



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:39 am BST

PDB ID : 2PKR  
Title : Crystal structure of (A+CTE)4 chimeric form of photosynthetic glyceraldehyde-3-phosphate dehydrogenase, complexed with NADP  
Authors : Fermani, S.; Falini, G.; Ripamonti, A.  
Deposited on : 2007-04-18  
Resolution : 2.40 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

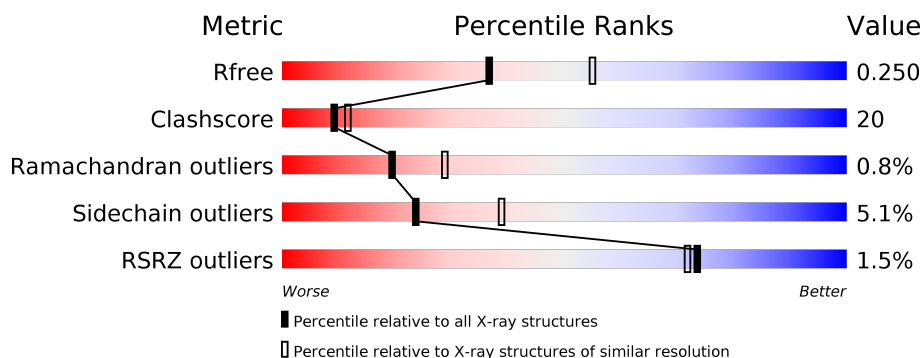
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 3907 (2.40-2.40)                                      |
| Clashscore            | 141614                      | 4398 (2.40-2.40)                                      |
| Ramachandran outliers | 138981                      | 4318 (2.40-2.40)                                      |
| Sidechain outliers    | 138945                      | 4319 (2.40-2.40)                                      |
| RSRZ outliers         | 127900                      | 3811 (2.40-2.40)                                      |

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 on 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     | 365    | <div> <div>3%</div> <div>67% 19% 5% • 8%</div> </div> |
| 1   | B     | 365    | <div> <div>63% 24% • • 8%</div> </div>                |
| 1   | C     | 365    | <div> <div>68% 22% • 8%</div> </div>                  |
| 1   | D     | 365    | <div> <div>3%</div> <div>69% 20% • 8%</div> </div>    |
| 1   | H     | 365    | <div> <div>2%</div> <div>68% 19% • • 8%</div> </div>  |
| 1   | I     | 365    | <div> <div>70% 19% • 8%</div> </div>                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | L     | 365    |  |
| 1   | M     | 365    |  |
| 1   | O     | 365    |  |
| 1   | P     | 365    |  |
| 1   | Q     | 365    |  |
| 1   | R     | 365    |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | SO4  | B     | 364 | -         | -        | X       | -                |
| 2   | SO4  | D     | 364 | -         | -        | X       | -                |
| 2   | SO4  | H     | 364 | -         | -        | X       | -                |
| 2   | SO4  | I     | 366 | -         | -        | X       | -                |
| 2   | SO4  | M     | 370 | -         | -        | X       | X                |
| 2   | SO4  | O     | 364 | -         | -        | X       | -                |
| 2   | SO4  | O     | 371 | -         | -        | X       | X                |
| 2   | SO4  | P     | 364 | -         | -        | X       | -                |
| 2   | SO4  | R     | 376 | -         | -        | X       | -                |
| 3   | NDP  | A     | 376 | X         | -        | -       | -                |
| 3   | NDP  | B     | 378 | X         | -        | -       | -                |
| 3   | NDP  | C     | 365 | X         | -        | -       | -                |
| 3   | NDP  | D     | 365 | X         | -        | -       | -                |
| 3   | NDP  | H     | 379 | X         | -        | -       | -                |
| 3   | NDP  | I     | 380 | X         | -        | -       | -                |
| 3   | NDP  | L     | 369 | X         | -        | -       | -                |
| 3   | NDP  | M     | 381 | X         | -        | -       | -                |
| 3   | NDP  | O     | 372 | X         | -        | -       | -                |
| 3   | NDP  | P     | 373 | X         | -        | -       | -                |
| 3   | NDP  | Q     | 375 | X         | -        | -       | -                |
| 3   | NDP  | R     | 377 | X         | -        | -       | -                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31248 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase Aor.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | O     | 337      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2542  | 1599 | 445 | 487 | 11 |         |         |       |
| 1   | R     | 337      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2542  | 1599 | 445 | 487 | 11 |         |         |       |
| 1   | P     | 337      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2542  | 1599 | 445 | 487 | 11 |         |         |       |
| 1   | Q     | 337      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2542  | 1599 | 445 | 487 | 11 |         |         |       |
| 1   | A     | 337      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2542  | 1599 | 445 | 487 | 11 |         |         |       |
| 1   | B     | 337      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2542  | 1599 | 445 | 487 | 11 |         |         |       |
| 1   | C     | 337      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2542  | 1599 | 445 | 487 | 11 |         |         |       |
| 1   | D     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2538  | 1597 | 444 | 486 | 11 |         |         |       |
| 1   | H     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2538  | 1597 | 444 | 486 | 11 |         |         |       |
| 1   | I     | 337      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2542  | 1599 | 445 | 487 | 11 |         |         |       |
| 1   | L     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2538  | 1597 | 444 | 486 | 11 |         |         |       |
| 1   | M     | 337      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2542  | 1599 | 445 | 487 | 11 |         |         |       |

