



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:37 AM UTC

PDB ID : 3G49 / pdb\_00003g49  
Title : N-(Pyridin-2-yl) Arylsulfonamide Inhibitors of 11b-Hydroxysteroid Dehydrogenase Type 1: Discovery of PF-915275  
Authors : Pauly, T.A.  
Deposited on : 2009-02-03  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

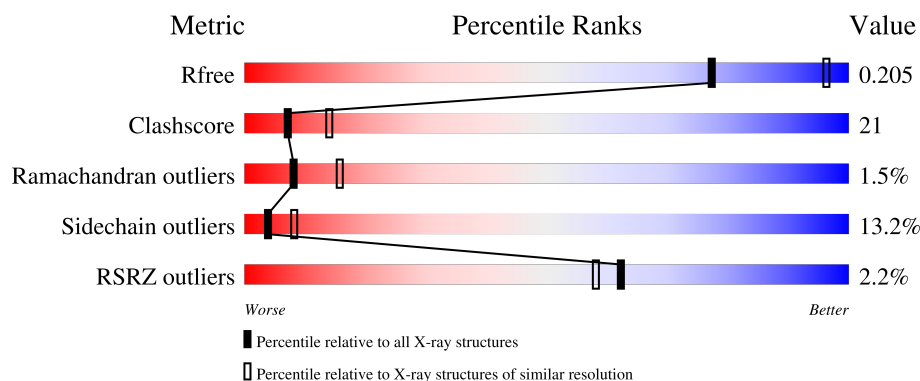
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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                      | 5829 (2.50-2.50)                                      |
| Clashscore            | 190562                      | 6492 (2.50-2.50)                                      |
| Ramachandran outliers | 187476                      | 6378 (2.50-2.50)                                      |
| Sidechain outliers    | 187428                      | 6380 (2.50-2.50)                                      |
| RSRZ outliers         | 180081                      | 5833 (2.50-2.50)                                      |

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     | 277    | <div> <div>48%</div> <div>33%</div> <div>12%</div> <div>• 5%</div> </div>               |
| 1   | B     | 277    | <div> <div>3%</div> <div>46%</div> <div>38%</div> <div>12%</div> <div>5%</div> </div>   |
| 1   | C     | 277    | <div> <div>2%</div> <div>51%</div> <div>32%</div> <div>10%</div> <div>• 5%</div> </div> |
| 1   | D     | 277    | <div> <div>3%</div> <div>43%</div> <div>38%</div> <div>12%</div> <div>• 5%</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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3   | 3G4  | A     | 2004 | -         | -        | X       | -                |
| 3   | 3G4  | D     | 2007 | -         | -        | X       | -                |

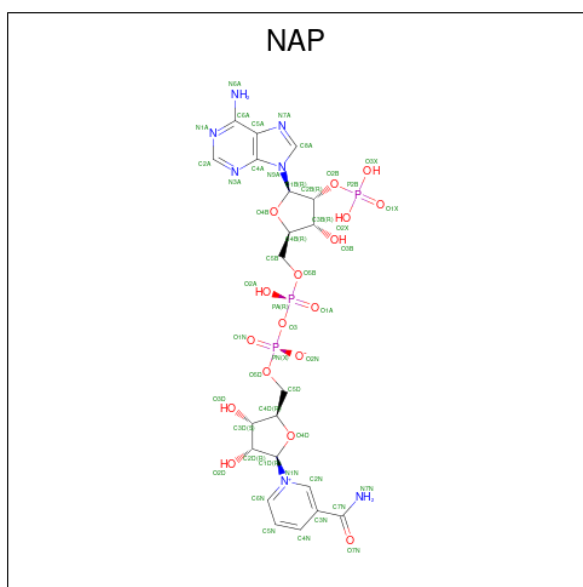


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 11-beta-hydroxysteroid dehydrogenase 1.

| Mol | Chain | Residues | Atoms         |           |          |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|---------|-------|
| 1   | A     | 263      | Total<br>2017 | C<br>1296 | N<br>337 | O<br>369 | S<br>15 | 0       | 0       | 0     |
| 1   | B     | 263      | Total<br>2017 | C<br>1296 | N<br>337 | O<br>369 | S<br>15 | 0       | 0       | 0     |
| 1   | C     | 263      | Total<br>2017 | C<br>1296 | N<br>337 | O<br>369 | S<br>15 | 0       | 0       | 0     |
| 1   | D     | 263      | Total<br>2017 | C<br>1296 | N<br>337 | O<br>369 | S<br>15 | 0       | 0       | 0     |

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



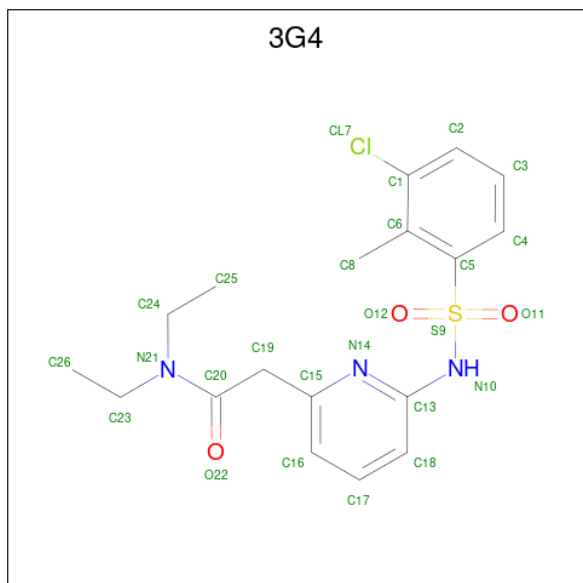
| Mol | Chain | Residues | Atoms       |         |        |         | ZeroOcc | AltConf |   |
|-----|-------|----------|-------------|---------|--------|---------|---------|---------|---|
| 2   | A     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3  | 0       | 0 |
| 2   | B     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3  | 0       | 0 |

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| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 17 | 3 |         |         |
| 2   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 48    | 21 | 7 | 17 | 3 |         |         |

- Molecule 3 is 2-(6-[(3-chloro-2-methylphenyl)sulfonyl]amino)pyridin-2-yl)-N,N-diethylacetamide (CCD ID: 3G4) (formula:  $C_{18}H_{22}ClN_3O_3S$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---|---------|---------|
| 3   | A     | 1        | Total | C  | Cl | N | O | S | 0       | 0       |
|     |       |          | 26    | 18 | 1  | 3 | 3 | 1 |         |         |
| 3   | D     | 1        | Total | C  | Cl | N | O | S | 0       | 0       |
|     |       |          | 26    | 18 | 1  | 3 | 3 | 1 |         |         |

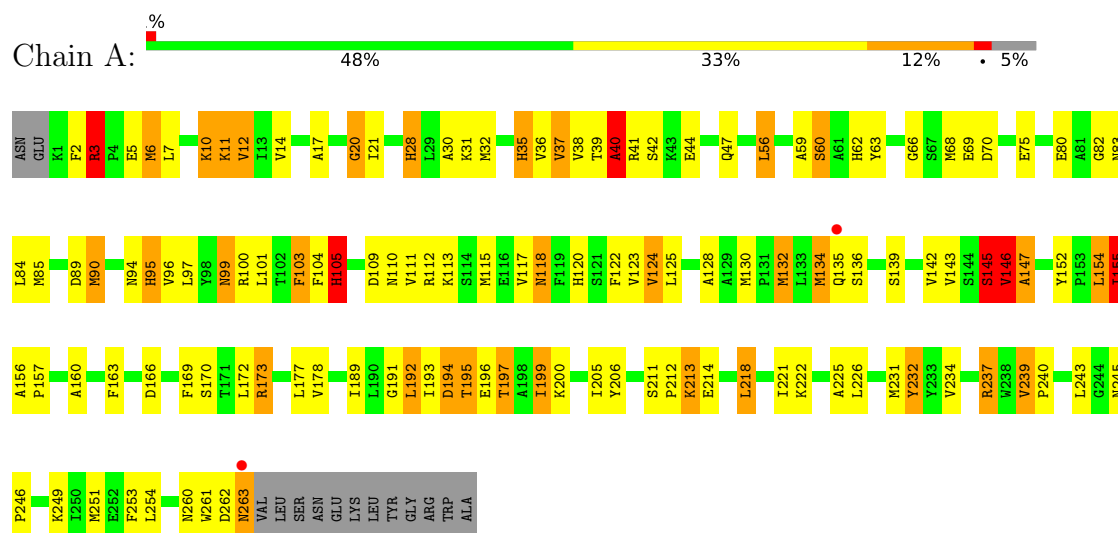
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 46       | Total | O  | 0       | 0       |
|     |       |          | 46    | 46 |         |         |
| 4   | B     | 28       | Total | O  | 0       | 0       |
|     |       |          | 28    | 28 |         |         |
| 4   | C     | 48       | Total | O  | 0       | 0       |
|     |       |          | 48    | 48 |         |         |
| 4   | D     | 46       | Total | O  | 0       | 0       |
|     |       |          | 46    | 46 |         |         |

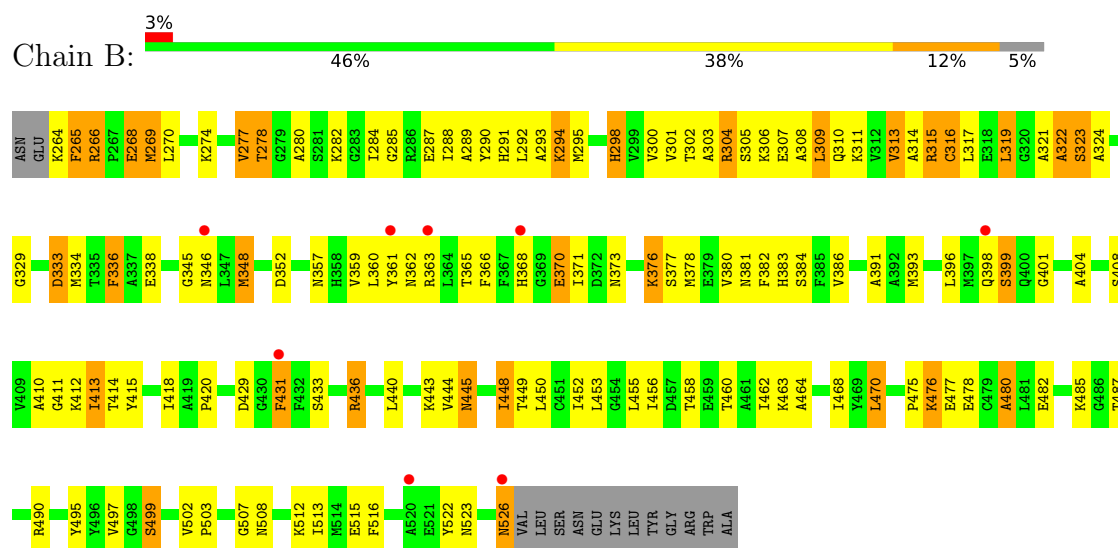
### 3 Residue-property plots

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: 11-beta-hydroxysteroid dehydrogenase 1

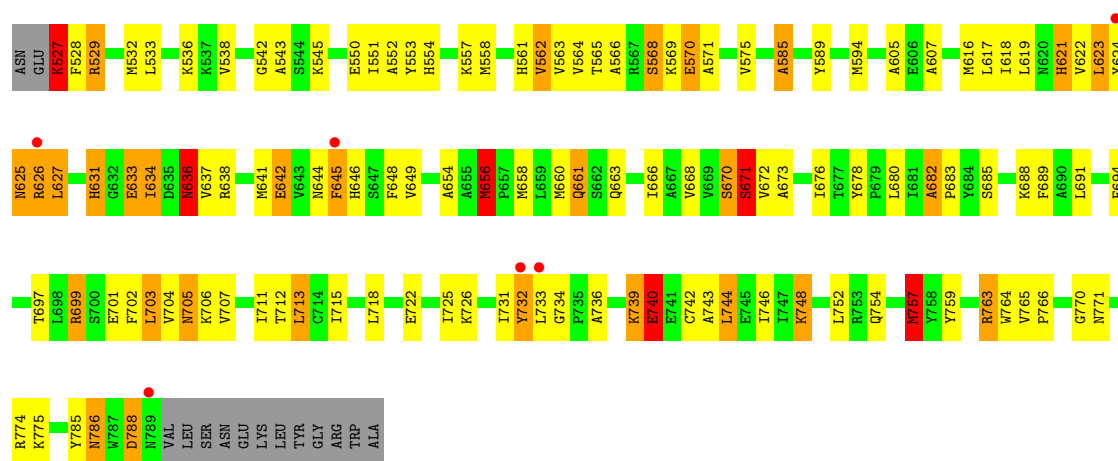


#### • Molecule 1: 11-beta-hydroxysteroid dehydrogenase 1

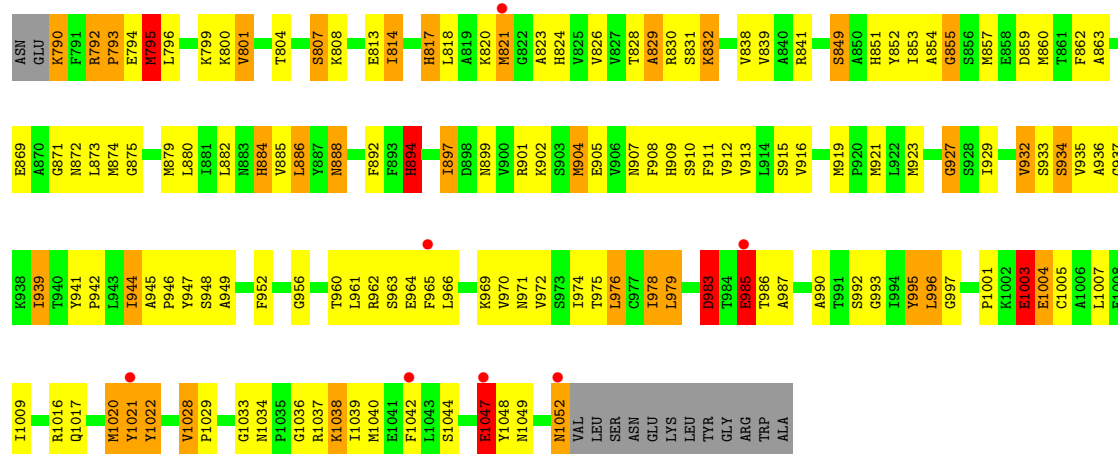


#### • Molecule 1: 11-beta-hydroxysteroid dehydrogenase 1





• Molecule 1: 11-beta-hydroxysteroid dehydrogenase 1



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 78.21Å 83.60Å 179.20Å<br>90.00° 90.00° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 41.27 – 2.50<br>41.27 – 2.50                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 91.8 (41.27-2.50)<br>91.8 (41.27-2.50)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.76 (at 2.51Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.1.24, CNS                                          | Depositor        |
| R, $R_{free}$                                                           | 0.189 , 0.225<br>0.213 , 0.205                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1935 reflections (5.08%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 27.8                                                        | Xtriage          |
| Anisotropy                                                              | 0.408                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.38 , 43.2                                                 | 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                                                   | 8480                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 31.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: NAP, 3G4

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     | 2.07         | 54/2056 (2.6%)  | 1.76        | 39/2777 (1.4%)   |
| 1   | B     | 1.98         | 43/2056 (2.1%)  | 1.72        | 34/2777 (1.2%)   |
| 1   | C     | 1.97         | 36/2056 (1.8%)  | 1.72        | 23/2777 (0.8%)   |
| 1   | D     | 2.03         | 51/2056 (2.5%)  | 1.81        | 42/2777 (1.5%)   |
| All | All   | 2.01         | 184/8224 (2.2%) | 1.75        | 138/11108 (1.2%) |

