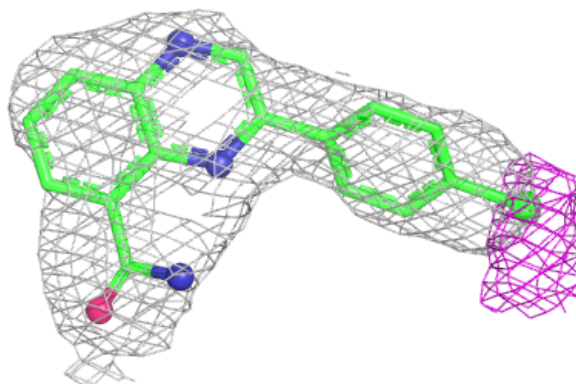
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | CNQ  | A     | 1   | 20/20 | 0.86 | 0.11 | 31,50,65,67                 | 0     |
| 2   | CNQ  | C     | 3   | 20/20 | 0.86 | 0.12 | 11,40,56,58                 | 0     |
| 2   | CNQ  | B     | 2   | 20/20 | 0.88 | 0.12 | 34,45,49,50                 | 0     |
| 2   | CNQ  | D     | 4   | 20/20 | 0.88 | 0.16 | 52,84,101,101               | 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.

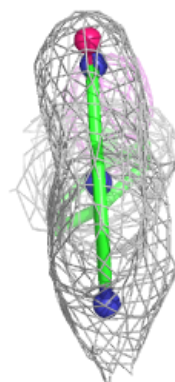
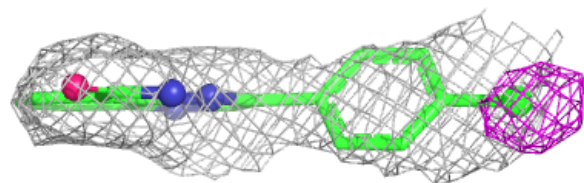
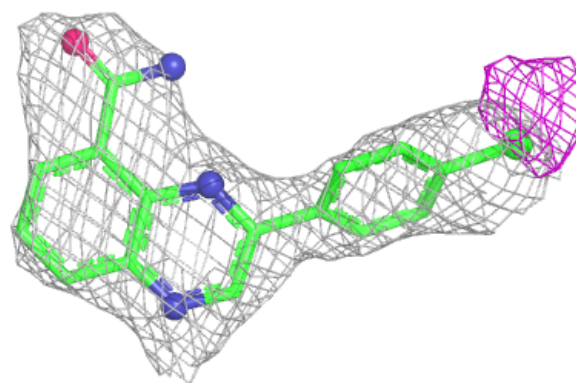


**Electron density around CNQ C 3:**

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

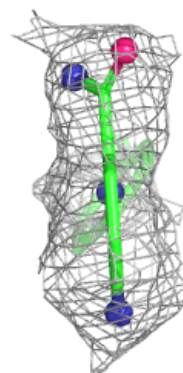
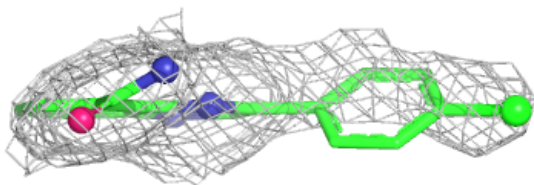
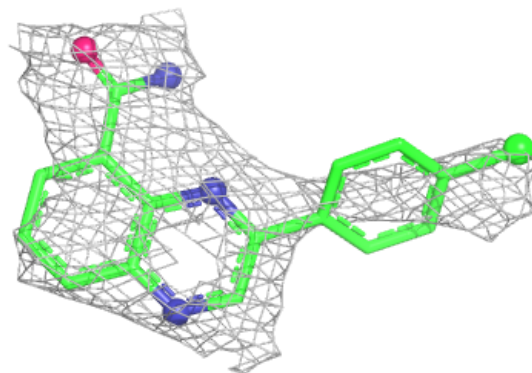
**Electron density around CNQ B 2:**

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



**Electron density around CNQ D 4:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.