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



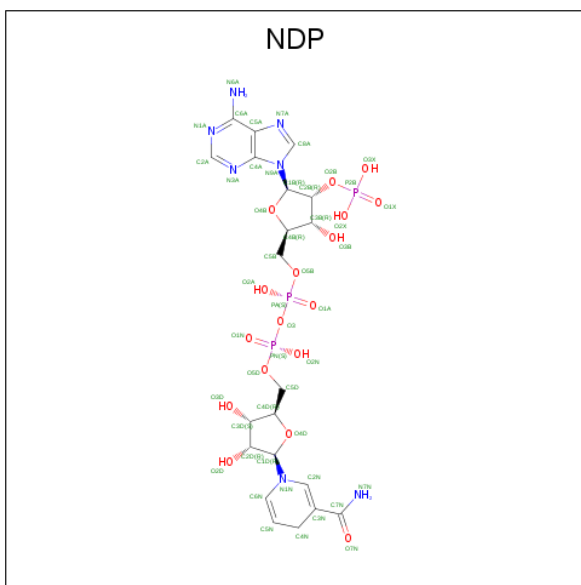
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | O     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | O     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | O     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | R     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | R     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | R     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | P     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | P     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | P     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | Q     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | Q     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | Q     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | Q     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | I     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | I     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | I     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | L     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | L     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms       |         |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 3   | O     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 3   | R     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 3   | P     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 3   | Q     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 3   | A     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 3   | B     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 3   | C     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 3   | D     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 3   | H     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 3   | I     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 3   | L     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 3   | M     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |

- Molecule 4 is water.