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                   |
| 1   | D     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (184) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 1   | C     | 757  | MET  | SD-CE | -12.98 | 1.47        | 1.79     |
| 1   | B     | 269  | MET  | SD-CE | -11.26 | 1.51        | 1.79     |
| 1   | C     | 733  | LEU  | C-O   | 11.15  | 1.39        | 1.24     |
| 1   | A     | 134  | MET  | SD-CE | 11.02  | 2.07        | 1.79     |
| 1   | C     | 558  | MET  | SD-CE | -10.79 | 1.52        | 1.79     |
| 1   | A     | 32   | MET  | SD-CE | -10.77 | 1.52        | 1.79     |
| 1   | A     | 117  | VAL  | CA-CB | 10.72  | 1.67        | 1.54     |
| 1   | B     | 334  | MET  | SD-CE | -10.42 | 1.53        | 1.79     |
| 1   | D     | 902  | LYS  | C-O   | -9.40  | 1.13        | 1.24     |
| 1   | D     | 1020 | MET  | SD-CE | -8.82  | 1.57        | 1.79     |
| 1   | B     | 448  | ILE  | C-O   | -8.71  | 1.14        | 1.24     |
| 1   | C     | 625  | ASN  | C-N   | 8.69   | 1.45        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | B     | 346  | ASN  | C-O   | 8.65  | 1.34        | 1.24     |
| 1   | A     | 117  | VAL  | C-O   | -8.65 | 1.14        | 1.24     |
| 1   | A     | 104  | PHE  | C-O   | 8.42  | 1.34        | 1.23     |
| 1   | B     | 366  | PHE  | C-O   | 8.23  | 1.33        | 1.23     |
| 1   | C     | 668  | VAL  | C-O   | -8.15 | 1.15        | 1.24     |
| 1   | D     | 1021 | TYR  | C-N   | -8.13 | 1.22        | 1.33     |
| 1   | A     | 212  | PRO  | C-N   | 8.11  | 1.44        | 1.34     |
| 1   | D     | 942  | PRO  | C-O   | -7.98 | 1.14        | 1.23     |
| 1   | D     | 987  | ALA  | CA-CB | -7.94 | 1.41        | 1.53     |
| 1   | A     | 12   | VAL  | C-O   | -7.91 | 1.15        | 1.23     |
| 1   | D     | 1034 | ASN  | CA-C  | 7.85  | 1.62        | 1.52     |
| 1   | A     | 96   | VAL  | C-O   | -7.78 | 1.14        | 1.23     |
| 1   | A     | 120  | HIS  | N-CA  | 7.72  | 1.55        | 1.46     |
| 1   | D     | 854  | ALA  | C-O   | -7.63 | 1.14        | 1.24     |
| 1   | A     | 10   | LYS  | CA-C  | -7.55 | 1.43        | 1.52     |
| 1   | A     | 173  | ARG  | CD-NE | 7.53  | 1.56        | 1.46     |
| 1   | B     | 313  | VAL  | CA-C  | 7.44  | 1.61        | 1.52     |
| 1   | A     | 96   | VAL  | CA-CB | 7.44  | 1.63        | 1.55     |
| 1   | A     | 169  | PHE  | C-O   | -7.37 | 1.15        | 1.24     |
| 1   | A     | 142  | VAL  | CA-CB | 7.36  | 1.62        | 1.53     |
| 1   | A     | 196  | GLU  | N-CA  | -7.31 | 1.37        | 1.46     |
| 1   | A     | 143  | VAL  | CA-CB | -7.30 | 1.45        | 1.54     |
| 1   | C     | 694  | PHE  | C-O   | -7.17 | 1.15        | 1.24     |
| 1   | D     | 964  | GLU  | C-O   | 7.13  | 1.32        | 1.24     |
| 1   | B     | 464  | ALA  | C-O   | -7.12 | 1.15        | 1.24     |
| 1   | A     | 221  | ILE  | CA-CB | 7.02  | 1.62        | 1.54     |
| 1   | B     | 378  | MET  | C-O   | -7.00 | 1.15        | 1.24     |
| 1   | A     | 195  | THR  | CA-CB | 6.89  | 1.64        | 1.53     |
| 1   | D     | 975  | THR  | C-O   | 6.81  | 1.31        | 1.24     |
| 1   | C     | 736  | ALA  | CA-CB | -6.80 | 1.41        | 1.53     |
| 1   | A     | 130  | MET  | N-CA  | 6.75  | 1.52        | 1.46     |
| 1   | C     | 682  | ALA  | CA-CB | 6.74  | 1.62        | 1.53     |
| 1   | A     | 130  | MET  | CA-C  | 6.73  | 1.60        | 1.52     |
| 1   | C     | 763  | ARG  | NE-CZ | 6.71  | 1.40        | 1.33     |
| 1   | A     | 155  | ILE  | CA-CB | -6.69 | 1.45        | 1.54     |
| 1   | B     | 368  | HIS  | CB-CG | 6.68  | 1.59        | 1.50     |
| 1   | A     | 37   | VAL  | CA-CB | 6.67  | 1.62        | 1.54     |
| 1   | C     | 713  | LEU  | CA-C  | -6.66 | 1.44        | 1.52     |
| 1   | B     | 399  | SER  | C-O   | -6.62 | 1.15        | 1.24     |
| 1   | D     | 841  | ARG  | NE-CZ | 6.60  | 1.40        | 1.33     |
| 1   | D     | 921  | MET  | C-O   | 6.58  | 1.31        | 1.24     |
| 1   | D     | 919  | MET  | SD-CE | 6.56  | 1.96        | 1.79     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | D     | 888  | ASN  | CA-C   | 6.53  | 1.60        | 1.52     |
| 1   | C     | 763  | ARG  | CA-C   | 6.53  | 1.61        | 1.52     |
| 1   | A     | 146  | VAL  | CA-CB  | -6.46 | 1.47        | 1.54     |
| 1   | A     | 42   | SER  | CA-CB  | 6.40  | 1.61        | 1.53     |
| 1   | C     | 713  | LEU  | C-O    | -6.32 | 1.16        | 1.24     |
| 1   | B     | 460  | THR  | CA-CB  | 6.32  | 1.63        | 1.53     |
| 1   | C     | 552  | ALA  | CA-CB  | -6.31 | 1.43        | 1.53     |
| 1   | C     | 754  | GLN  | CD-OE1 | 6.31  | 1.35        | 1.23     |
| 1   | B     | 396  | LEU  | C-O    | 6.30  | 1.32        | 1.24     |
| 1   | B     | 513  | ILE  | CA-CB  | 6.30  | 1.62        | 1.54     |
| 1   | D     | 1028 | VAL  | CA-C   | 6.27  | 1.59        | 1.52     |
| 1   | D     | 894  | HIS  | CA-CB  | 6.24  | 1.61        | 1.53     |
| 1   | A     | 115  | MET  | C-O    | -6.22 | 1.16        | 1.24     |
| 1   | C     | 654  | ALA  | CA-CB  | -6.21 | 1.43        | 1.53     |
| 1   | B     | 414  | THR  | C-O    | 6.19  | 1.31        | 1.23     |
| 1   | A     | 194  | ASP  | CA-C   | 6.17  | 1.61        | 1.52     |
| 1   | B     | 513  | ILE  | C-O    | 6.17  | 1.31        | 1.24     |
| 1   | D     | 795  | MET  | N-CA   | 6.15  | 1.54        | 1.46     |
| 1   | D     | 929  | ILE  | CA-C   | -6.14 | 1.45        | 1.52     |
| 1   | D     | 939  | ILE  | CA-CB  | 6.12  | 1.62        | 1.54     |
| 1   | A     | 239  | VAL  | CA-CB  | 6.10  | 1.62        | 1.54     |
| 1   | B     | 345  | GLY  | C-N    | 6.09  | 1.41        | 1.33     |
| 1   | B     | 277  | VAL  | C-O    | -6.09 | 1.17        | 1.24     |
| 1   | D     | 874  | MET  | SD-CE  | -6.09 | 1.64        | 1.79     |
| 1   | C     | 545  | LYS  | CA-C   | 6.04  | 1.59        | 1.53     |
| 1   | A     | 212  | PRO  | CA-C   | 6.01  | 1.59        | 1.52     |
| 1   | A     | 262  | ASP  | CA-C   | -6.01 | 1.44        | 1.52     |
| 1   | A     | 132  | MET  | SD-CE  | -6.00 | 1.64        | 1.79     |
| 1   | D     | 801  | VAL  | C-O    | -5.97 | 1.17        | 1.24     |
| 1   | B     | 361  | TYR  | CA-CB  | 5.97  | 1.62        | 1.53     |
| 1   | C     | 689  | PHE  | C-O    | -5.97 | 1.17        | 1.24     |
| 1   | A     | 225  | ALA  | C-O    | -5.94 | 1.17        | 1.24     |
| 1   | C     | 661  | GLN  | CD-NE2 | 5.94  | 1.45        | 1.33     |
| 1   | C     | 542  | GLY  | CA-C   | 5.93  | 1.57        | 1.51     |
| 1   | D     | 855  | GLY  | C-O    | -5.93 | 1.17        | 1.24     |
| 1   | B     | 411  | GLY  | C-O    | -5.92 | 1.17        | 1.23     |
| 1   | D     | 990  | ALA  | CA-CB  | -5.91 | 1.43        | 1.53     |
| 1   | B     | 393  | MET  | SD-CE  | -5.91 | 1.64        | 1.79     |
| 1   | A     | 226  | LEU  | CA-C   | 5.91  | 1.62        | 1.52     |
| 1   | D     | 820  | LYS  | C-N    | -5.88 | 1.25        | 1.33     |
| 1   | B     | 284  | ILE  | CA-CB  | -5.87 | 1.46        | 1.54     |
| 1   | C     | 625  | ASN  | CA-C   | 5.86  | 1.59        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | D     | 952  | PHE  | CA-C    | 5.86  | 1.60        | 1.52     |
| 1   | B     | 470  | LEU  | C-O     | -5.86 | 1.16        | 1.24     |
| 1   | A     | 163  | PHE  | CA-C    | 5.83  | 1.60        | 1.52     |
| 1   | D     | 1003 | GLU  | C-O     | -5.83 | 1.17        | 1.24     |
| 1   | D     | 970  | VAL  | CA-C    | 5.82  | 1.59        | 1.52     |
| 1   | C     | 746  | ILE  | N-CA    | 5.80  | 1.53        | 1.46     |
| 1   | B     | 468  | ILE  | C-O     | -5.79 | 1.17        | 1.24     |
| 1   | D     | 929  | ILE  | CA-CB   | -5.79 | 1.47        | 1.54     |
| 1   | D     | 897  | ILE  | CG1-CD1 | 5.79  | 1.74        | 1.51     |
| 1   | A     | 63   | TYR  | CA-C    | -5.74 | 1.45        | 1.52     |
| 1   | A     | 124  | VAL  | CA-CB   | -5.72 | 1.47        | 1.54     |
| 1   | A     | 35   | HIS  | C-O     | 5.71  | 1.30        | 1.23     |
| 1   | D     | 934  | SER  | CA-C    | -5.71 | 1.45        | 1.52     |
| 1   | A     | 111  | VAL  | C-O     | -5.68 | 1.17        | 1.24     |
| 1   | B     | 449  | THR  | C-O     | 5.67  | 1.30        | 1.24     |
| 1   | D     | 1039 | ILE  | C-N     | 5.67  | 1.41        | 1.33     |
| 1   | A     | 40   | ALA  | C-O     | -5.66 | 1.16        | 1.24     |
| 1   | D     | 934  | SER  | C-O     | -5.65 | 1.17        | 1.23     |
| 1   | C     | 746  | ILE  | C-O     | -5.64 | 1.17        | 1.24     |
| 1   | D     | 1036 | GLY  | C-O     | 5.64  | 1.31        | 1.23     |
| 1   | D     | 978  | ILE  | C-O     | 5.64  | 1.30        | 1.24     |
| 1   | C     | 726  | LYS  | CA-C    | 5.64  | 1.59        | 1.52     |
| 1   | A     | 130  | MET  | C-O     | 5.63  | 1.30        | 1.24     |
| 1   | B     | 414  | THR  | N-CA    | -5.63 | 1.39        | 1.45     |
| 1   | C     | 624  | TYR  | CA-CB   | 5.63  | 1.61        | 1.53     |
| 1   | A     | 14   | VAL  | C-O     | -5.63 | 1.18        | 1.24     |
| 1   | B     | 295  | MET  | CG-SD   | 5.59  | 1.94        | 1.80     |
| 1   | B     | 373  | ASN  | CA-CB   | 5.57  | 1.62        | 1.53     |
| 1   | B     | 436  | ARG  | CA-C    | -5.55 | 1.45        | 1.52     |
| 1   | A     | 232  | TYR  | CA-C    | -5.55 | 1.46        | 1.52     |
| 1   | B     | 334  | MET  | C-O     | -5.54 | 1.16        | 1.24     |
| 1   | C     | 649  | VAL  | CA-CB   | 5.53  | 1.60        | 1.54     |
| 1   | D     | 993  | GLY  | C-O     | 5.53  | 1.32        | 1.24     |
| 1   | A     | 205  | ILE  | C-O     | -5.52 | 1.17        | 1.24     |
| 1   | C     | 672  | VAL  | N-CA    | -5.50 | 1.40        | 1.46     |
| 1   | D     | 937  | GLY  | CA-C    | 5.50  | 1.59        | 1.51     |
| 1   | D     | 838  | VAL  | CA-C    | 5.49  | 1.59        | 1.52     |
| 1   | A     | 115  | MET  | SD-CE   | 5.45  | 1.93        | 1.79     |
| 1   | D     | 886  | LEU  | CA-C    | -5.45 | 1.46        | 1.52     |
| 1   | C     | 763  | ARG  | CA-CB   | 5.44  | 1.62        | 1.53     |
| 1   | A     | 125  | LEU  | CA-C    | -5.43 | 1.45        | 1.52     |
| 1   | C     | 656  | MET  | N-CA    | 5.43  | 1.52        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | D     | 830  | ARG  | CZ-NH2 | -5.43 | 1.26        | 1.33     |
| 1   | C     | 732  | TYR  | C-N    | 5.41  | 1.41        | 1.33     |
| 1   | D     | 1022 | TYR  | CA-C   | -5.40 | 1.47        | 1.53     |
| 1   | D     | 983  | ASP  | C-O    | -5.40 | 1.17        | 1.24     |
| 1   | D     | 990  | ALA  | CA-C   | 5.39  | 1.60        | 1.52     |
| 1   | B     | 303  | ALA  | C-O    | -5.37 | 1.19        | 1.24     |
| 1   | D     | 813  | GLU  | C-O    | -5.36 | 1.17        | 1.24     |
| 1   | C     | 670  | SER  | C-O    | 5.35  | 1.29        | 1.24     |
| 1   | C     | 605  | ALA  | C-O    | -5.34 | 1.18        | 1.24     |
| 1   | B     | 368  | HIS  | CG-ND1 | 5.33  | 1.44        | 1.38     |
| 1   | A     | 128  | ALA  | C-O    | -5.33 | 1.17        | 1.24     |
| 1   | A     | 199  | ILE  | CA-CB  | 5.32  | 1.60        | 1.54     |
| 1   | D     | 874  | MET  | CG-SD  | 5.31  | 1.94        | 1.80     |
| 1   | B     | 348  | MET  | SD-CE  | 5.31  | 1.92        | 1.79     |
| 1   | D     | 897  | ILE  | CA-CB  | 5.31  | 1.61        | 1.54     |
| 1   | B     | 294  | LYS  | CB-CG  | 5.30  | 1.68        | 1.52     |
| 1   | B     | 413  | ILE  | CA-C   | 5.28  | 1.59        | 1.52     |
| 1   | A     | 246  | PRO  | C-O    | -5.28 | 1.17        | 1.24     |
| 1   | A     | 145  | SER  | C-O    | -5.27 | 1.17        | 1.23     |
| 1   | B     | 303  | ALA  | CA-CB  | 5.27  | 1.60        | 1.53     |
| 1   | B     | 444  | VAL  | CA-CB  | 5.26  | 1.60        | 1.54     |
| 1   | C     | 585  | ALA  | CA-CB  | -5.26 | 1.44        | 1.53     |
| 1   | D     | 828  | THR  | CA-C   | -5.24 | 1.46        | 1.52     |
| 1   | D     | 932  | VAL  | C-O    | 5.22  | 1.30        | 1.24     |
| 1   | D     | 808  | LYS  | CA-C   | -5.21 | 1.46        | 1.52     |
| 1   | D     | 974  | ILE  | C-O    | 5.20  | 1.30        | 1.24     |
| 1   | A     | 36   | VAL  | C-O    | -5.20 | 1.18        | 1.24     |
| 1   | C     | 739  | LYS  | C-O    | 5.18  | 1.30        | 1.24     |
| 1   | A     | 66   | GLY  | C-O    | -5.16 | 1.18        | 1.23     |
| 1   | C     | 585  | ALA  | C-O    | 5.16  | 1.30        | 1.24     |
| 1   | D     | 1042 | PHE  | N-CA   | -5.15 | 1.40        | 1.46     |
| 1   | A     | 245  | ASN  | C-O    | 5.15  | 1.30        | 1.24     |
| 1   | B     | 391  | ALA  | CA-CB  | -5.14 | 1.45        | 1.53     |
| 1   | A     | 195  | THR  | C-O    | -5.13 | 1.17        | 1.23     |
| 1   | B     | 440  | LEU  | C-O    | 5.13  | 1.30        | 1.24     |
| 1   | B     | 490  | ARG  | CA-C   | -5.12 | 1.46        | 1.53     |
| 1   | C     | 699  | ARG  | CA-C   | 5.11  | 1.59        | 1.52     |
| 1   | B     | 480  | ALA  | CA-CB  | 5.10  | 1.61        | 1.53     |
| 1   | D     | 939  | ILE  | CA-C   | -5.10 | 1.48        | 1.52     |
| 1   | A     | 90   | MET  | SD-CE  | 5.09  | 1.92        | 1.79     |
| 1   | D     | 854  | ALA  | CA-CB  | -5.05 | 1.46        | 1.53     |
| 1   | B     | 268  | GLU  | CA-C   | 5.03  | 1.59        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | B     | 290 | TYR  | N-CA  | 5.02  | 1.52        | 1.46     |
| 1   | A     | 123 | VAL  | CA-C  | 5.02  | 1.59        | 1.52     |
| 1   | B     | 324 | ALA  | CA-CB | 5.02  | 1.62        | 1.53     |
| 1   | C     | 663 | GLN  | CG-CD | -5.01 | 1.39        | 1.52     |