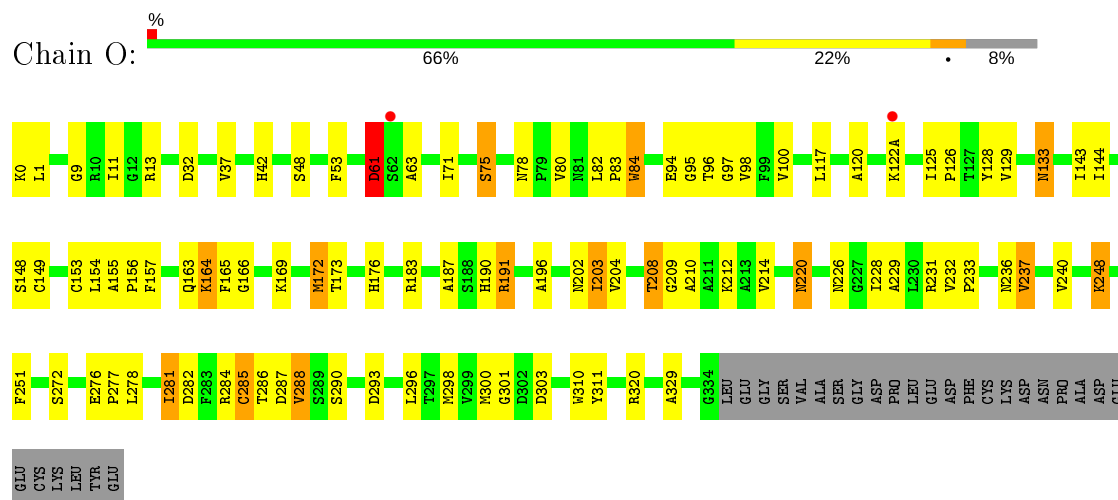
| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 4   | O     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 4   | H     | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 4   | I     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 4   | L     | 4        | Total<br>4 | O<br>4 | 0       | 0       |
| 4   | M     | 2        | Total<br>2 | O<br>2 | 0       | 0       |



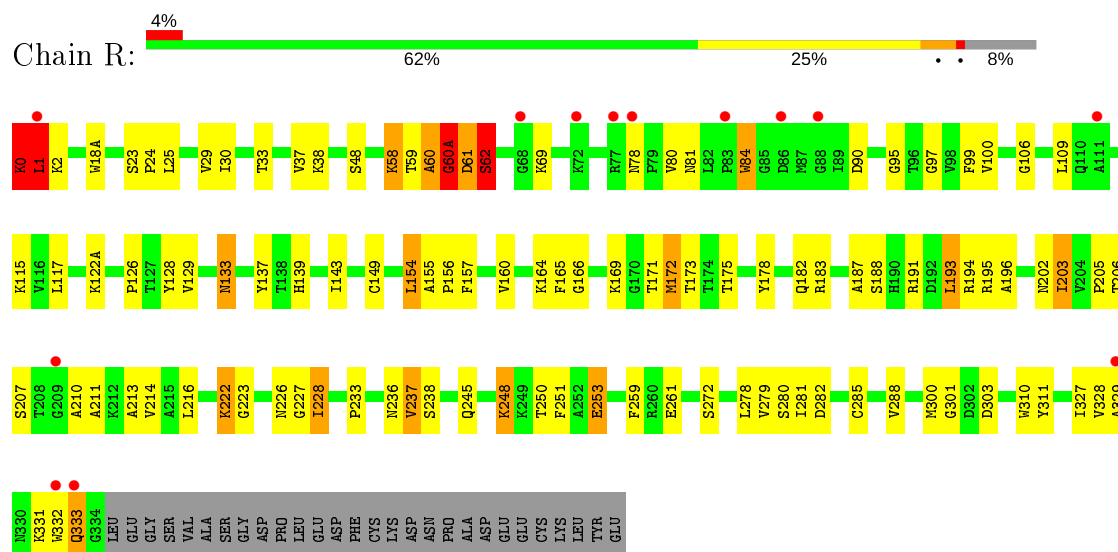
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Glyceraldehyde-3-phosphate dehydrogenase Aor