All (138) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1   | D     | 839  | VAL  | N-CA-C    | -13.33 | 97.89       | 110.42   |
| 1   | D     | 1021 | TYR  | CA-C-O    | -12.10 | 107.24      | 120.43   |
| 1   | A     | 173  | ARG  | NE-CZ-NH2 | 10.51  | 128.66      | 119.20   |
| 1   | A     | 56   | LEU  | N-CA-C    | 10.09  | 125.13      | 113.02   |
| 1   | B     | 373  | ASN  | N-CA-C    | -9.72  | 100.24      | 111.03   |
| 1   | D     | 921  | MET  | CA-C-N    | 9.50   | 133.95      | 120.28   |
| 1   | D     | 921  | MET  | C-N-CA    | 9.50   | 133.95      | 120.28   |
| 1   | C     | 733  | LEU  | O-C-N     | -9.46  | 110.79      | 122.24   |
| 1   | A     | 69   | GLU  | N-CA-C    | -8.29  | 103.16      | 113.20   |
| 1   | D     | 831  | SER  | N-CA-C    | 8.28   | 121.50      | 108.67   |
| 1   | C     | 562  | VAL  | N-CA-C    | 8.15   | 119.85      | 108.12   |
| 1   | A     | 109  | ASP  | N-CA-C    | -8.13  | 102.39      | 111.82   |
| 1   | B     | 289  | ALA  | N-CA-C    | -7.59  | 102.70      | 110.97   |
| 1   | B     | 345  | GLY  | CA-C-N    | 7.57   | 131.31      | 120.79   |
| 1   | B     | 345  | GLY  | C-N-CA    | 7.57   | 131.31      | 120.79   |
| 1   | A     | 173  | ARG  | NE-CZ-NH1 | -7.54  | 113.96      | 121.50   |
| 1   | A     | 199  | ILE  | N-CA-C    | -7.52  | 103.46      | 110.53   |
| 1   | D     | 1021 | TYR  | CB-CA-C   | -7.45  | 97.45       | 109.75   |
| 1   | C     | 636  | ASN  | CB-CA-C   | 7.36   | 122.69      | 109.29   |
| 1   | C     | 788  | ASP  | N-CA-C    | 7.35   | 119.99      | 111.02   |
| 1   | C     | 625  | ASN  | N-CA-CB   | -7.29  | 98.33       | 110.95   |
| 1   | A     | 191  | GLY  | N-CA-C    | -7.24  | 100.80      | 112.31   |
| 1   | D     | 995  | TYR  | CB-CA-C   | -7.08  | 97.46       | 109.72   |
| 1   | B     | 444  | VAL  | CB-CA-C   | 7.01   | 120.26      | 111.15   |
| 1   | B     | 345  | GLY  | CA-C-O    | -6.96  | 113.28      | 120.66   |
| 1   | B     | 333  | ASP  | N-CA-C    | 6.94   | 119.58      | 108.41   |
| 1   | A     | 146  | VAL  | N-CA-CB   | -6.88  | 102.87      | 110.51   |
| 1   | C     | 642  | GLU  | N-CA-C    | 6.86   | 118.45      | 110.97   |
| 1   | A     | 263  | ASN  | CA-C-O    | 6.79   | 132.34      | 120.80   |
| 1   | D     | 970  | VAL  | N-CA-C    | 6.78   | 117.79      | 108.84   |
| 1   | B     | 361  | TYR  | N-CA-CB   | 6.72   | 120.20      | 110.06   |
| 1   | B     | 284  | ILE  | N-CA-C    | -6.72  | 103.68      | 111.00   |
| 1   | B     | 313  | VAL  | N-CA-C    | 6.66   | 116.68      | 110.42   |
| 1   | D     | 1001 | PRO  | N-CA-C    | 6.64   | 121.37      | 110.55   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | C     | 740 | GLU  | N-CA-CB   | 6.57  | 119.88      | 110.16   |
| 1   | B     | 431 | PHE  | CB-CA-C   | 6.49  | 121.01      | 110.95   |
| 1   | B     | 515 | GLU  | CA-C-N    | 6.46  | 129.18      | 120.65   |
| 1   | B     | 515 | GLU  | C-N-CA    | 6.46  | 129.18      | 120.65   |
| 1   | C     | 699 | ARG  | NE-CZ-NH2 | 6.43  | 124.99      | 119.20   |
| 1   | A     | 245 | ASN  | CA-C-N    | 6.42  | 126.35      | 119.28   |
| 1   | A     | 245 | ASN  | C-N-CA    | 6.42  | 126.35      | 119.28   |
| 1   | D     | 979 | LEU  | CA-C-N    | -6.40 | 115.51      | 122.55   |
| 1   | D     | 979 | LEU  | C-N-CA    | -6.40 | 115.51      | 122.55   |
| 1   | A     | 35  | HIS  | N-CA-C    | -6.38 | 99.29       | 109.76   |
| 1   | D     | 879 | MET  | N-CA-C    | 6.37  | 118.77      | 108.32   |
| 1   | D     | 942 | PRO  | CA-C-O    | -6.27 | 114.11      | 121.95   |
| 1   | D     | 905 | GLU  | CB-CA-C   | -6.27 | 100.26      | 110.79   |
| 1   | A     | 262 | ASP  | CB-CA-C   | -6.23 | 100.40      | 110.74   |
| 1   | D     | 912 | VAL  | N-CA-C    | -6.19 | 104.71      | 110.53   |
| 1   | A     | 103 | PHE  | N-CA-CB   | 6.19  | 119.18      | 109.83   |
| 1   | D     | 863 | ALA  | N-CA-C    | 6.17  | 117.70      | 110.97   |
| 1   | C     | 733 | LEU  | CA-C-N    | 6.12  | 131.47      | 121.87   |
| 1   | C     | 733 | LEU  | C-N-CA    | 6.12  | 131.47      | 121.87   |
| 1   | A     | 110 | ASN  | N-CA-C    | 6.12  | 117.75      | 111.14   |
| 1   | B     | 316 | CYS  | N-CA-C    | -6.09 | 104.76      | 111.82   |
| 1   | A     | 105 | HIS  | N-CA-C    | 6.09  | 119.96      | 111.56   |
| 1   | D     | 915 | SER  | N-CA-C    | -6.08 | 104.73      | 111.36   |
| 1   | B     | 298 | HIS  | N-CA-C    | -6.06 | 99.41       | 109.46   |
| 1   | A     | 89  | ASP  | N-CA-C    | 6.04  | 120.85      | 112.45   |
| 1   | D     | 990 | ALA  | N-CA-C    | 6.04  | 118.65      | 111.71   |
| 1   | A     | 31  | LYS  | N-CA-CB   | 6.01  | 120.53      | 110.32   |
| 1   | A     | 192 | LEU  | CB-CA-C   | -6.00 | 99.03       | 109.64   |
| 1   | D     | 910 | SER  | CA-C-N    | 5.97  | 128.56      | 120.38   |
| 1   | D     | 910 | SER  | C-N-CA    | 5.97  | 128.56      | 120.38   |
| 1   | C     | 722 | GLU  | N-CA-C    | 5.96  | 117.65      | 111.03   |
| 1   | C     | 701 | GLU  | N-CA-C    | -5.94 | 104.49      | 110.97   |
| 1   | B     | 516 | PHE  | N-CA-C    | 5.92  | 117.43      | 110.97   |
| 1   | B     | 495 | TYR  | N-CA-C    | 5.92  | 118.37      | 108.96   |
| 1   | D     | 904 | MET  | CA-C-O    | -5.90 | 114.30      | 120.55   |
| 1   | D     | 793 | PRO  | N-CD-CG   | -5.87 | 94.40       | 103.20   |
| 1   | A     | 218 | LEU  | CA-C-N    | 5.85  | 128.40      | 120.38   |
| 1   | A     | 218 | LEU  | C-N-CA    | 5.85  | 128.40      | 120.38   |
| 1   | D     | 956 | GLY  | N-CA-C    | -5.84 | 99.35       | 113.18   |
| 1   | D     | 962 | ARG  | NE-CZ-NH2 | -5.83 | 113.95      | 119.20   |
| 1   | A     | 30  | ALA  | CA-C-O    | -5.82 | 114.25      | 120.42   |
| 1   | B     | 499 | SER  | N-CA-C    | 5.82  | 117.62      | 108.96   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | B     | 362  | ASN  | CB-CA-C  | -5.81 | 100.40      | 110.45   |
| 1   | C     | 672  | VAL  | CB-CA-C  | 5.76  | 119.26      | 111.88   |
| 1   | A     | 28   | HIS  | CB-CA-C  | -5.74 | 100.93      | 110.68   |
| 1   | C     | 527  | LYS  | CB-CA-C  | 5.73  | 120.98      | 110.10   |
| 1   | A     | 96   | VAL  | CA-C-N   | 5.72  | 129.49      | 121.02   |
| 1   | A     | 96   | VAL  | C-N-CA   | 5.72  | 129.49      | 121.02   |
| 1   | B     | 420  | PRO  | CA-C-O   | 5.72  | 128.24      | 119.55   |
| 1   | C     | 645  | PHE  | CB-CA-C  | 5.68  | 121.00      | 112.31   |
| 1   | D     | 897  | ILE  | CB-CA-C  | -5.66 | 104.40      | 112.22   |
| 1   | D     | 997  | GLY  | CA-C-O   | -5.65 | 115.68      | 121.62   |
| 1   | D     | 814  | ILE  | CB-CA-C  | -5.61 | 104.87      | 111.94   |
| 1   | A     | 135  | GLN  | CB-CA-C  | 5.60  | 120.98      | 110.63   |
| 1   | B     | 458  | THR  | N-CA-C   | -5.58 | 102.64      | 110.50   |
| 1   | C     | 734  | GLY  | N-CA-C   | 5.58  | 123.72      | 112.34   |
| 1   | D     | 821  | MET  | CB-CA-C  | 5.58  | 121.05      | 109.95   |
| 1   | A     | 135  | GLN  | O-C-N    | -5.58 | 115.70      | 122.22   |
| 1   | A     | 191  | GLY  | CA-C-O   | -5.58 | 116.45      | 122.47   |
| 1   | B     | 512  | LYS  | CA-C-N   | 5.57  | 128.09      | 120.46   |
| 1   | B     | 512  | LYS  | C-N-CA   | 5.57  | 128.09      | 120.46   |
| 1   | A     | 245  | ASN  | CB-CA-C  | 5.54  | 121.09      | 110.17   |
| 1   | B     | 373  | ASN  | CB-CA-C  | -5.52 | 102.39      | 110.95   |
| 1   | C     | 625  | ASN  | O-C-N    | -5.49 | 116.11      | 123.14   |
| 1   | D     | 1016 | ARG  | CG-CD-NE | 5.47  | 124.04      | 112.00   |
| 1   | C     | 668  | VAL  | N-CA-C   | 5.42  | 115.38      | 107.37   |
| 1   | A     | 163  | PHE  | N-CA-C   | 5.41  | 117.60      | 111.11   |
| 1   | D     | 888  | ASN  | O-C-N    | -5.40 | 117.09      | 123.41   |
| 1   | D     | 965  | PHE  | CB-CA-C  | 5.40  | 121.03      | 110.67   |
| 1   | B     | 309  | LEU  | N-CA-C   | 5.39  | 117.24      | 111.36   |
| 1   | B     | 462  | ILE  | CB-CA-C  | -5.36 | 104.82      | 112.22   |
| 1   | D     | 1017 | GLN  | N-CA-C   | 5.36  | 117.78      | 110.55   |
| 1   | B     | 285  | GLY  | N-CA-C   | 5.34  | 119.61      | 112.77   |
| 1   | D     | 817  | HIS  | N-CA-C   | -5.32 | 105.49      | 111.28   |
| 1   | B     | 365  | THR  | N-CA-C   | 5.31  | 116.59      | 108.52   |
| 1   | D     | 985  | GLU  | CB-CA-C  | 5.31  | 120.99      | 110.42   |
| 1   | C     | 553  | TYR  | N-CA-C   | -5.31 | 105.57      | 111.36   |
| 1   | D     | 821  | MET  | CA-C-O   | 5.30  | 125.90      | 119.11   |
| 1   | D     | 1022 | TYR  | N-CA-C   | -5.29 | 97.24       | 107.44   |
| 1   | A     | 3    | ARG  | CB-CA-C  | 5.28  | 117.18      | 110.16   |
| 1   | A     | 12   | VAL  | N-CA-C   | 5.26  | 115.48      | 108.27   |
| 1   | D     | 831  | SER  | CB-CA-C  | -5.25 | 102.00      | 110.77   |
| 1   | A     | 37   | VAL  | CB-CA-C  | 5.24  | 118.39      | 110.63   |
| 1   | D     | 828  | THR  | O-C-N    | 5.23  | 129.50      | 123.17   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 20  | GLY  | N-CA-C    | 5.23  | 125.57      | 113.18   |
| 1   | C     | 671 | SER  | N-CA-C    | 5.20  | 116.19      | 108.86   |
| 1   | A     | 56  | LEU  | CB-CA-C   | -5.20 | 101.12      | 110.37   |
| 1   | A     | 3   | ARG  | CA-C-N    | 5.16  | 126.29      | 119.84   |
| 1   | A     | 3   | ARG  | C-N-CA    | 5.16  | 126.29      | 119.84   |
| 1   | C     | 703 | LEU  | CB-CG-CD2 | 5.15  | 126.14      | 110.70   |
| 1   | D     | 905 | GLU  | CA-CB-CG  | 5.14  | 124.37      | 114.10   |
| 1   | C     | 726 | LYS  | N-CA-C    | 5.13  | 116.56      | 110.97   |
| 1   | D     | 869 | GLU  | N-CA-C    | 5.13  | 117.77      | 111.82   |
| 1   | A     | 212 | PRO  | N-CA-C    | 5.12  | 118.53      | 110.80   |
| 1   | D     | 992 | SER  | N-CA-C    | -5.10 | 102.36      | 109.96   |
| 1   | B     | 463 | LYS  | N-CA-C    | -5.10 | 105.64      | 111.14   |
| 1   | B     | 475 | PRO  | N-CA-C    | 5.10  | 119.09      | 111.14   |
| 1   | B     | 265 | PHE  | N-CA-C    | 5.06  | 117.23      | 110.35   |
| 1   | B     | 336 | PHE  | N-CA-C    | 5.05  | 116.79      | 111.28   |
| 1   | A     | 10  | LYS  | N-CA-C    | -5.05 | 102.04      | 110.17   |
| 1   | D     | 808 | LYS  | CA-C-O    | -5.03 | 115.56      | 121.10   |
| 1   | C     | 685 | SER  | N-CA-C    | 5.02  | 116.75      | 111.28   |
| 1   | B     | 396 | LEU  | CA-C-N    | -5.00 | 112.71      | 120.31   |
| 1   | B     | 396 | LEU  | C-N-CA    | -5.00 | 112.71      | 120.31   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | B     | 507 | GLY  | Peptide |
| 1   | D     | 927 | GLY  | Peptide |

## 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     | 2017  | 0        | 2053     | 87      | 0            |
| 1   | B     | 2017  | 0        | 2050     | 70      | 0            |
| 1   | C     | 2017  | 0        | 2050     | 92      | 0            |
| 1   | D     | 2017  | 0        | 2050     | 101     | 0            |
| 2   | A     | 48    | 0        | 25       | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | B     | 48    | 0        | 25       | 2       | 0            |
| 2   | C     | 48    | 0        | 25       | 2       | 0            |
| 2   | D     | 48    | 0        | 25       | 2       | 0            |
| 3   | A     | 26    | 0        | 22       | 15      | 0            |
| 3   | D     | 26    | 0        | 22       | 15      | 0            |
| 4   | A     | 46    | 0        | 0        | 2       | 0            |
| 4   | B     | 28    | 0        | 0        | 3       | 0            |
| 4   | C     | 48    | 0        | 0        | 2       | 0            |
| 4   | D     | 46    | 0        | 0        | 5       | 0            |
| All | All   | 8480  | 0        | 8347     | 346     | 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 21.

All (346) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:134:MET:SD   | 1:A:134:MET:CE   | 2.07                     | 1.41              |
| 1:D:985:GLU:HB3  | 4:D:2239:HOH:O   | 1.11                     | 1.23              |
| 1:C:527:LYS:C    | 1:C:527:LYS:HD3  | 1.83                     | 1.02              |
| 1:B:526:ASN:N    | 1:B:526:ASN:HD22 | 1.60                     | 1.00              |
| 1:D:892:PHE:HB2  | 1:D:894:HIS:HE1  | 1.28                     | 0.98              |
| 1:B:360:LEU:H    | 1:B:381:ASN:HD21 | 1.13                     | 0.96              |
| 1:D:857:MET:HG3  | 1:D:884:HIS:CD2  | 2.02                     | 0.94              |
| 1:D:888:ASN:HD21 | 1:D:899:ASN:HD21 | 0.96                     | 0.94              |
| 1:C:631:HIS:CE1  | 1:C:633:GLU:OE2  | 2.22                     | 0.93              |
| 1:B:363:ARG:NH1  | 4:B:2283:HOH:O   | 2.05                     | 0.90              |
| 1:D:888:ASN:ND2  | 1:D:899:ASN:HD21 | 1.68                     | 0.90              |
| 1:C:594:MET:HG3  | 1:C:621:HIS:CD2  | 2.11                     | 0.86              |
| 1:C:561:HIS:CE1  | 1:C:585:ALA:HB1  | 2.09                     | 0.86              |
| 1:D:792:ARG:O    | 1:D:795:MET:HG3  | 1.75                     | 0.85              |
| 1:A:3:ARG:O      | 1:A:6:MET:HG3    | 1.77                     | 0.84              |
| 1:B:526:ASN:HD22 | 1:B:526:ASN:H    | 1.21                     | 0.84              |
| 1:C:594:MET:HG3  | 1:C:621:HIS:HD2  | 1.43                     | 0.83              |
| 1:C:774:ARG:HG3  | 1:D:939:ILE:HG22 | 1.62                     | 0.80              |
| 1:C:561:HIS:ND1  | 1:C:585:ALA:HB3  | 1.97                     | 0.79              |
| 1:D:888:ASN:HD21 | 1:D:899:ASN:ND2  | 1.78                     | 0.79              |
| 1:A:206:TYR:CD1  | 3:A:2004:3G4:CL7 | 2.73                     | 0.78              |
| 1:C:631:HIS:HE1  | 1:C:633:GLU:OE2  | 1.66                     | 0.78              |
| 1:A:95:HIS:ND1   | 1:A:122:PHE:HE1  | 1.81                     | 0.78              |
| 1:A:206:TYR:CE1  | 3:A:2004:3G4:CL7 | 2.74                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:570:GLU:H    | 1:C:570:GLU:CD   | 1.94                     | 0.75              |
| 1:A:124:VAL:HG22 | 1:B:371:ILE:HD13 | 1.66                     | 0.75              |
| 1:A:95:HIS:CE1   | 1:A:122:PHE:CE1  | 2.74                     | 0.75              |
| 1:C:786:ASN:C    | 1:C:786:ASN:HD22 | 1.94                     | 0.75              |
| 1:C:527:LYS:C    | 1:C:527:LYS:CD   | 2.57                     | 0.75              |
| 1:A:68:MET:HG3   | 1:A:95:HIS:CD2   | 2.22                     | 0.75              |
| 1:C:561:HIS:ND1  | 1:C:585:ALA:CB   | 2.50                     | 0.75              |
| 1:A:95:HIS:CE1   | 1:A:122:PHE:HE1  | 2.05                     | 0.74              |
| 1:B:526:ASN:N    | 1:B:526:ASN:ND2  | 2.33                     | 0.74              |
| 1:D:892:PHE:HB2  | 1:D:894:HIS:CE1  | 2.20                     | 0.74              |
| 1:A:95:HIS:HD1   | 1:A:122:PHE:HE1  | 1.36                     | 0.73              |
| 1:A:11:LYS:HE3   | 1:A:85:MET:O     | 1.89                     | 0.72              |
| 1:D:995:TYR:CD2  | 3:D:2007:3G4:CL7 | 2.79                     | 0.72              |
| 1:A:28:HIS:HE1   | 1:A:214:GLU:O    | 1.74                     | 0.71              |
| 1:D:824:HIS:ND1  | 1:D:849:SER:HB2  | 2.05                     | 0.71              |
| 1:A:146:VAL:HG11 | 1:A:152:TYR:OH   | 1.90                     | 0.70              |
| 1:A:160:ALA:HB2  | 1:B:431:PHE:HB2  | 1.72                     | 0.70              |
| 1:D:947:TYR:CZ   | 3:D:2007:3G4:H19 | 2.25                     | 0.70              |
| 1:B:304:ARG:HB2  | 2:B:2003:NAP:O1X | 1.91                     | 0.70              |
| 1:C:623:LEU:H    | 1:C:644:ASN:HD21 | 1.40                     | 0.70              |
| 1:B:523:ASN:OD1  | 1:B:526:ASN:ND2  | 2.25                     | 0.69              |
| 1:C:638:ARG:HA   | 1:D:909:HIS:HE1  | 1.56                     | 0.69              |
| 1:A:197:THR:HG21 | 2:A:2002:NAP:O1A | 1.94                     | 0.68              |
| 1:D:860:MET:SD   | 1:D:913:VAL:HG21 | 2.34                     | 0.68              |
| 1:C:554:HIS:CE1  | 1:C:744:LEU:HB2  | 2.29                     | 0.68              |
| 1:C:646:HIS:HE1  | 1:D:901:ARG:HA   | 1.59                     | 0.68              |
| 1:D:1049:ASN:ND2 | 1:D:1052:ASN:OD1 | 2.26                     | 0.68              |
| 1:D:1044:SER:HA  | 1:D:1047:GLU:HG2 | 1.77                     | 0.67              |
| 1:D:817:HIS:CE1  | 1:D:1007:LEU:HB2 | 2.30                     | 0.67              |
| 1:C:671:SER:HB2  | 1:C:673:ALA:H    | 1.59                     | 0.67              |
| 1:B:313:VAL:O    | 1:B:314:ALA:C    | 2.38                     | 0.66              |
| 1:B:526:ASN:H    | 1:B:526:ASN:ND2  | 1.89                     | 0.66              |
| 1:B:412:LYS:HG2  | 1:B:452:ILE:HD12 | 1.78                     | 0.66              |
| 1:A:35:HIS:CD2   | 1:A:59:ALA:HB3   | 2.31                     | 0.66              |
| 1:D:857:MET:HG3  | 1:D:884:HIS:NE2  | 2.12                     | 0.65              |
| 1:B:410:ALA:HB2  | 1:B:415:TYR:CD1  | 2.32                     | 0.65              |
| 1:C:732:TYR:CE2  | 1:D:1047:GLU:HB3 | 2.31                     | 0.65              |
| 1:A:206:TYR:CG   | 3:A:2004:3G4:CL7 | 2.87                     | 0.65              |
| 1:D:944:ILE:HD13 | 3:D:2007:3G4:H3  | 1.78                     | 0.64              |
| 1:C:561:HIS:CE1  | 1:C:585:ALA:CB   | 2.79                     | 0.64              |
| 1:C:561:HIS:HE1  | 1:C:585:ALA:HB1  | 1.62                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:239:VAL:N     | 1:A:240:PRO:CD    | 2.61                     | 0.64              |
| 1:B:300:VAL:HG23  | 1:B:348:MET:SD    | 2.37                     | 0.64              |
| 1:A:194:ASP:HA    | 1:A:199:ILE:HD11  | 1.78                     | 0.63              |
| 1:C:625:ASN:HD21  | 1:C:636:ASN:ND2   | 1.96                     | 0.63              |
| 1:A:7:LEU:HD11    | 1:A:90:MET:HE1    | 1.81                     | 0.63              |
| 1:C:645:PHE:CE1   | 1:D:904:MET:HE3   | 2.34                     | 0.62              |
| 1:C:636:ASN:C     | 1:C:636:ASN:HD22  | 2.07                     | 0.62              |
| 1:D:886:LEU:H     | 1:D:907:ASN:HD21  | 1.47                     | 0.62              |
| 1:D:947:TYR:CE2   | 3:D:2007:3G4:H19  | 2.35                     | 0.62              |
| 1:B:523:ASN:CG    | 1:B:526:ASN:HD21  | 2.08                     | 0.62              |
| 1:A:206:TYR:CZ    | 3:A:2004:3G4:CL7  | 2.90                     | 0.62              |
| 1:D:1005:CYS:O    | 1:D:1009:ILE:HG13 | 2.00                     | 0.61              |
| 1:D:851:HIS:CD2   | 1:D:873:LEU:HD22  | 2.35                     | 0.61              |
| 1:D:857:MET:HG3   | 1:D:884:HIS:HD2   | 1.62                     | 0.61              |
| 1:D:884:HIS:CE1   | 1:D:911:PHE:CE1   | 2.88                     | 0.61              |
| 1:D:1020:MET:HE1  | 1:D:1022:TYR:HB2  | 1.82                     | 0.61              |
| 1:C:625:ASN:HD21  | 1:C:636:ASN:HD21  | 1.49                     | 0.61              |
| 1:D:1044:SER:HA   | 1:D:1047:GLU:CG   | 2.31                     | 0.61              |
| 1:B:523:ASN:CG    | 1:B:526:ASN:ND2   | 2.60                     | 0.60              |
| 1:C:562:VAL:O     | 1:C:562:VAL:HG23  | 2.01                     | 0.60              |
| 1:C:570:GLU:N     | 1:C:570:GLU:OE1   | 2.35                     | 0.60              |
| 1:D:960:THR:O     | 1:D:961:LEU:C     | 2.43                     | 0.60              |
| 1:A:103:PHE:HB2   | 1:A:105:HIS:HE1   | 1.67                     | 0.60              |
| 3:A:2004:3G4:H26B | 3:A:2004:3G4:C15  | 2.31                     | 0.60              |
| 1:B:278:THR:O     | 1:B:357:ASN:HB3   | 2.02                     | 0.60              |
| 1:D:995:TYR:C     | 1:D:996:LEU:HD23  | 2.26                     | 0.60              |
| 1:C:699:ARG:O     | 1:C:703:LEU:HG    | 2.02                     | 0.59              |
| 1:A:231:MET:HE3   | 1:A:231:MET:O     | 2.01                     | 0.59              |
| 3:D:2007:3G4:H19  | 3:D:2007:3G4:H26A | 1.84                     | 0.59              |
| 1:A:146:VAL:HG12  | 1:A:152:TYR:HE1   | 1.67                     | 0.59              |
| 3:A:2004:3G4:H8B  | 3:A:2004:3G4:O11  | 2.01                     | 0.59              |
| 3:A:2004:3G4:H18  | 3:A:2004:3G4:C5   | 2.33                     | 0.59              |
| 1:D:1021:TYR:CG   | 1:D:1029:PRO:HB3  | 2.37                     | 0.59              |
| 1:C:699:ARG:NH2   | 4:C:2393:HOH:O    | 2.36                     | 0.58              |
| 1:C:625:ASN:O     | 1:C:626:ARG:C     | 2.46                     | 0.58              |
| 1:B:270:LEU:HD23  | 1:B:292:LEU:HD22  | 1.86                     | 0.58              |
| 1:B:497:VAL:HG21  | 1:B:502:VAL:HG12  | 1.86                     | 0.58              |
| 1:D:884:HIS:ND1   | 1:D:911:PHE:HE1   | 2.01                     | 0.58              |
| 1:A:152:TYR:HB3   | 1:B:522:TYR:OH    | 2.02                     | 0.58              |
| 1:B:360:LEU:N     | 1:B:381:ASN:HD21  | 1.95                     | 0.57              |
| 1:C:656:MET:HE1   | 1:C:666:ILE:HD11  | 1.86                     | 0.57              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:2007:3G4:H23A | 3:D:2007:3G4:C15 | 2.33                     | 0.57              |
| 1:D:884:HIS:HD1   | 1:D:911:PHE:HE1  | 1.52                     | 0.57              |
| 1:D:935:VAL:HG23  | 1:D:979:LEU:O    | 2.03                     | 0.57              |
| 1:B:293:ALA:HB2   | 1:B:316:CYS:HB3  | 1.85                     | 0.57              |
| 1:B:380:VAL:O     | 1:B:384:SER:OG   | 2.23                     | 0.57              |
| 1:B:412:LYS:NZ    | 1:B:429:ASP:OD2  | 2.33                     | 0.57              |
| 1:D:852:TYR:CD1   | 1:D:852:TYR:C    | 2.81                     | 0.57              |
| 1:B:265:PHE:CD1   | 1:B:269:MET:CE   | 2.88                     | 0.57              |
| 3:D:2007:3G4:H8B  | 3:D:2007:3G4:O11 | 2.04                     | 0.57              |
| 1:A:156:ALA:HB3   | 1:A:157:PRO:HD3  | 1.86                     | 0.56              |
| 1:C:627:LEU:N     | 1:C:627:LEU:HD23 | 2.18                     | 0.56              |
| 1:D:884:HIS:CE1   | 1:D:911:PHE:HE1  | 2.23                     | 0.56              |
| 1:C:774:ARG:HG3   | 1:D:939:ILE:CG2  | 2.32                     | 0.56              |
| 1:C:616:MET:SD    | 1:C:618:ILE:HD11 | 2.46                     | 0.56              |
| 1:A:44:GLU:CD     | 1:A:44:GLU:H     | 2.15                     | 0.55              |
| 1:D:945:ALA:N     | 1:D:946:PRO:CD   | 2.68                     | 0.55              |
| 1:A:118:ASN:N     | 1:A:118:ASN:ND2  | 2.54                     | 0.55              |
| 1:C:757:MET:HE1   | 1:C:759:TYR:HB2  | 1.87                     | 0.55              |
| 1:D:892:PHE:CB    | 1:D:894:HIS:HE1  | 2.12                     | 0.55              |
| 1:D:936:ALA:HA    | 1:D:939:ILE:O    | 2.07                     | 0.55              |
| 1:A:195:THR:HA    | 1:A:213:LYS:HE2  | 1.88                     | 0.55              |
| 1:A:206:TYR:CD2   | 3:A:2004:3G4:CL7 | 2.97                     | 0.55              |
| 1:A:118:ASN:N     | 1:A:118:ASN:HD22 | 2.05                     | 0.54              |
| 1:C:551:ILE:HG13  | 1:C:743:ALA:HB1  | 1.87                     | 0.54              |
| 1:D:1005:CYS:HB2  | 1:D:1022:TYR:CE2 | 2.42                     | 0.54              |
| 3:D:2007:3G4:H23A | 3:D:2007:3G4:C16 | 2.37                     | 0.54              |
| 1:A:166:ASP:O     | 1:A:170:SER:HB2  | 2.07                     | 0.54              |
| 1:B:266:ARG:H     | 1:B:269:MET:HE2  | 1.71                     | 0.54              |
| 1:C:532:MET:O     | 1:C:536:LYS:HE3  | 2.07                     | 0.54              |
| 1:D:947:TYR:CZ    | 3:D:2007:3G4:C19 | 2.90                     | 0.54              |
| 1:B:436:ARG:NH1   | 1:B:448:ILE:O    | 2.41                     | 0.54              |
| 3:A:2004:3G4:O11  | 3:A:2004:3G4:C8  | 2.56                     | 0.54              |
| 1:B:329:GLY:HA3   | 1:B:336:PHE:CZ   | 2.42                     | 0.54              |
| 1:A:95:HIS:ND1    | 1:A:122:PHE:CE1  | 2.68                     | 0.54              |
| 1:A:39:THR:O      | 1:A:40:ALA:HB2   | 2.09                     | 0.53              |
| 1:B:429:ASP:O     | 1:B:433:SER:HB2  | 2.07                     | 0.53              |
| 1:A:62:HIS:ND1    | 1:A:84:LEU:HD22  | 2.24                     | 0.53              |
| 1:D:1021:TYR:CD1  | 1:D:1029:PRO:HB3 | 2.44                     | 0.53              |
| 1:D:855:GLY:HA3   | 1:D:862:PHE:CE1  | 2.44                     | 0.53              |
| 1:A:90:MET:HA     | 1:A:139:SER:O    | 2.08                     | 0.52              |
| 1:C:554:HIS:HE1   | 1:C:740:GLU:O    | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:948:SER:O    | 1:D:949:ALA:C    | 2.49                     | 0.52              |
| 1:D:995:TYR:CG   | 3:D:2007:3G4:CL7 | 2.99                     | 0.52              |
| 1:A:260:ASN:HB2  | 1:B:470:LEU:HD11 | 1.92                     | 0.52              |
| 1:B:265:PHE:CD1  | 1:B:269:MET:HE1  | 2.45                     | 0.52              |
| 1:A:35:HIS:CD2   | 1:A:59:ALA:CB    | 2.93                     | 0.52              |
| 1:D:944:ILE:HG13 | 1:D:944:ILE:O    | 2.09                     | 0.52              |
| 1:A:2:PHE:CD2    | 1:A:222:LYS:HE2  | 2.45                     | 0.52              |
| 1:C:527:LYS:HD3  | 1:C:528:PHE:N    | 2.23                     | 0.52              |
| 4:C:2072:HOH:O   | 1:D:897:ILE:HD11 | 2.10                     | 0.51              |
| 1:B:359:VAL:CG1  | 2:B:2003:NAP:H3D | 2.41                     | 0.51              |
| 1:C:594:MET:CG   | 1:C:621:HIS:CD2  | 2.90                     | 0.51              |
| 1:A:206:TYR:CE2  | 3:A:2004:3G4:CL7 | 3.01                     | 0.51              |
| 1:D:985:GLU:CB   | 4:D:2239:HOH:O   | 1.98                     | 0.51              |
| 1:B:502:VAL:N    | 1:B:503:PRO:HD2  | 2.26                     | 0.51              |
| 1:D:985:GLU:HA   | 4:D:2239:HOH:O   | 2.10                     | 0.51              |
| 1:A:146:VAL:HG12 | 1:A:147:ALA:N    | 2.24                     | 0.51              |
| 1:B:333:ASP:OD1  | 1:B:333:ASP:C    | 2.52                     | 0.51              |
| 1:C:634:ILE:HD12 | 1:D:916:VAL:HG21 | 1.93                     | 0.51              |
| 1:D:880:LEU:HD11 | 1:D:882:LEU:HD21 | 1.92                     | 0.51              |
| 1:D:985:GLU:CA   | 4:D:2239:HOH:O   | 2.49                     | 0.51              |
| 1:B:382:PHE:O    | 1:B:383:HIS:C    | 2.54                     | 0.51              |
| 1:B:321:ALA:C    | 1:B:323:SER:N    | 2.69                     | 0.50              |
| 1:C:634:ILE:CD1  | 1:D:916:VAL:HG21 | 2.42                     | 0.50              |
| 1:C:636:ASN:ND2  | 1:C:636:ASN:C    | 2.70                     | 0.50              |
| 3:A:2004:3G4:C5  | 3:A:2004:3G4:C18 | 2.89                     | 0.50              |
| 1:B:291:HIS:HE1  | 1:B:477:GLU:O    | 1.94                     | 0.50              |
| 1:D:888:ASN:ND2  | 1:D:899:ASN:ND2  | 2.49                     | 0.50              |
| 1:C:786:ASN:HD21 | 1:C:788:ASP:HB2  | 1.76                     | 0.50              |
| 1:B:485:LYS:HD2  | 4:B:2278:HOH:O   | 2.12                     | 0.50              |
| 1:A:68:MET:HG3   | 1:A:95:HIS:NE2   | 2.27                     | 0.49              |
| 1:B:308:ALA:HA   | 1:B:311:LYS:HE2  | 1.94                     | 0.49              |
| 1:C:621:HIS:HD1  | 1:C:648:PHE:HE1  | 1.58                     | 0.49              |
| 1:C:671:SER:HB2  | 1:C:673:ALA:N    | 2.27                     | 0.49              |
| 1:A:100:ARG:HD3  | 4:A:2308:HOH:O   | 2.11                     | 0.49              |
| 1:A:263:ASN:ND2  | 4:A:2235:HOH:O   | 2.42                     | 0.49              |
| 1:B:386:VAL:HG13 | 1:B:431:PHE:CZ   | 2.47                     | 0.49              |
| 1:A:11:LYS:HD3   | 1:A:85:MET:O     | 2.13                     | 0.49              |
| 1:A:35:HIS:ND1   | 1:A:60:SER:OG    | 2.46                     | 0.49              |
| 1:C:543:ALA:HB3  | 1:C:564:VAL:HB   | 1.94                     | 0.49              |
| 1:C:676:ILE:HG22 | 1:D:1037:ARG:HG3 | 1.94                     | 0.49              |
| 1:A:166:ASP:O    | 1:A:170:SER:CB   | 2.60                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:502:VAL:N    | 1:B:503:PRO:CD   | 2.76                     | 0.49              |
| 3:D:2007:3G4:O11 | 3:D:2007:3G4:C8  | 2.60                     | 0.48              |
| 1:C:617:LEU:HD21 | 1:C:619:LEU:HD21 | 1.95                     | 0.48              |
| 1:C:786:ASN:HB2  | 1:D:996:LEU:HD11 | 1.94                     | 0.48              |
| 1:A:194:ASP:OD1  | 1:A:213:LYS:HG2  | 2.14                     | 0.48              |
| 1:B:380:VAL:HG12 | 1:B:381:ASN:HD22 | 1.77                     | 0.48              |
| 1:A:44:GLU:HA    | 1:A:47:GLN:NE2   | 2.29                     | 0.48              |
| 1:A:199:ILE:O    | 1:A:200:LYS:C    | 2.55                     | 0.48              |
| 1:C:621:HIS:CE1  | 1:C:648:PHE:CE1  | 3.02                     | 0.48              |
| 1:A:7:LEU:HD11   | 1:A:90:MET:CE    | 2.44                     | 0.48              |
| 1:B:360:LEU:H    | 1:B:381:ASN:ND2  | 1.96                     | 0.48              |
| 1:C:682:ALA:N    | 1:C:683:PRO:HD2  | 2.28                     | 0.48              |
| 1:B:277:VAL:HG12 | 1:B:280:ALA:HB2  | 1.96                     | 0.48              |
| 1:A:21:ILE:HD11  | 1:A:193:ILE:HG21 | 1.95                     | 0.48              |
| 1:A:97:LEU:H     | 1:A:118:ASN:ND2  | 2.11                     | 0.48              |
| 1:D:1052:ASN:N   | 1:D:1052:ASN:ND2 | 2.61                     | 0.48              |
| 1:B:410:ALA:HB2  | 1:B:415:TYR:HD1  | 1.76                     | 0.47              |
| 1:A:172:LEU:O    | 1:A:173:ARG:C    | 2.53                     | 0.47              |
| 1:B:301:VAL:HG23 | 1:B:309:LEU:HD22 | 1.96                     | 0.47              |
| 1:C:786:ASN:C    | 1:C:786:ASN:ND2  | 2.66                     | 0.47              |
| 1:A:5:GLU:CD     | 1:A:5:GLU:H      | 2.21                     | 0.47              |
| 1:B:280:ALA:HB3  | 1:B:301:VAL:HB   | 1.96                     | 0.47              |
| 1:D:996:LEU:HD23 | 1:D:996:LEU:N    | 2.30                     | 0.47              |
| 1:B:321:ALA:C    | 1:B:323:SER:H    | 2.22                     | 0.47              |
| 1:A:146:VAL:HG22 | 1:A:243:LEU:HD11 | 1.97                     | 0.47              |
| 1:C:713:LEU:HD13 | 1:C:715:ILE:HD11 | 1.97                     | 0.47              |
| 1:D:829:ALA:O    | 1:D:855:GLY:N    | 2.44                     | 0.47              |
| 1:D:886:LEU:N    | 1:D:907:ASN:HD21 | 2.09                     | 0.47              |
| 1:C:770:GLY:O    | 1:C:771:ASN:C    | 2.57                     | 0.47              |
| 1:A:154:LEU:C    | 1:A:155:ILE:HG23 | 2.40                     | 0.46              |
| 1:B:270:LEU:HD23 | 1:B:292:LEU:CD2  | 2.45                     | 0.46              |
| 1:C:527:LYS:HD3  | 1:C:527:LYS:O    | 2.12                     | 0.46              |
| 1:C:627:LEU:N    | 1:C:627:LEU:CD2  | 2.78                     | 0.46              |
| 1:D:807:SER:OG   | 2:D:2001:NAP:O3B | 2.29                     | 0.46              |
| 1:D:976:LEU:HD13 | 1:D:978:ILE:HD11 | 1.97                     | 0.46              |
| 1:A:6:MET:O      | 1:A:7:LEU:HD22   | 2.15                     | 0.46              |
| 1:C:621:HIS:ND1  | 1:C:648:PHE:HE1  | 2.13                     | 0.46              |
| 1:D:1021:TYR:OH  | 1:D:1033:GLY:CA  | 2.63                     | 0.46              |
| 1:C:527:LYS:CD   | 1:C:527:LYS:O    | 2.64                     | 0.46              |
| 1:C:682:ALA:N    | 1:C:683:PRO:CD   | 2.79                     | 0.46              |
| 1:A:37:VAL:HG23  | 1:A:85:MET:SD    | 2.56                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:538:VAL:HG22 | 1:C:616:MET:HB3   | 1.96                     | 0.46              |
| 1:A:97:LEU:H     | 1:A:118:ASN:HD21  | 1.63                     | 0.46              |
| 1:C:699:ARG:NH1  | 1:C:711:ILE:HG22  | 2.30                     | 0.46              |
| 1:C:731:ILE:N    | 1:C:731:ILE:HD12  | 2.31                     | 0.46              |
| 1:D:792:ARG:HD2  | 1:D:793:PRO:HD2   | 1.97                     | 0.46              |
| 1:B:497:VAL:HG23 | 1:B:497:VAL:O     | 2.15                     | 0.45              |
| 2:A:2002:NAP:H2D | 3:A:2004:3G4:H19A | 1.97                     | 0.45              |
| 1:B:315:ARG:O    | 1:B:319:LEU:HG    | 2.16                     | 0.45              |
| 1:D:908:PHE:O    | 1:D:911:PHE:HB2   | 2.15                     | 0.45              |
| 1:A:17:ALA:HB3   | 1:A:38:VAL:HB     | 1.97                     | 0.45              |
| 1:B:455:LEU:O    | 1:B:456:ILE:HD13  | 2.15                     | 0.45              |
| 1:A:7:LEU:HA     | 1:A:10:LYS:HG3    | 1.97                     | 0.45              |
| 1:B:293:ALA:O    | 1:B:294:LYS:C     | 2.59                     | 0.45              |
| 1:B:497:VAL:HG21 | 1:B:502:VAL:CG1   | 2.46                     | 0.45              |
| 1:A:197:THR:CG2  | 2:A:2002:NAP:O1A  | 2.63                     | 0.45              |
| 1:A:239:VAL:N    | 1:A:240:PRO:HD2   | 2.32                     | 0.45              |
| 1:D:944:ILE:CD1  | 3:D:2007:3G4:H3   | 2.44                     | 0.45              |
| 1:A:41:ARG:HB2   | 2:A:2002:NAP:O1X  | 2.17                     | 0.45              |
| 1:C:568:SER:HB2  | 1:C:571:ALA:HB3   | 2.00                     | 0.45              |
| 1:D:1028:VAL:O   | 1:D:1029:PRO:C    | 2.60                     | 0.45              |
| 1:C:732:TYR:CE2  | 1:D:1047:GLU:CB   | 2.99                     | 0.44              |
| 1:B:269:MET:C    | 1:B:270:LEU:HD12  | 2.42                     | 0.44              |
| 1:C:658:MET:HE3  | 1:C:658:MET:HB2   | 1.83                     | 0.44              |
| 1:D:884:HIS:HE1  | 1:D:911:PHE:CD1   | 2.35                     | 0.44              |
| 1:C:562:VAL:O    | 1:C:562:VAL:CG2   | 2.64                     | 0.44              |
| 1:C:705:ASN:HB3  | 1:C:707:VAL:HG23  | 1.98                     | 0.44              |
| 1:B:404:ALA:HB2  | 1:B:487:THR:HG21  | 1.98                     | 0.44              |
| 1:B:410:ALA:HA   | 1:B:413:ILE:O     | 2.17                     | 0.44              |
| 1:C:765:VAL:HG13 | 1:D:1040:MET:HE2  | 1.99                     | 0.44              |
| 1:D:790:LYS:HE3  | 1:D:792:ARG:HH22  | 1.82                     | 0.44              |
| 1:B:352:ASP:O    | 1:B:401:GLY:HA3   | 2.18                     | 0.44              |
| 1:C:702:PHE:O    | 1:C:703:LEU:C     | 2.60                     | 0.44              |
| 1:C:688:LYS:O    | 1:C:691:LEU:HB2   | 2.18                     | 0.44              |
| 1:C:678:TYR:HB3  | 1:D:1048:TYR:OH   | 2.18                     | 0.44              |
| 1:C:528:PHE:HB2  | 1:C:752:LEU:HD11  | 2.00                     | 0.44              |
| 1:D:927:GLY:O    | 1:D:972:VAL:HA    | 2.18                     | 0.43              |
| 1:D:933:SER:OG   | 1:D:934:SER:N     | 2.51                     | 0.43              |
| 1:D:892:PHE:CB   | 1:D:894:HIS:CE1   | 2.96                     | 0.43              |
| 1:D:935:VAL:HB   | 3:D:2007:3G4:O12  | 2.18                     | 0.43              |
| 1:A:145:SER:HB3  | 3:A:2004:3G4:HN10 | 1.84                     | 0.43              |
| 1:C:631:HIS:ND1  | 1:C:633:GLU:OE2   | 2.49                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:637:VAL:HA    | 1:C:683:PRO:HB3   | 2.00                     | 0.43              |
| 1:D:1020:MET:SD   | 1:D:1020:MET:C    | 3.02                     | 0.43              |
| 1:D:799:LYS:O     | 1:D:823:ALA:HB1   | 2.19                     | 0.43              |
| 1:D:851:HIS:HD2   | 1:D:873:LEU:HD22  | 1.81                     | 0.43              |
| 1:A:6:MET:C       | 1:A:7:LEU:HD22    | 2.43                     | 0.43              |
| 1:A:11:LYS:CE     | 1:A:85:MET:O      | 2.63                     | 0.43              |
| 1:A:251:MET:HB3   | 1:B:413:ILE:HD13  | 1.99                     | 0.43              |
| 1:D:853:ILE:HD13  | 1:D:853:ILE:HG21  | 1.75                     | 0.43              |
| 1:C:764:TRP:C     | 1:C:766:PRO:HD2   | 2.43                     | 0.43              |
| 1:D:832:LYS:H     | 1:D:832:LYS:CD    | 2.32                     | 0.43              |
| 1:A:189:ILE:HB    | 1:A:232:TYR:CD1   | 2.54                     | 0.43              |
| 3:A:2004:3G4:H25A | 3:A:2004:3G4:H26A | 2.00                     | 0.43              |
| 2:D:2001:NAP:H2A  | 4:D:2017:HOH:O    | 2.19                     | 0.43              |
| 1:D:947:TYR:OH    | 3:D:2007:3G4:N14  | 2.45                     | 0.43              |
| 1:D:1038:LYS:HB3  | 1:D:1038:LYS:HE2  | 1.86                     | 0.42              |
| 1:A:68:MET:C      | 1:A:70:ASP:H      | 2.25                     | 0.42              |
| 1:C:764:TRP:O     | 1:C:765:VAL:C     | 2.62                     | 0.42              |
| 1:D:817:HIS:HB3   | 1:D:821:MET:HE3   | 2.01                     | 0.42              |
| 1:D:859:ASP:OD1   | 1:D:859:ASP:C     | 2.62                     | 0.42              |
| 1:A:145:SER:O     | 1:A:146:VAL:C     | 2.63                     | 0.42              |
| 1:C:563:VAL:HG11  | 1:C:607:ALA:HB2   | 2.01                     | 0.42              |
| 1:A:62:HIS:N      | 1:A:62:HIS:CD2    | 2.87                     | 0.42              |
| 1:B:455:LEU:C     | 1:B:456:ILE:HD13  | 2.44                     | 0.42              |
| 1:C:671:SER:HB3   | 2:C:2000:NAP:H5N  | 2.00                     | 0.42              |
| 1:D:817:HIS:NE2   | 1:D:1003:GLU:HG2  | 2.34                     | 0.42              |
| 3:D:2007:3G4:H25A | 3:D:2007:3G4:H23  | 1.76                     | 0.42              |
| 1:A:237:ARG:O     | 1:A:237:ARG:HG3   | 2.19                     | 0.42              |
| 1:B:376:LYS:O     | 1:B:377:SER:C     | 2.61                     | 0.42              |
| 1:D:832:LYS:HB2   | 1:D:832:LYS:HE2   | 1.94                     | 0.42              |
| 1:B:370:GLU:H     | 1:B:370:GLU:CD    | 2.28                     | 0.42              |
| 1:C:670:SER:O     | 2:C:2000:NAP:H6N  | 2.20                     | 0.42              |
| 1:B:445:ASN:H     | 1:B:445:ASN:HD22  | 1.67                     | 0.42              |
| 1:C:550:GLU:HG3   | 1:C:739:LYS:HG3   | 2.01                     | 0.42              |
| 1:C:571:ALA:O     | 1:C:575:VAL:HG23  | 2.19                     | 0.42              |
| 1:D:790:LYS:CE    | 1:D:792:ARG:HH22  | 2.33                     | 0.42              |
| 1:B:298:HIS:CE1   | 1:B:322:ALA:HB1   | 2.55                     | 0.41              |
| 1:D:814:ILE:O     | 1:D:818:LEU:HG    | 2.20                     | 0.41              |
| 1:A:3:ARG:O       | 1:A:6:MET:CG      | 2.60                     | 0.41              |
| 1:A:173:ARG:HH11  | 1:A:173:ARG:HD3   | 1.50                     | 0.41              |
| 1:A:253:PHE:O     | 1:A:254:LEU:C     | 2.63                     | 0.41              |
| 1:C:528:PHE:CD1   | 1:C:748:LYS:HE2   | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:826:VAL:HA   | 1:D:851:HIS:O    | 2.20                     | 0.41              |
| 1:B:288:ILE:HG13 | 1:B:480:ALA:HB1  | 2.02                     | 0.41              |
| 1:A:82:GLY:HA3   | 1:A:132:MET:HE1  | 2.02                     | 0.41              |
| 1:B:415:TYR:HB2  | 1:B:418:ILE:HD11 | 2.03                     | 0.41              |
| 1:C:589:TYR:CD1  | 1:C:589:TYR:C    | 2.98                     | 0.41              |
| 1:B:482:GLU:CD   | 4:B:2278:HOH:O   | 2.63                     | 0.41              |
| 1:D:871:GLY:O    | 1:D:875:GLY:N    | 2.53                     | 0.41              |
| 1:B:287:GLU:HG3  | 1:B:476:LYS:HB2  | 2.03                     | 0.41              |
| 1:C:638:ARG:O    | 1:C:642:GLU:HG2  | 2.21                     | 0.41              |
| 1:D:821:MET:HE1  | 1:D:1007:LEU:CD1 | 2.51                     | 0.41              |
| 1:A:44:GLU:HA    | 1:A:47:GLN:HE21  | 1.85                     | 0.41              |
| 3:A:2004:3G4:H23 | 3:A:2004:3G4:H19 | 1.91                     | 0.41              |
| 1:C:529:ARG:HH11 | 1:C:529:ARG:HG3  | 1.86                     | 0.41              |
| 1:C:625:ASN:ND2  | 1:C:636:ASN:ND2  | 2.64                     | 0.41              |
| 1:C:641:MET:SD   | 1:C:645:PHE:CD1  | 3.14                     | 0.41              |
| 1:D:885:VAL:HG21 | 1:D:947:TYR:HE2  | 1.86                     | 0.41              |
| 1:D:944:ILE:O    | 1:D:944:ILE:CG1  | 2.66                     | 0.41              |
| 1:D:871:GLY:O    | 1:D:872:ASN:C    | 2.64                     | 0.41              |
| 1:A:94:ASN:O     | 2:A:2002:NAP:H4D | 2.21                     | 0.40              |
| 1:A:154:LEU:O    | 1:A:155:ILE:HG23 | 2.21                     | 0.40              |
| 1:A:178:VAL:HG11 | 1:A:261:TRP:CZ3  | 2.56                     | 0.40              |
| 1:C:670:SER:HB3  | 1:C:715:ILE:HD13 | 2.03                     | 0.40              |
| 1:C:785:TYR:OH   | 1:D:941:TYR:HB3  | 2.21                     | 0.40              |
| 1:D:882:LEU:O    | 1:D:932:VAL:HG23 | 2.21                     | 0.40              |
| 1:A:99:ASN:HD22  | 1:A:99:ASN:HA    | 1.66                     | 0.40              |
| 1:A:234:VAL:HG21 | 1:A:239:VAL:HG12 | 2.03                     | 0.40              |
| 1:A:11:LYS:C     | 1:A:12:VAL:CG2   | 2.93                     | 0.40              |
| 1:A:70:ASP:OD1   | 1:A:70:ASP:C     | 2.64                     | 0.40              |
| 1:A:231:MET:HE3  | 1:A:231:MET:C    | 2.46                     | 0.40              |
| 1:B:317:LEU:HA   | 1:B:317:LEU:HD23 | 1.81                     | 0.40              |
| 1:C:623:LEU:H    | 1:C:644:ASN:ND2  | 2.12                     | 0.40              |
| 1:D:1004:GLU:HB3 | 1:D:1022:TYR:OH  | 2.21                     | 0.40              |
| 1:B:268:GLU:C    | 1:B:270:LEU:H    | 2.30                     | 0.40              |
| 1:C:533:LEU:O    | 1:C:536:LYS:HB2  | 2.21                     | 0.40              |
| 1:C:565:THR:O    | 1:C:566:ALA:HB2  | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|-----------|----------|----------|-------------|----|
| 1   | A     | 261/277 (94%)   | 233 (89%) | 23 (9%)  | 5 (2%)   | 6           | 11 |
| 1   | B     | 261/277 (94%)   | 228 (87%) | 29 (11%) | 4 (2%)   | 8           | 16 |
| 1   | C     | 261/277 (94%)   | 238 (91%) | 20 (8%)  | 3 (1%)   | 11          | 22 |
| 1   | D     | 261/277 (94%)   | 244 (94%) | 13 (5%)  | 4 (2%)   | 8           | 16 |
| All | All   | 1044/1108 (94%) | 943 (90%) | 85 (8%)  | 16 (2%)  | 8           | 16 |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 154  | LEU  |
| 1   | B     | 322  | ALA  |
| 1   | A     | 20   | GLY  |
| 1   | C     | 742  | CYS  |
| 1   | B     | 319  | LEU  |
| 1   | C     | 680  | LEU  |
| 1   | B     | 323  | SER  |
| 1   | D     | 983  | ASP  |
| 1   | D     | 985  | GLU  |
| 1   | A     | 147  | ALA  |
| 1   | C     | 633  | GLU  |
| 1   | A     | 40   | ALA  |
| 1   | D     | 829  | ALA  |
| 1   | D     | 1047 | GLU  |
| 1   | A     | 155  | ILE  |
| 1   | B     | 508  | ASN  |

### 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     | 214/226 (95%) | 188 (88%) | 26 (12%)  | 5           | 10 |
| 1   | B     | 214/226 (95%) | 188 (88%) | 26 (12%)  | 5           | 10 |
| 1   | C     | 214/226 (95%) | 182 (85%) | 32 (15%)  | 3           | 6  |
| 1   | D     | 214/226 (95%) | 185 (86%) | 29 (14%)  | 3           | 8  |
| All | All   | 856/904 (95%) | 743 (87%) | 113 (13%) | 4           | 8  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | ARG  |
| 1   | A     | 6   | MET  |
| 1   | A     | 11  | LYS  |
| 1   | A     | 56  | LEU  |
| 1   | A     | 60  | SER  |
| 1   | A     | 75  | GLU  |
| 1   | A     | 80  | GLU  |
| 1   | A     | 83  | ASN  |
| 1   | A     | 95  | HIS  |
| 1   | A     | 99  | ASN  |
| 1   | A     | 101 | LEU  |
| 1   | A     | 105 | HIS  |
| 1   | A     | 112 | ARG  |
| 1   | A     | 113 | LYS  |
| 1   | A     | 118 | ASN  |
| 1   | A     | 136 | SER  |
| 1   | A     | 145 | SER  |
| 1   | A     | 146 | VAL  |
| 1   | A     | 177 | LEU  |
| 1   | A     | 192 | LEU  |
| 1   | A     | 197 | THR  |
| 1   | A     | 211 | SER  |
| 1   | A     | 213 | LYS  |
| 1   | A     | 218 | LEU  |
| 1   | A     | 237 | ARG  |
| 1   | A     | 249 | LYS  |
| 1   | B     | 264 | LYS  |
| 1   | B     | 266 | ARG  |
| 1   | B     | 274 | LYS  |
| 1   | B     | 278 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 282 | LYS  |
| 1   | B     | 302 | THR  |
| 1   | B     | 304 | ARG  |
| 1   | B     | 305 | SER  |
| 1   | B     | 306 | LYS  |
| 1   | B     | 307 | GLU  |
| 1   | B     | 310 | GLN  |
| 1   | B     | 315 | ARG  |
| 1   | B     | 338 | GLU  |
| 1   | B     | 370 | GLU  |
| 1   | B     | 376 | LYS  |
| 1   | B     | 398 | GLN  |
| 1   | B     | 399 | SER  |
| 1   | B     | 408 | SER  |
| 1   | B     | 443 | LYS  |
| 1   | B     | 445 | ASN  |
| 1   | B     | 450 | LEU  |
| 1   | B     | 453 | LEU  |
| 1   | B     | 476 | LYS  |
| 1   | B     | 478 | GLU  |
| 1   | B     | 499 | SER  |
| 1   | B     | 526 | ASN  |
| 1   | C     | 527 | LYS  |
| 1   | C     | 529 | ARG  |
| 1   | C     | 557 | LYS  |
| 1   | C     | 568 | SER  |
| 1   | C     | 569 | LYS  |
| 1   | C     | 570 | GLU  |
| 1   | C     | 621 | HIS  |
| 1   | C     | 622 | VAL  |
| 1   | C     | 623 | LEU  |
| 1   | C     | 626 | ARG  |
| 1   | C     | 627 | LEU  |
| 1   | C     | 631 | HIS  |
| 1   | C     | 634 | ILE  |
| 1   | C     | 636 | ASN  |
| 1   | C     | 656 | MET  |
| 1   | C     | 660 | MET  |
| 1   | C     | 661 | GLN  |
| 1   | C     | 671 | SER  |
| 1   | C     | 697 | THR  |
| 1   | C     | 704 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 705  | ASN  |
| 1   | C     | 706  | LYS  |
| 1   | C     | 712  | THR  |
| 1   | C     | 718  | LEU  |
| 1   | C     | 725  | ILE  |
| 1   | C     | 740  | GLU  |
| 1   | C     | 744  | LEU  |
| 1   | C     | 748  | LYS  |
| 1   | C     | 757  | MET  |
| 1   | C     | 763  | ARG  |
| 1   | C     | 775  | LYS  |
| 1   | C     | 786  | ASN  |
| 1   | D     | 790  | LYS  |
| 1   | D     | 792  | ARG  |
| 1   | D     | 794  | GLU  |
| 1   | D     | 795  | MET  |
| 1   | D     | 796  | LEU  |
| 1   | D     | 800  | LYS  |
| 1   | D     | 801  | VAL  |
| 1   | D     | 804  | THR  |
| 1   | D     | 807  | SER  |
| 1   | D     | 832  | LYS  |
| 1   | D     | 849  | SER  |
| 1   | D     | 884  | HIS  |
| 1   | D     | 894  | HIS  |
| 1   | D     | 923  | MET  |
| 1   | D     | 944  | ILE  |
| 1   | D     | 963  | SER  |
| 1   | D     | 966  | LEU  |
| 1   | D     | 969  | LYS  |
| 1   | D     | 971  | ASN  |
| 1   | D     | 976  | LEU  |
| 1   | D     | 983  | ASP  |
| 1   | D     | 985  | GLU  |
| 1   | D     | 986  | THR  |
| 1   | D     | 996  | LEU  |
| 1   | D     | 1003 | GLU  |
| 1   | D     | 1004 | GLU  |
| 1   | D     | 1038 | LYS  |
| 1   | D     | 1047 | GLU  |
| 1   | D     | 1052 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39)

such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 8    | GLN  |
| 1   | A     | 28   | HIS  |
| 1   | A     | 47   | GLN  |
| 1   | A     | 62   | HIS  |
| 1   | A     | 83   | ASN  |
| 1   | A     | 99   | ASN  |
| 1   | A     | 118  | ASN  |
| 1   | A     | 182  | ASN  |
| 1   | A     | 245  | ASN  |
| 1   | A     | 260  | ASN  |
| 1   | B     | 291  | HIS  |
| 1   | B     | 310  | GLN  |
| 1   | B     | 357  | ASN  |
| 1   | B     | 362  | ASN  |
| 1   | B     | 373  | ASN  |
| 1   | B     | 381  | ASN  |
| 1   | B     | 445  | ASN  |
| 1   | B     | 523  | ASN  |
| 1   | B     | 526  | ASN  |
| 1   | C     | 534  | GLN  |
| 1   | C     | 554  | HIS  |
| 1   | C     | 588  | HIS  |
| 1   | C     | 609  | ASN  |
| 1   | C     | 625  | ASN  |
| 1   | C     | 631  | HIS  |
| 1   | C     | 636  | ASN  |
| 1   | C     | 644  | ASN  |
| 1   | C     | 646  | HIS  |
| 1   | C     | 705  | ASN  |
| 1   | C     | 754  | GLN  |
| 1   | C     | 786  | ASN  |
| 1   | D     | 836  | GLN  |
| 1   | D     | 883  | ASN  |
| 1   | D     | 888  | ASN  |
| 1   | D     | 894  | HIS  |
| 1   | D     | 907  | ASN  |
| 1   | D     | 909  | HIS  |
| 1   | D     | 1049 | ASN  |
| 1   | D     | 1052 | 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 ⓘ

6 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 2   | NAP  | B     | 2003 | -    | 50,52,52     | 2.07 | 12 (24%)    | 71,80,80    | 2.51 | 25 (35%)    |
| 2   | NAP  | D     | 2001 | -    | 50,52,52     | 1.52 | 7 (14%)     | 71,80,80    | 2.04 | 23 (32%)    |
| 3   | 3G4  | D     | 2007 | -    | 27,27,27     | 3.45 | 8 (29%)     | 36,38,38    | 2.06 | 7 (19%)     |
| 2   | NAP  | C     | 2000 | -    | 50,52,52     | 1.67 | 9 (18%)     | 71,80,80    | 2.17 | 23 (32%)    |
| 2   | NAP  | A     | 2002 | -    | 50,52,52     | 1.84 | 12 (24%)    | 71,80,80    | 2.68 | 23 (32%)    |
| 3   | 3G4  | A     | 2004 | -    | 27,27,27     | 2.94 | 6 (22%)     | 36,38,38    | 2.25 | 7 (19%)     |

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   | NAP  | B     | 2003 | -    | -       | 4/35/67/67 | 0/5/5/5 |
| 2   | NAP  | D     | 2001 | -    | -       | 5/35/67/67 | 0/5/5/5 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|------|------|---------|-------------|---------|
| 3   | 3G4  | D     | 2007 | -    | -       | 10/23/23/23 | 0/2/2/2 |
| 2   | NAP  | C     | 2000 | -    | -       | 7/35/67/67  | 0/5/5/5 |
| 2   | NAP  | A     | 2002 | -    | -       | 4/35/67/67  | 0/5/5/5 |
| 3   | 3G4  | A     | 2004 | -    | -       | 6/23/23/23  | 0/2/2/2 |

All (54) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 3   | D     | 2007 | 3G4  | C19-C20 | -10.41 | 1.40        | 1.52     |
| 3   | A     | 2004 | 3G4  | C19-C20 | -9.10  | 1.42        | 1.52     |
| 3   | D     | 2007 | 3G4  | C5-S9   | -8.99  | 1.65        | 1.77     |
| 3   | D     | 2007 | 3G4  | S9-N10  | -8.43  | 1.50        | 1.63     |
| 3   | A     | 2004 | 3G4  | C5-S9   | -8.33  | 1.66        | 1.77     |
| 2   | B     | 2003 | NAP  | PA-O3   | 7.37   | 1.67        | 1.59     |
| 2   | C     | 2000 | NAP  | C4A-N3A | 6.97   | 1.47        | 1.34     |
| 3   | A     | 2004 | 3G4  | S9-N10  | -6.68  | 1.53        | 1.63     |
| 2   | B     | 2003 | NAP  | C4A-N3A | 6.24   | 1.46        | 1.34     |
| 2   | A     | 2002 | NAP  | PA-O3   | 5.16   | 1.65        | 1.59     |
| 2   | A     | 2002 | NAP  | C4A-N3A | 4.83   | 1.43        | 1.34     |
| 3   | D     | 2007 | 3G4  | C6-C5   | -4.15  | 1.37        | 1.41     |
| 2   | D     | 2001 | NAP  | C4A-N3A | 4.11   | 1.42        | 1.34     |
| 2   | A     | 2002 | NAP  | C5A-N7A | -3.85  | 1.32        | 1.39     |
| 2   | B     | 2003 | NAP  | C5A-C4A | -3.81  | 1.32        | 1.39     |
| 2   | A     | 2002 | NAP  | PN-O3   | 3.76   | 1.63        | 1.59     |
| 2   | D     | 2001 | NAP  | C4A-N9A | -3.68  | 1.30        | 1.37     |
| 2   | B     | 2003 | NAP  | C8A-N7A | 3.63   | 1.38        | 1.31     |
| 2   | D     | 2001 | NAP  | O4D-C4D | -3.54  | 1.37        | 1.45     |
| 2   | A     | 2002 | NAP  | C8A-N7A | 3.33   | 1.38        | 1.31     |
| 2   | B     | 2003 | NAP  | C8A-N9A | -3.29  | 1.32        | 1.37     |
| 2   | A     | 2002 | NAP  | C4A-N9A | -3.13  | 1.31        | 1.37     |
| 2   | D     | 2001 | NAP  | C8A-N7A | 3.12   | 1.37        | 1.31     |
| 3   | D     | 2007 | 3G4  | C13-N14 | -2.88  | 1.28        | 1.34     |
| 2   | B     | 2003 | NAP  | C4A-N9A | -2.85  | 1.31        | 1.37     |
| 2   | D     | 2001 | NAP  | PA-O3   | 2.80   | 1.62        | 1.59     |
| 3   | A     | 2004 | 3G4  | O12-S9  | 2.80   | 1.46        | 1.43     |
| 2   | C     | 2000 | NAP  | C5A-C4A | -2.76  | 1.34        | 1.39     |
| 2   | B     | 2003 | NAP  | C2A-N1A | 2.74   | 1.38        | 1.33     |
| 2   | B     | 2003 | NAP  | C7N-N7N | 2.73   | 1.38        | 1.33     |
| 2   | C     | 2000 | NAP  | C8A-N7A | 2.67   | 1.36        | 1.31     |
| 2   | C     | 2000 | NAP  | C4A-N9A | -2.67  | 1.32        | 1.37     |
| 3   | A     | 2004 | 3G4  | C1-C6   | -2.57  | 1.35        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | C     | 2000 | NAP  | C7N-N7N | 2.57  | 1.37        | 1.33     |
| 2   | C     | 2000 | NAP  | P2B-O2B | 2.50  | 1.63        | 1.59     |
| 3   | D     | 2007 | 3G4  | C4-C5   | 2.47  | 1.42        | 1.39     |
| 2   | D     | 2001 | NAP  | C2D-C3D | -2.42 | 1.46        | 1.53     |
| 2   | A     | 2002 | NAP  | PN-O1N  | 2.37  | 1.59        | 1.50     |
| 2   | A     | 2002 | NAP  | C3D-C4D | -2.35 | 1.47        | 1.53     |
| 2   | D     | 2001 | NAP  | O4B-C4B | -2.35 | 1.39        | 1.45     |
| 2   | C     | 2000 | NAP  | C3B-C2B | -2.34 | 1.47        | 1.53     |
| 2   | A     | 2002 | NAP  | O5B-C5B | -2.33 | 1.35        | 1.44     |
| 2   | A     | 2002 | NAP  | C3B-C2B | -2.32 | 1.47        | 1.53     |
| 3   | D     | 2007 | 3G4  | C1-C6   | 2.30  | 1.43        | 1.39     |
| 3   | D     | 2007 | 3G4  | O22-C20 | -2.22 | 1.18        | 1.23     |
| 2   | B     | 2003 | NAP  | O4D-C4D | -2.17 | 1.40        | 1.45     |
| 2   | B     | 2003 | NAP  | C6N-N1N | -2.15 | 1.30        | 1.35     |
| 2   | B     | 2003 | NAP  | PN-O3   | -2.13 | 1.57        | 1.59     |
| 3   | A     | 2004 | 3G4  | C3-C4   | 2.10  | 1.42        | 1.38     |
| 2   | B     | 2003 | NAP  | O3D-C3D | 2.10  | 1.48        | 1.43     |
| 2   | A     | 2002 | NAP  | P2B-O2B | 2.08  | 1.63        | 1.59     |
| 2   | C     | 2000 | NAP  | C5A-N7A | -2.04 | 1.35        | 1.39     |
| 2   | C     | 2000 | NAP  | O5B-C5B | -2.02 | 1.36        | 1.44     |
| 2   | A     | 2002 | NAP  | C2N-N1N | -2.00 | 1.32        | 1.35     |

All (108) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 2002 | NAP  | O4B-C1B-N9A | 10.71 | 128.66      | 108.09   |
| 3   | A     | 2004 | 3G4  | O12-S9-O11  | -8.41 | 109.31      | 119.52   |
| 3   | D     | 2007 | 3G4  | O12-S9-O11  | -7.42 | 110.51      | 119.52   |
| 2   | A     | 2002 | NAP  | N3A-C2A-N1A | -7.15 | 117.76      | 128.58   |
| 2   | B     | 2003 | NAP  | N3A-C2A-N1A | -6.82 | 118.26      | 128.58   |
| 3   | D     | 2007 | 3G4  | C13-N14-C15 | 6.68  | 122.80      | 118.16   |
| 2   | D     | 2001 | NAP  | C5A-C4A-N9A | 6.24  | 112.61      | 105.81   |
| 2   | C     | 2000 | NAP  | N9A-C8A-N7A | -6.07 | 105.33      | 113.94   |
| 2   | B     | 2003 | NAP  | O2N-PN-O3   | -6.03 | 90.97       | 107.27   |
| 2   | B     | 2003 | NAP  | C4D-O4D-C1D | 5.98  | 115.40      | 109.92   |
| 2   | A     | 2002 | NAP  | C5A-C4A-N9A | 5.85  | 112.18      | 105.81   |
| 2   | B     | 2003 | NAP  | O3-PA-O1A   | -5.53 | 94.07       | 110.70   |
| 2   | B     | 2003 | NAP  | C5A-C4A-N9A | 5.46  | 111.77      | 105.81   |
| 3   | A     | 2004 | 3G4  | C13-N14-C15 | 5.44  | 121.94      | 118.16   |
| 2   | A     | 2002 | NAP  | C5A-C4A-N3A | -5.23 | 119.52      | 126.72   |
| 3   | A     | 2004 | 3G4  | O22-C20-N21 | -5.07 | 113.09      | 122.12   |
| 2   | D     | 2001 | NAP  | C4A-C5A-N7A | -4.94 | 104.93      | 110.58   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | B     | 2003 | NAP  | N9A-C8A-N7A | -4.91 | 106.97      | 113.94   |
| 2   | A     | 2002 | NAP  | C4D-O4D-C1D | 4.83  | 114.35      | 109.92   |
| 2   | C     | 2000 | NAP  | N3A-C2A-N1A | -4.76 | 121.37      | 128.58   |
| 2   | A     | 2002 | NAP  | O3B-C3B-C2B | -4.70 | 98.03       | 111.19   |
| 2   | B     | 2003 | NAP  | C4A-C5A-N7A | -4.69 | 105.21      | 110.58   |
| 2   | A     | 2002 | NAP  | O3B-C3B-C4B | -4.65 | 97.73       | 111.08   |
| 2   | C     | 2000 | NAP  | O3B-C3B-C2B | -4.63 | 98.24       | 111.19   |
| 2   | D     | 2001 | NAP  | O4B-C1B-N9A | 4.43  | 116.59      | 108.09   |
| 2   | D     | 2001 | NAP  | O2N-PN-O1N  | 4.36  | 132.73      | 112.44   |
| 2   | A     | 2002 | NAP  | O3D-C3D-C4D | -4.18 | 99.07       | 111.08   |
| 2   | B     | 2003 | NAP  | C3N-C7N-N7N | 4.12  | 122.81      | 117.74   |
| 2   | C     | 2000 | NAP  | C4A-N9A-C8A | 4.07  | 110.01      | 105.74   |
| 2   | B     | 2003 | NAP  | C5A-C4A-N3A | -4.06 | 121.13      | 126.72   |
| 2   | A     | 2002 | NAP  | C4A-C5A-N7A | -4.00 | 106.01      | 110.58   |
| 2   | A     | 2002 | NAP  | C2B-C3B-C4B | 3.95  | 110.48      | 101.99   |
| 2   | B     | 2003 | NAP  | O2A-PA-O3   | 3.94  | 117.92      | 107.27   |
| 2   | C     | 2000 | NAP  | O2X-P2B-O2B | 3.87  | 120.91      | 105.85   |
| 2   | A     | 2002 | NAP  | C2A-N3A-C4A | 3.77  | 121.03      | 111.83   |
| 2   | A     | 2002 | NAP  | C2B-C1B-N9A | -3.66 | 107.73      | 113.75   |
| 2   | C     | 2000 | NAP  | C5A-N7A-C8A | 3.65  | 109.19      | 103.45   |
| 2   | C     | 2000 | NAP  | C4A-C5A-N7A | -3.63 | 106.43      | 110.58   |
| 2   | B     | 2003 | NAP  | O7N-C7N-C3N | -3.61 | 115.18      | 119.60   |
| 2   | B     | 2003 | NAP  | O3B-C3B-C4B | -3.61 | 100.72      | 111.08   |
| 2   | C     | 2000 | NAP  | O3X-P2B-O2B | -3.60 | 91.83       | 105.85   |
| 2   | D     | 2001 | NAP  | N3A-C2A-N1A | -3.59 | 123.15      | 128.58   |
| 2   | A     | 2002 | NAP  | O2B-C2B-C1B | 3.57  | 122.61      | 110.05   |
| 2   | A     | 2002 | NAP  | N9A-C8A-N7A | -3.56 | 108.88      | 113.94   |
| 2   | D     | 2001 | NAP  | O2B-C2B-C1B | 3.54  | 122.49      | 110.05   |
| 2   | C     | 2000 | NAP  | O4B-C1B-N9A | 3.49  | 114.80      | 108.09   |
| 2   | C     | 2000 | NAP  | C6A-C5A-N7A | 3.41  | 138.67      | 132.09   |
| 2   | C     | 2000 | NAP  | O4B-C1B-C2B | 3.41  | 112.46      | 106.59   |
| 2   | A     | 2002 | NAP  | O7N-C7N-N7N | 3.41  | 127.54      | 122.62   |
| 2   | B     | 2003 | NAP  | C2A-N3A-C4A | 3.39  | 120.11      | 111.83   |
| 2   | D     | 2001 | NAP  | O3X-P2B-O2B | -3.37 | 92.71       | 105.85   |
| 2   | D     | 2001 | NAP  | O3B-C3B-C4B | -3.34 | 101.50      | 111.08   |
| 2   | D     | 2001 | NAP  | N9A-C8A-N7A | -3.28 | 109.28      | 113.94   |
| 2   | A     | 2002 | NAP  | C2A-N1A-C6A | 3.27  | 124.11      | 118.73   |
| 2   | D     | 2001 | NAP  | C6A-C5A-N7A | 3.27  | 138.40      | 132.09   |
| 3   | A     | 2004 | 3G4  | C8-C6-C1    | -3.24 | 117.96      | 121.86   |
| 2   | C     | 2000 | NAP  | O2D-C2D-C3D | 3.23  | 122.17      | 111.82   |
| 2   | B     | 2003 | NAP  | O4B-C1B-N9A | 3.23  | 114.29      | 108.09   |
| 2   | C     | 2000 | NAP  | O7N-C7N-C3N | -3.15 | 115.74      | 119.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | B     | 2003 | NAP  | O2A-PA-O1A  | 3.11  | 126.89      | 112.44   |
| 2   | D     | 2001 | NAP  | O3X-P2B-O1X | 3.03  | 122.63      | 110.83   |
| 2   | C     | 2000 | NAP  | O5B-PA-O1A  | -3.01 | 97.00       | 108.94   |
| 2   | C     | 2000 | NAP  | C2B-C3B-C4B | 2.98  | 108.40      | 101.99   |
| 2   | C     | 2000 | NAP  | C5A-C4A-N9A | 2.95  | 109.03      | 105.81   |
| 2   | B     | 2003 | NAP  | O3-PN-O1N   | 2.95  | 119.59      | 110.70   |
| 2   | D     | 2001 | NAP  | C5A-C4A-N3A | -2.94 | 122.66      | 126.72   |
| 2   | A     | 2002 | NAP  | O7N-C7N-C3N | -2.90 | 116.06      | 119.60   |
| 3   | D     | 2007 | 3G4  | C4-C5-C6    | -2.87 | 118.51      | 121.19   |
| 2   | A     | 2002 | NAP  | C2D-C3D-C4D | 2.85  | 108.11      | 102.61   |
| 2   | B     | 2003 | NAP  | O2B-C2B-C1B | 2.79  | 119.84      | 110.05   |
| 2   | D     | 2001 | NAP  | O3-PN-O1N   | -2.78 | 102.34      | 110.70   |
| 3   | A     | 2004 | 3G4  | O22-C20-C19 | 2.72  | 125.94      | 121.61   |
| 3   | D     | 2007 | 3G4  | O22-C20-C19 | 2.71  | 125.92      | 121.61   |
| 2   | B     | 2003 | NAP  | C5N-C4N-C3N | -2.64 | 117.77      | 120.36   |
| 2   | A     | 2002 | NAP  | O2A-PA-O1A  | 2.63  | 124.67      | 112.44   |
| 2   | B     | 2003 | NAP  | C4A-N9A-C8A | 2.62  | 108.49      | 105.74   |
| 2   | C     | 2000 | NAP  | O2A-PA-O1A  | 2.62  | 124.62      | 112.44   |
| 2   | A     | 2002 | NAP  | C5A-N7A-C8A | 2.61  | 107.56      | 103.45   |
| 2   | B     | 2003 | NAP  | C5A-N7A-C8A | 2.56  | 107.48      | 103.45   |
| 2   | B     | 2003 | NAP  | C6A-C5A-N7A | 2.48  | 136.87      | 132.09   |
| 2   | B     | 2003 | NAP  | C2D-C3D-C4D | 2.48  | 107.39      | 102.61   |
| 2   | D     | 2001 | NAP  | C2D-C3D-C4D | 2.45  | 107.35      | 102.61   |
| 2   | D     | 2001 | NAP  | C5A-N7A-C8A | 2.40  | 107.22      | 103.45   |
| 2   | B     | 2003 | NAP  | O4B-C1B-C2B | 2.38  | 110.68      | 106.59   |
| 2   | D     | 2001 | NAP  | O5D-PN-O1N  | -2.35 | 99.63       | 108.94   |
| 2   | A     | 2002 | NAP  | O2A-PA-O5B  | -2.31 | 97.11       | 107.57   |
| 2   | D     | 2001 | NAP  | O4B-C4B-C3B | 2.31  | 109.73      | 105.15   |
| 2   | D     | 2001 | NAP  | C2B-C1B-N9A | 2.29  | 117.52      | 113.75   |
| 2   | C     | 2000 | NAP  | C5A-C6A-N6A | -2.28 | 117.64      | 123.29   |
| 3   | D     | 2007 | 3G4  | O22-C20-N21 | -2.28 | 118.07      | 122.12   |
| 2   | B     | 2003 | NAP  | C5A-C6A-N6A | -2.24 | 117.74      | 123.29   |
| 2   | C     | 2000 | NAP  | O3X-P2B-O2X | 2.20  | 116.06      | 107.80   |
| 2   | B     | 2003 | NAP  | O2X-P2B-O1X | 2.20  | 119.40      | 110.83   |
| 2   | D     | 2001 | NAP  | C5B-C4B-C3B | -2.18 | 107.36      | 115.21   |
| 2   | C     | 2000 | NAP  | O2B-P2B-O1X | -2.18 | 101.58      | 109.33   |
| 2   | D     | 2001 | NAP  | C5A-C6A-N6A | -2.18 | 117.90      | 123.29   |
| 2   | A     | 2002 | NAP  | C6A-C5A-N7A | 2.17  | 136.28      | 132.09   |
| 2   | D     | 2001 | NAP  | C1B-N9A-C8A | 2.13  | 131.83      | 127.09   |
| 2   | C     | 2000 | NAP  | C5A-C6A-N1A | 2.11  | 122.87      | 117.51   |
| 2   | A     | 2002 | NAP  | C6N-N1N-C1D | -2.07 | 115.67      | 119.73   |
| 3   | D     | 2007 | 3G4  | C8-C6-C1    | -2.07 | 119.36      | 121.86   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | C     | 2000 | NAP  | C5A-C4A-N3A | -2.05 | 123.90      | 126.72   |
| 3   | D     | 2007 | 3G4  | C6-C5-S9    | 2.04  | 123.83      | 122.02   |
| 2   | C     | 2000 | NAP  | C2A-N3A-C4A | 2.04  | 116.82      | 111.83   |
| 3   | A     | 2004 | 3G4  | C4-C5-C6    | -2.04 | 119.29      | 121.19   |
| 2   | D     | 2001 | NAP  | O3-PA-O1A   | -2.02 | 104.62      | 110.70   |
| 2   | D     | 2001 | NAP  | C2A-N3A-C4A | 2.01  | 116.75      | 111.83   |
| 3   | A     | 2004 | 3G4  | C5-S9-N10   | 2.00  | 109.66      | 107.30   |

There are no chirality outliers.

All (36) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | B     | 2003 | NAP  | C5B-O5B-PA-O1A  |
| 2   | C     | 2000 | NAP  | C5B-O5B-PA-O1A  |
| 2   | C     | 2000 | NAP  | C5B-O5B-PA-O3   |
| 2   | C     | 2000 | NAP  | C5D-O5D-PN-O2N  |
| 2   | D     | 2001 | NAP  | C5D-O5D-PN-O2N  |
| 3   | A     | 2004 | 3G4  | C6-C5-S9-O12    |
| 3   | A     | 2004 | 3G4  | C6-C5-S9-N10    |
| 3   | D     | 2007 | 3G4  | C6-C5-S9-O12    |
| 3   | D     | 2007 | 3G4  | C6-C5-S9-N10    |
| 3   | A     | 2004 | 3G4  | C25-C24-N21-C20 |
| 3   | A     | 2004 | 3G4  | C4-C5-S9-O12    |
| 3   | D     | 2007 | 3G4  | C4-C5-S9-O12    |
| 3   | D     | 2007 | 3G4  | C6-C5-S9-O11    |
| 3   | A     | 2004 | 3G4  | C25-C24-N21-C23 |
| 3   | D     | 2007 | 3G4  | C25-C24-N21-C20 |
| 3   | A     | 2004 | 3G4  | C4-C5-S9-N10    |
| 3   | D     | 2007 | 3G4  | C4-C5-S9-N10    |
| 3   | D     | 2007 | 3G4  | C25-C24-N21-C23 |
| 2   | C     | 2000 | NAP  | O4B-C4B-C5B-O5B |
| 2   | D     | 2001 | NAP  | C1B-C2B-O2B-P2B |
| 2   | A     | 2002 | NAP  | PN-O3-PA-O2A    |
| 2   | A     | 2002 | NAP  | C5B-O5B-PA-O1A  |
| 2   | D     | 2001 | NAP  | C5D-O5D-PN-O3   |
| 2   | D     | 2001 | NAP  | PN-O3-PA-O1A    |
| 2   | A     | 2002 | NAP  | O4D-C1D-N1N-C2N |
| 2   | C     | 2000 | NAP  | O4D-C1D-N1N-C6N |
| 3   | D     | 2007 | 3G4  | C13-N10-S9-O11  |
| 2   | B     | 2003 | NAP  | O4B-C4B-C5B-O5B |
| 2   | A     | 2002 | NAP  | O4D-C4D-C5D-O5D |
| 3   | D     | 2007 | 3G4  | C4-C5-S9-O11    |

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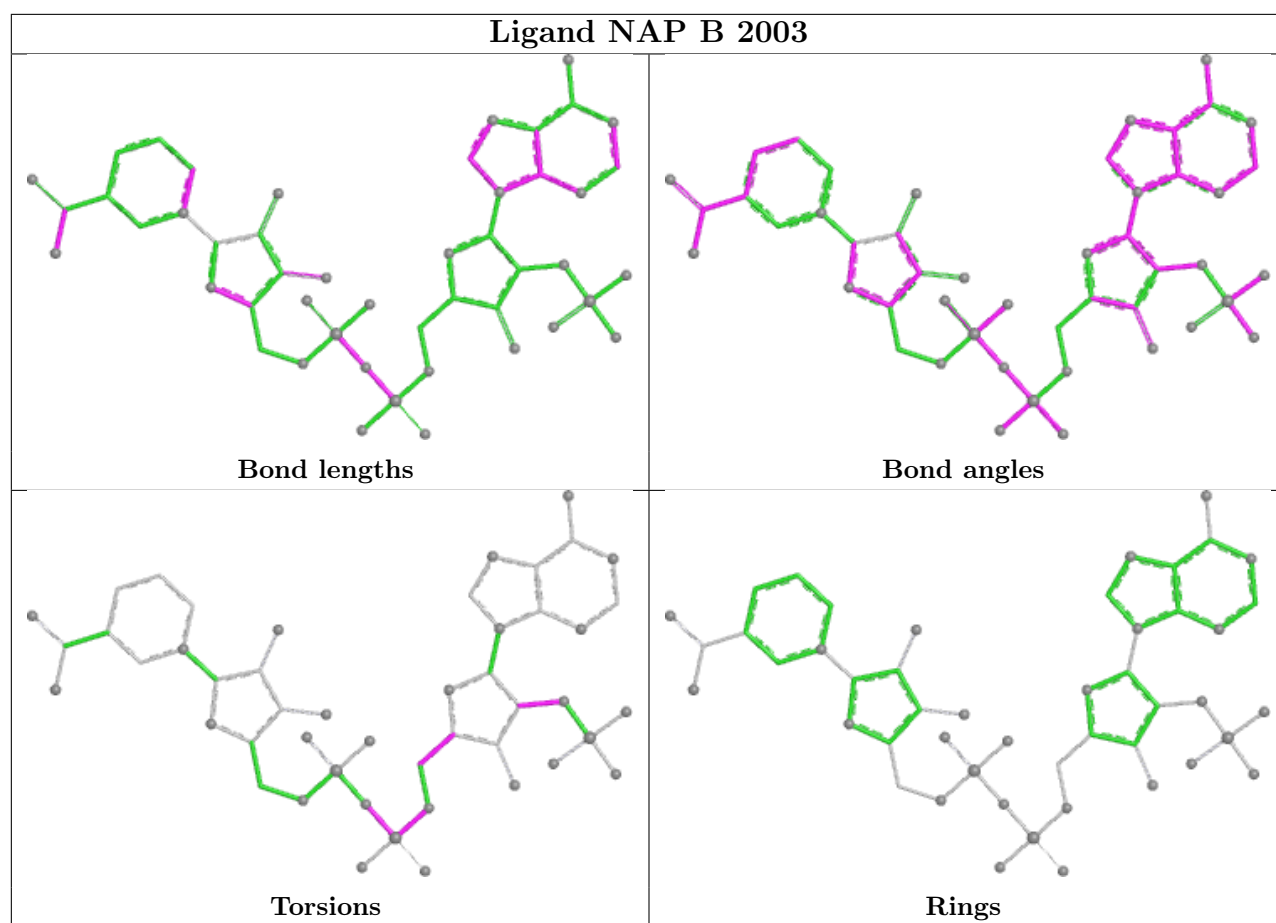
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | B     | 2003 | NAP  | PN-O3-PA-O1A    |
| 2   | C     | 2000 | NAP  | PN-O3-PA-O1A    |
| 2   | C     | 2000 | NAP  | PN-O3-PA-O2A    |
| 2   | D     | 2001 | NAP  | PN-O3-PA-O2A    |
| 2   | B     | 2003 | NAP  | C1B-C2B-O2B-P2B |
| 3   | D     | 2007 | 3G4  | C15-C19-C20-N21 |

There are no ring outliers.

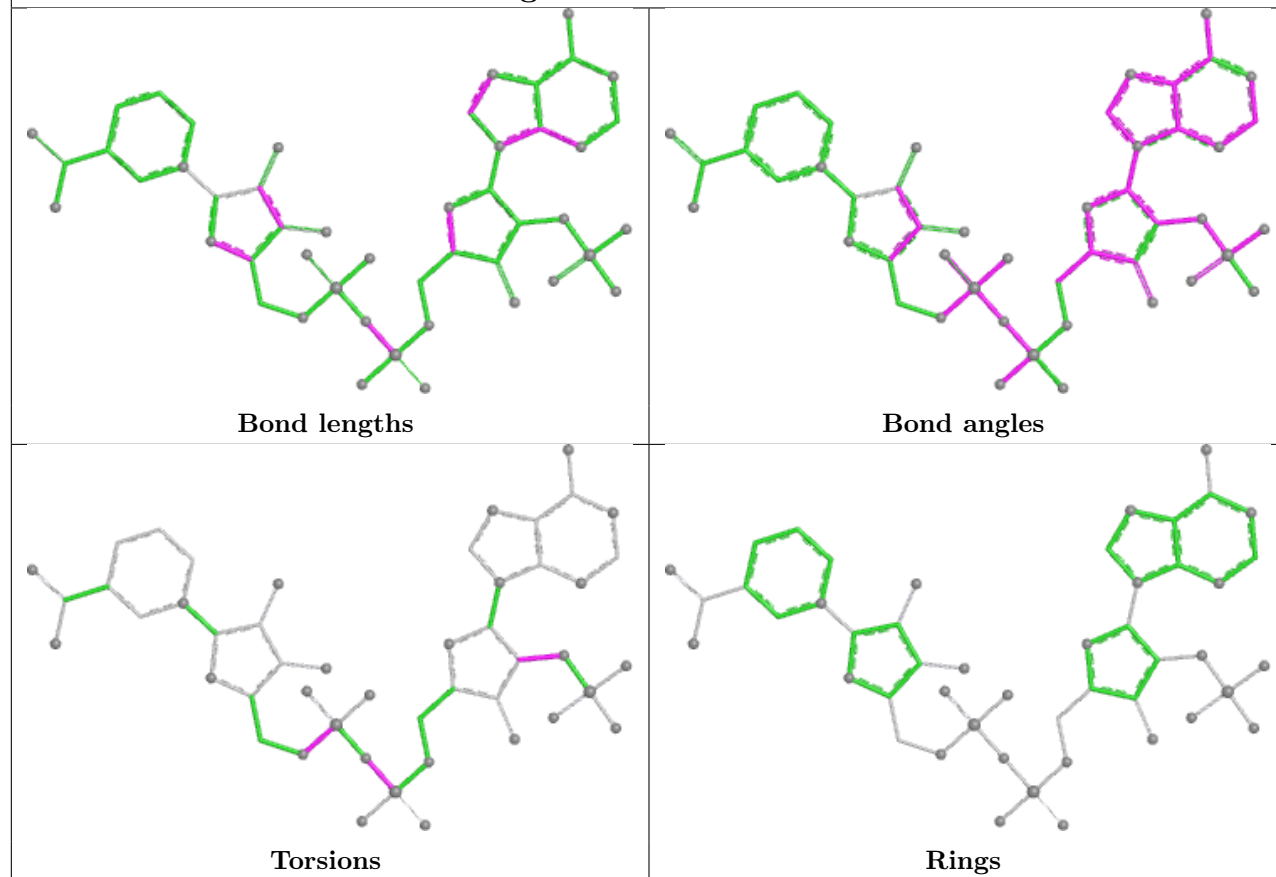
6 monomers are involved in 40 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | B     | 2003 | NAP  | 2       | 0            |
| 2   | D     | 2001 | NAP  | 2       | 0            |
| 3   | D     | 2007 | 3G4  | 15      | 0            |
| 2   | C     | 2000 | NAP  | 2       | 0            |
| 2   | A     | 2002 | NAP  | 5       | 0            |
| 3   | A     | 2004 | 3G4  | 15      | 0            |

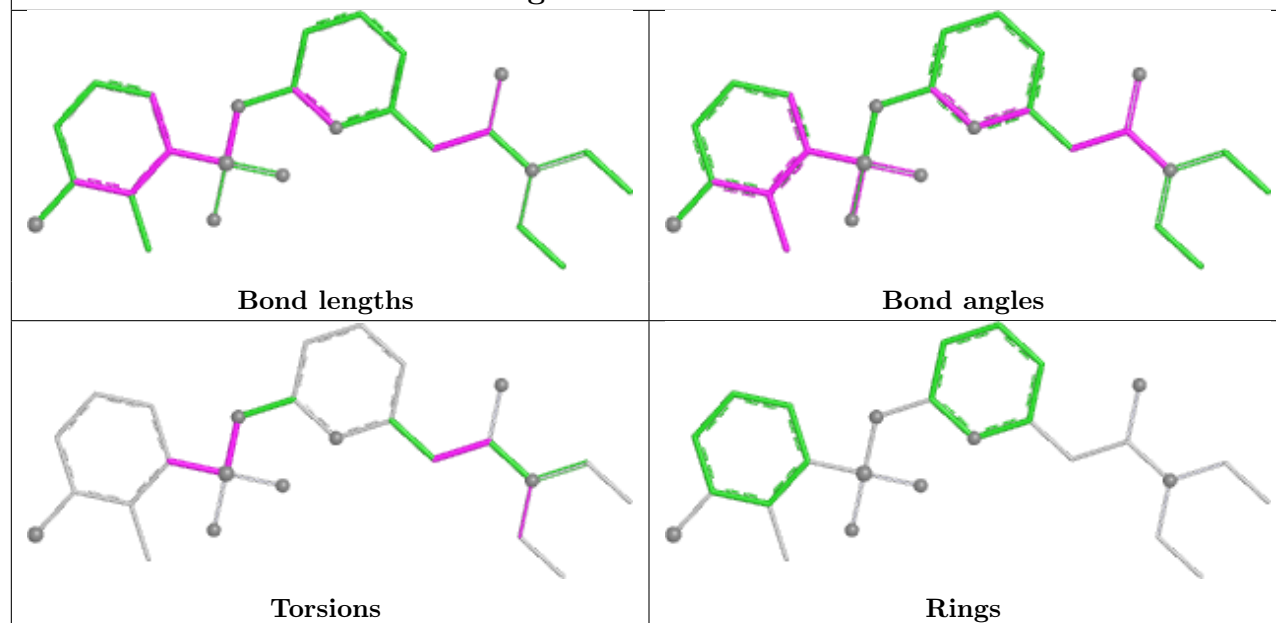
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

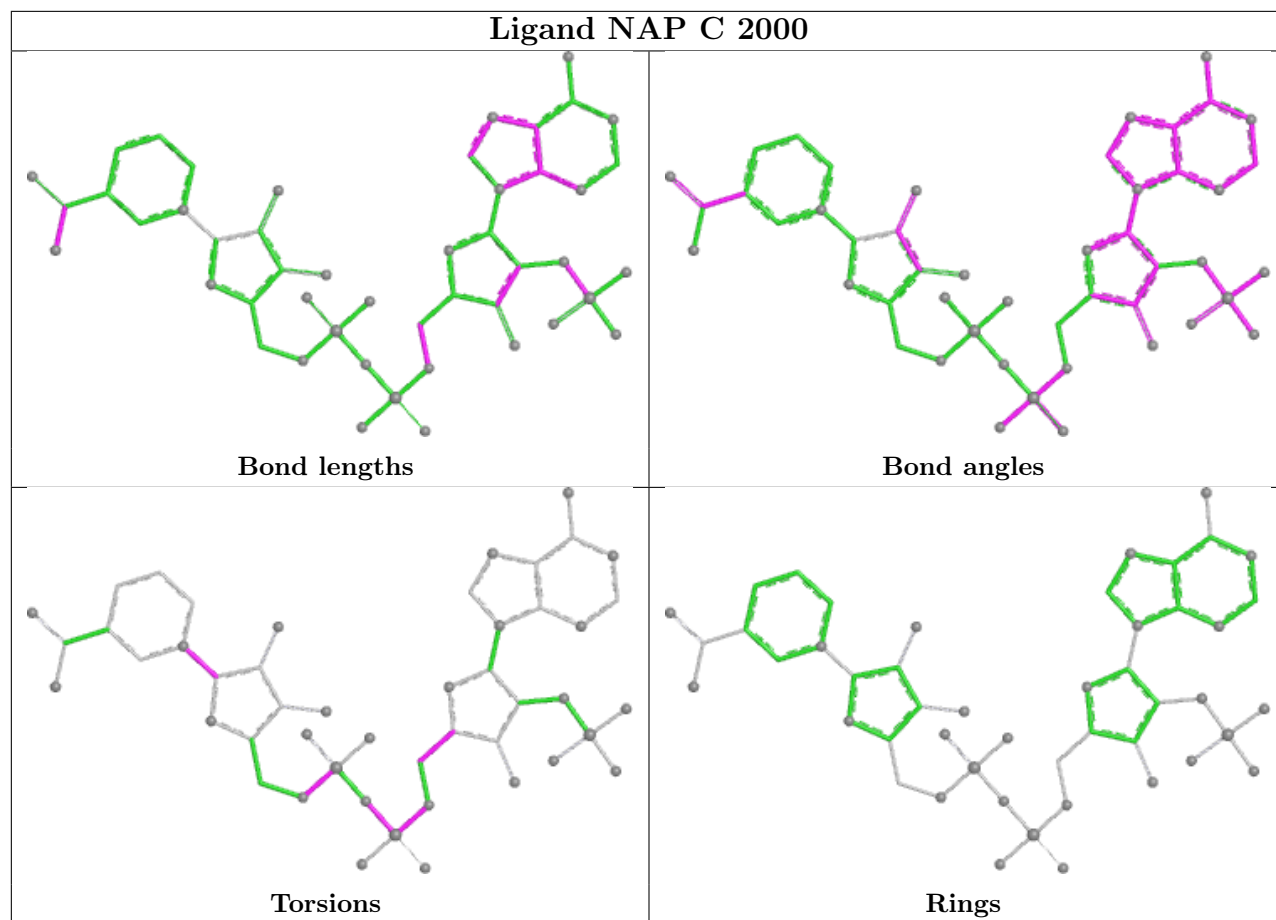


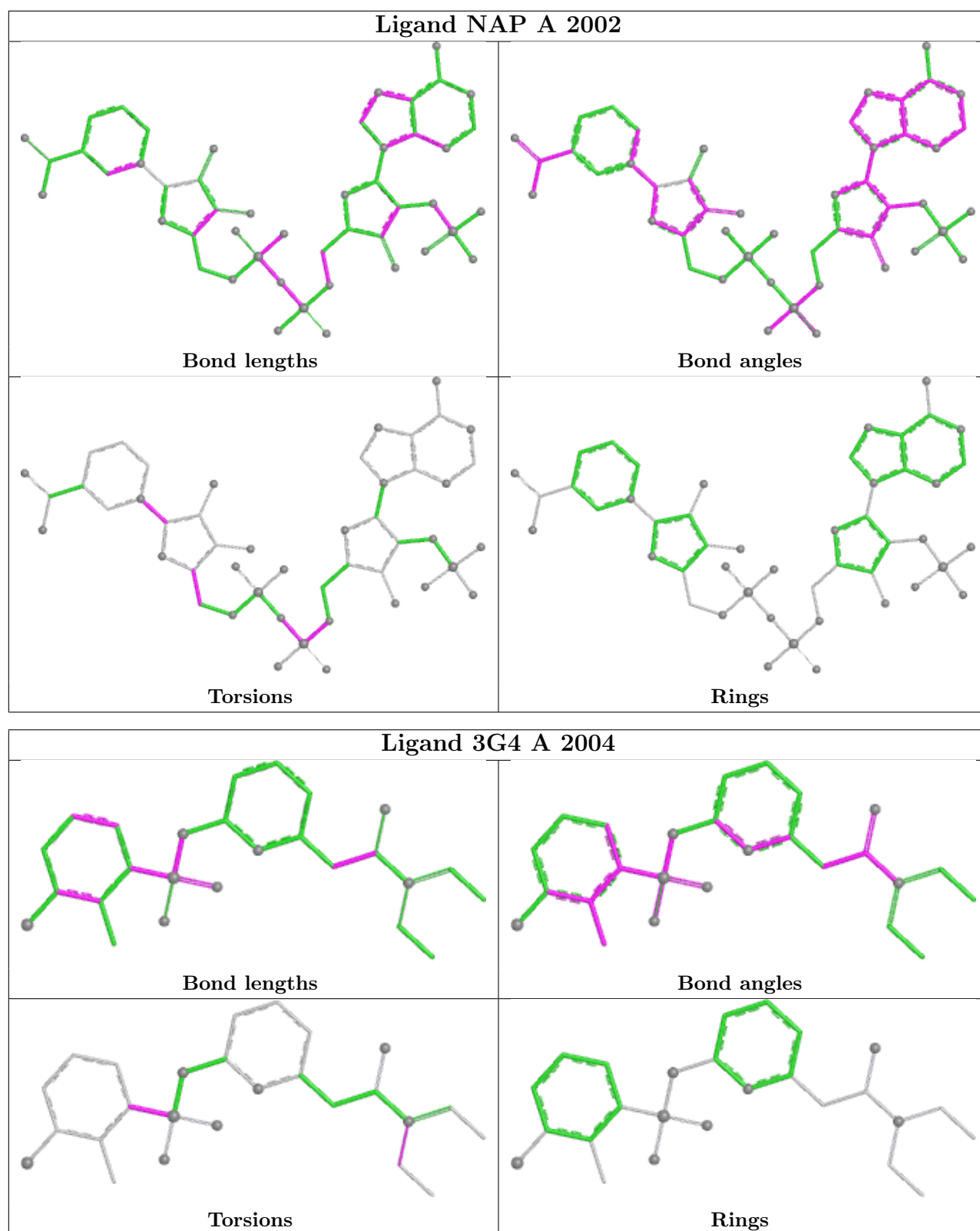
## Ligand NAP D 2001



## Ligand 3G4 D 2007







## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 263/277 (94%)   | -0.06  | 2 (0%) 82 80  | 17, 29, 41, 56        | 0     |
| 1   | B     | 263/277 (94%)   | 0.08   | 8 (3%) 52 48  | 16, 32, 45, 51        | 0     |
| 1   | C     | 263/277 (94%)   | 0.02   | 6 (2%) 61 57  | 16, 31, 45, 60        | 0     |
| 1   | D     | 263/277 (94%)   | -0.04  | 7 (2%) 56 51  | 16, 28, 41, 56        | 0     |
| All | All   | 1052/1108 (94%) | -0.00  | 23 (2%) 62 58 | 16, 30, 44, 60        | 0     |

All (23) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | C     | 733  | LEU  | 5.9  |
| 1   | D     | 1021 | TYR  | 5.5  |
| 1   | B     | 363  | ARG  | 5.0  |
| 1   | D     | 985  | GLU  | 3.6  |
| 1   | C     | 626  | ARG  | 3.6  |
| 1   | B     | 368  | HIS  | 3.2  |
| 1   | C     | 789  | ASN  | 3.1  |
| 1   | D     | 965  | PHE  | 2.8  |
| 1   | B     | 526  | ASN  | 2.7  |
| 1   | D     | 1042 | PHE  | 2.6  |
| 1   | D     | 821  | MET  | 2.6  |
| 1   | A     | 135  | GLN  | 2.5  |
| 1   | C     | 624  | TYR  | 2.5  |
| 1   | C     | 732  | TYR  | 2.5  |
| 1   | C     | 645  | PHE  | 2.4  |
| 1   | B     | 398  | GLN  | 2.4  |
| 1   | D     | 1047 | GLU  | 2.3  |
| 1   | B     | 346  | ASN  | 2.3  |
| 1   | D     | 1052 | ASN  | 2.3  |
| 1   | B     | 361  | TYR  | 2.2  |
| 1   | B     | 431  | PHE  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 520 | ALA  | 2.0  |
| 1   | A     | 263 | ASN  | 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](#)

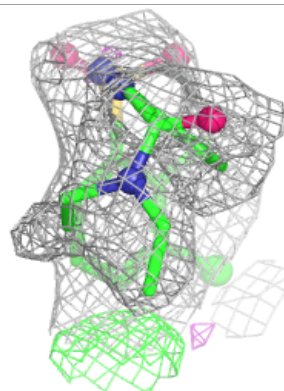
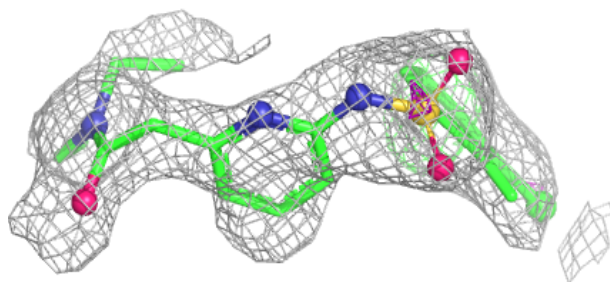
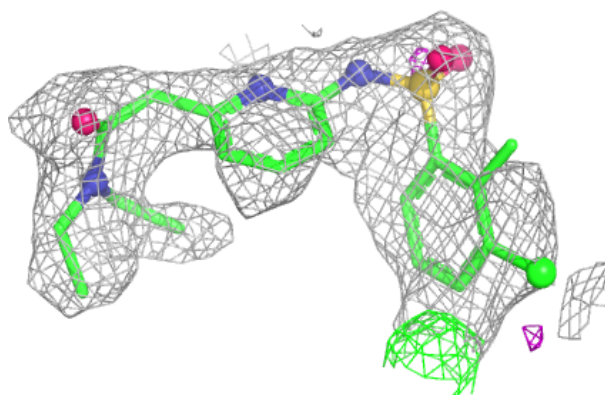
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | 3G4  | A     | 2004 | 26/26 | 0.86 | 0.14 | 41,48,60,67                 | 0     |
| 3   | 3G4  | D     | 2007 | 26/26 | 0.90 | 0.14 | 29,38,60,68                 | 0     |
| 2   | NAP  | C     | 2000 | 48/48 | 0.97 | 0.06 | 18,26,36,39                 | 0     |
| 2   | NAP  | D     | 2001 | 48/48 | 0.97 | 0.06 | 11,22,28,30                 | 0     |
| 2   | NAP  | A     | 2002 | 48/48 | 0.97 | 0.06 | 15,25,29,32                 | 0     |
| 2   | NAP  | B     | 2003 | 48/48 | 0.97 | 0.06 | 15,27,33,42                 | 0     |

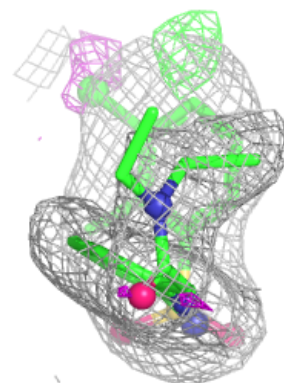
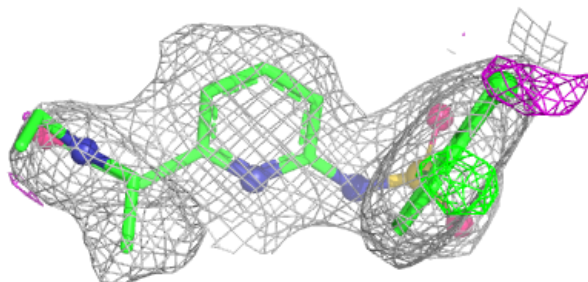
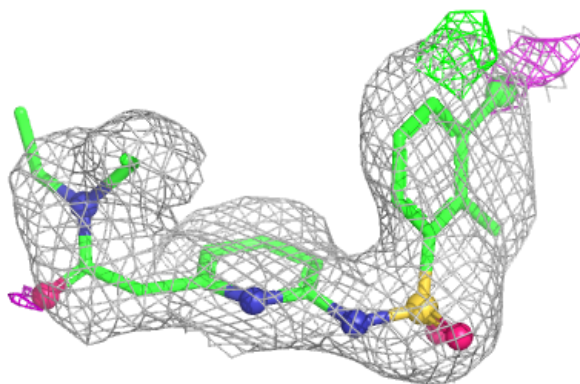
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 3G4 A 2004:**

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

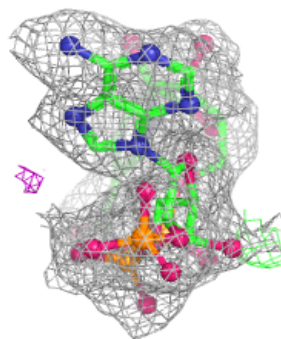
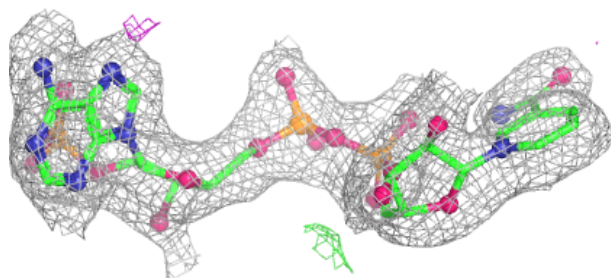
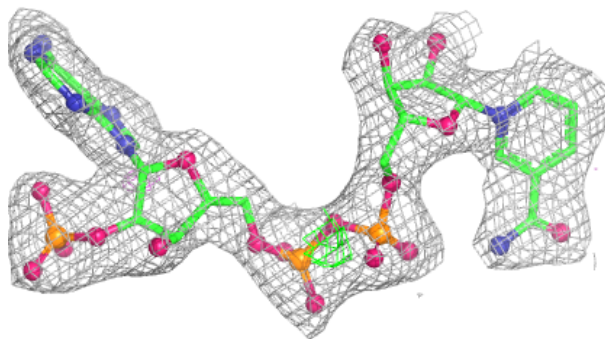
**Electron density around 3G4 D 2007:**

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

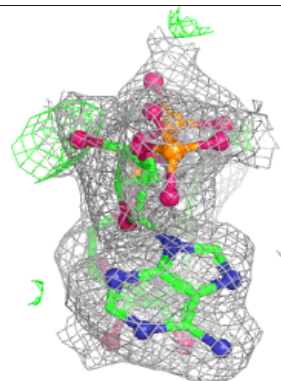
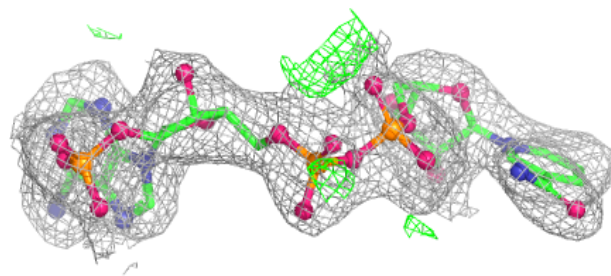
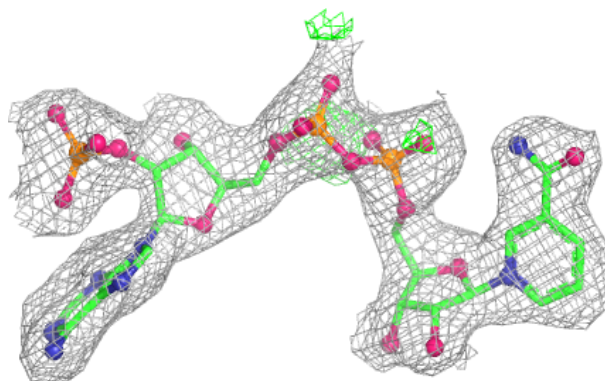


**Electron density around NAP C 2000:**

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

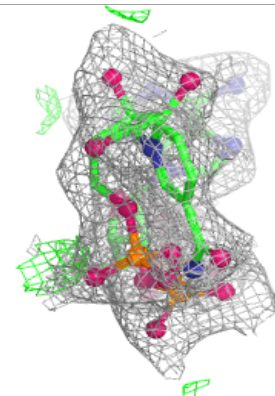
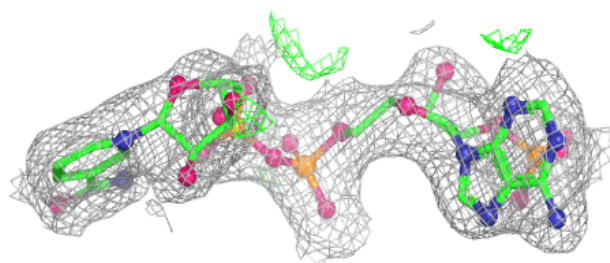
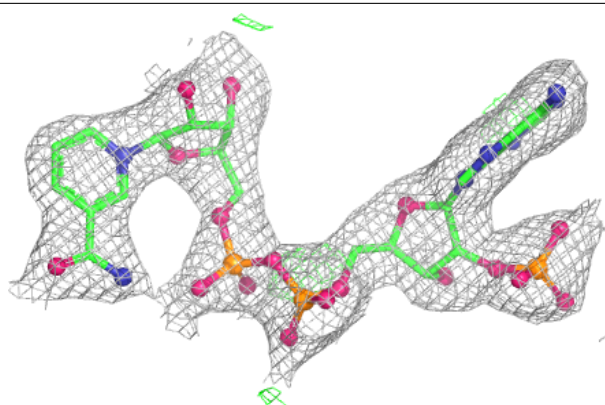
**Electron density around NAP D 2001:**

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

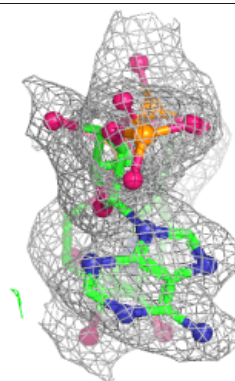
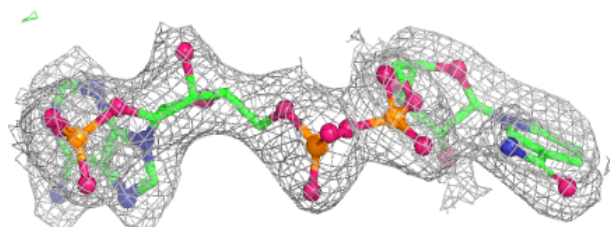
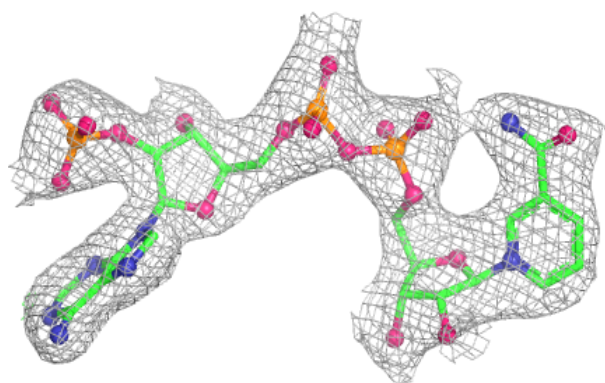


**Electron density around NAP A 2002:**

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

**Electron density around NAP B 2003:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.