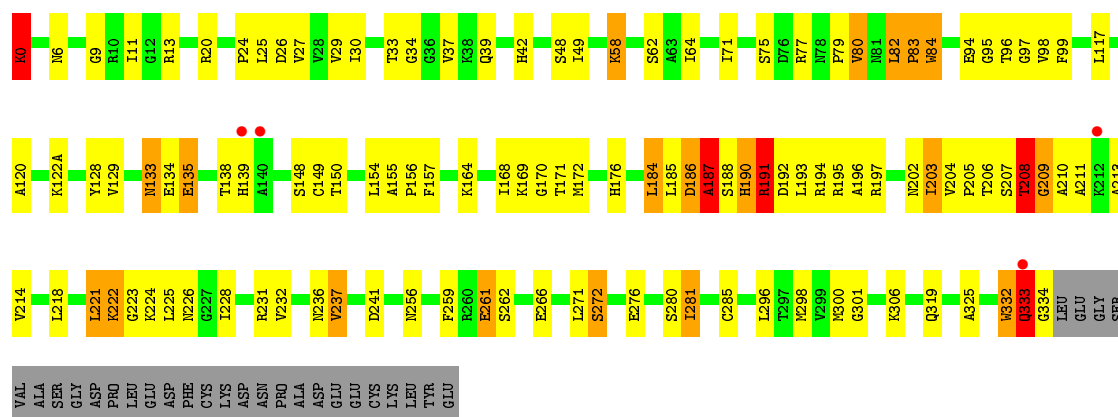


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor



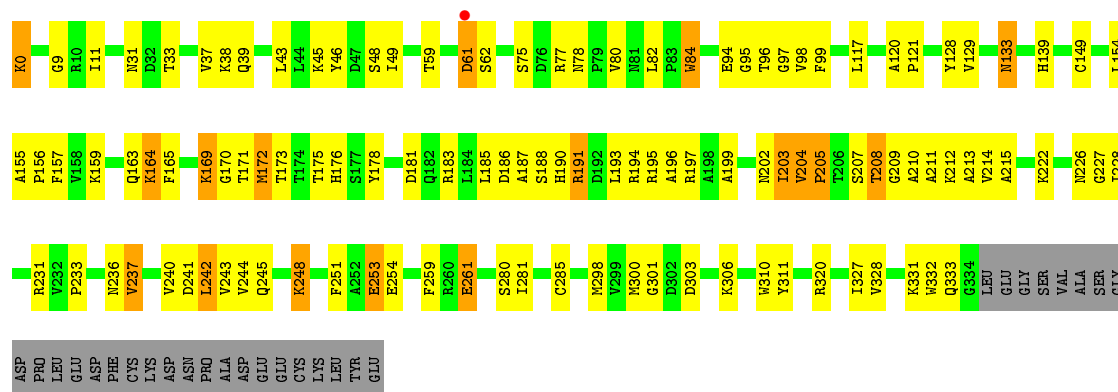
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor





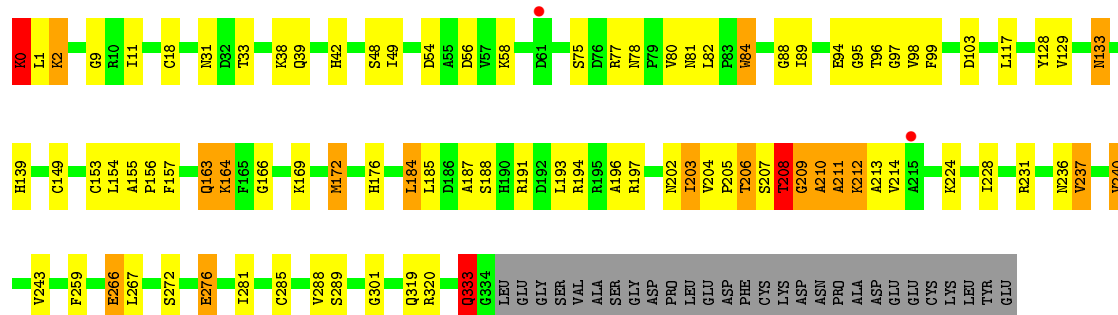
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor

Chain Q: 61% 27% 5% 8%



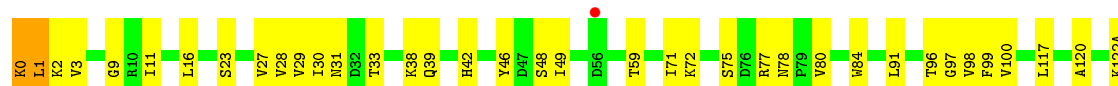
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor

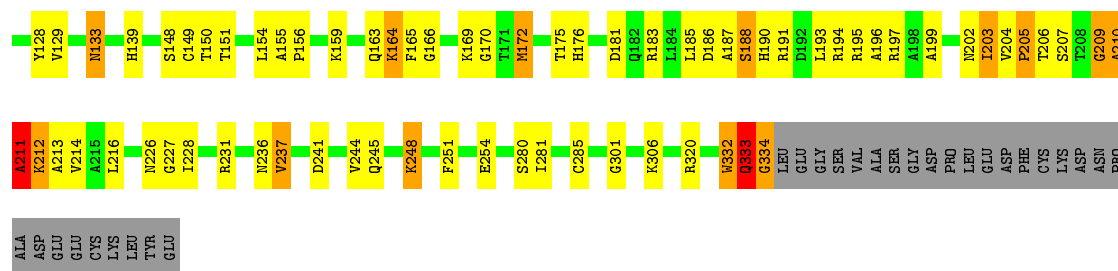
Chain A: 67% 19% 5% 8%



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor

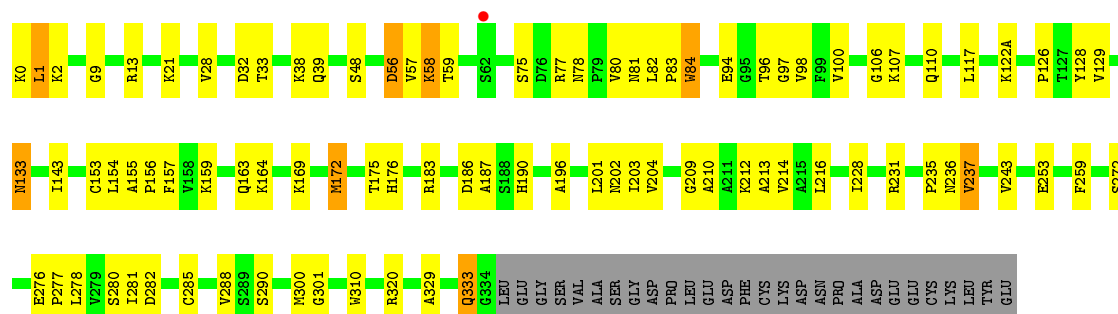
Chain B: 63% 24% 8%





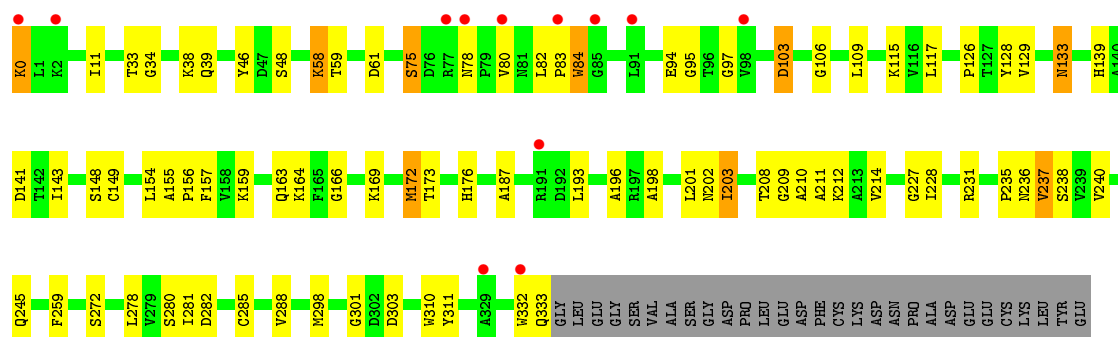
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor

Chain C: 68% 22% 8%



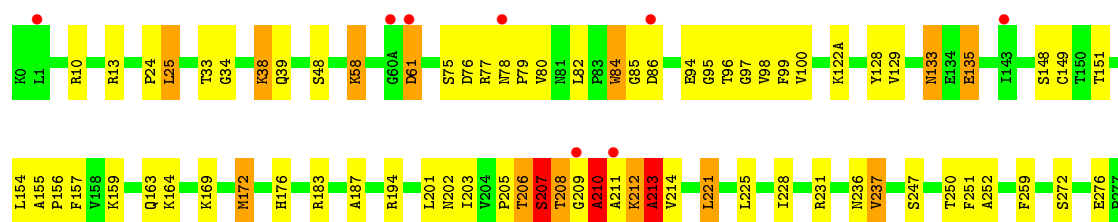
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor

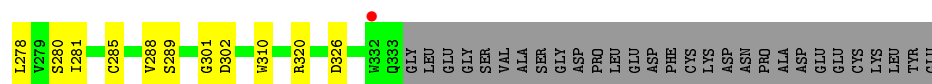
Chain D: 3% 69% 20% 8%



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor

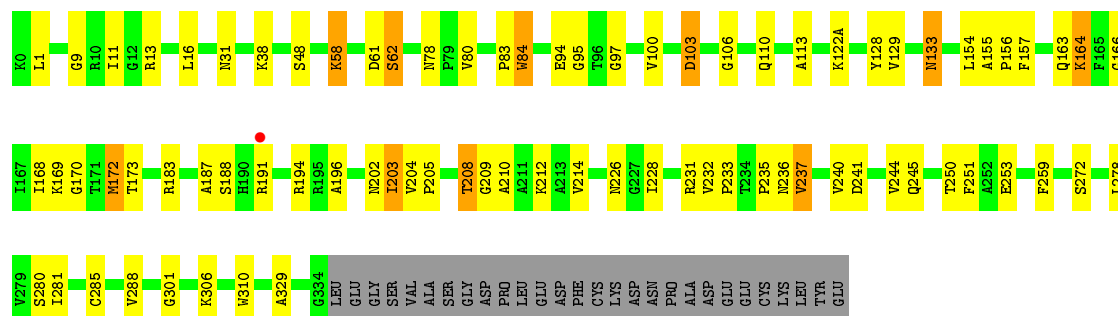
Chain H: 2% 68% 19% 8%





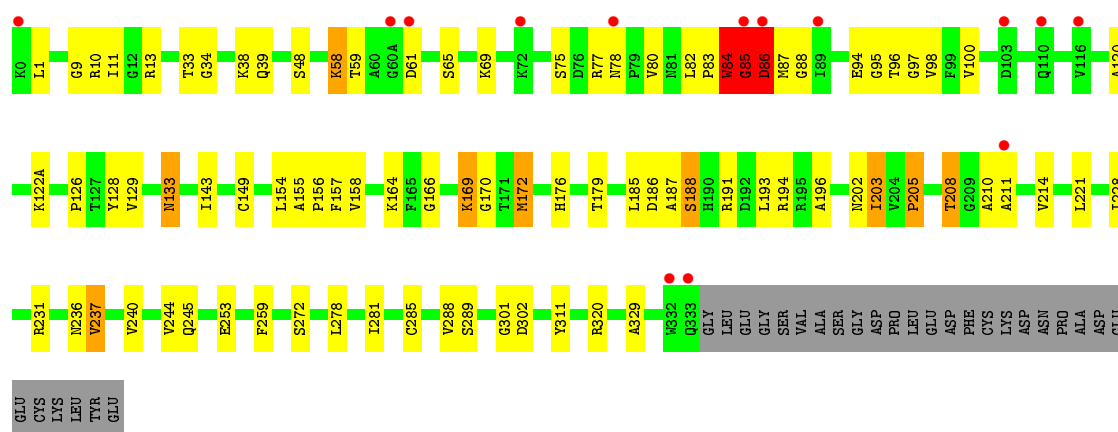
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor

Chain I: 70% 19% 8%



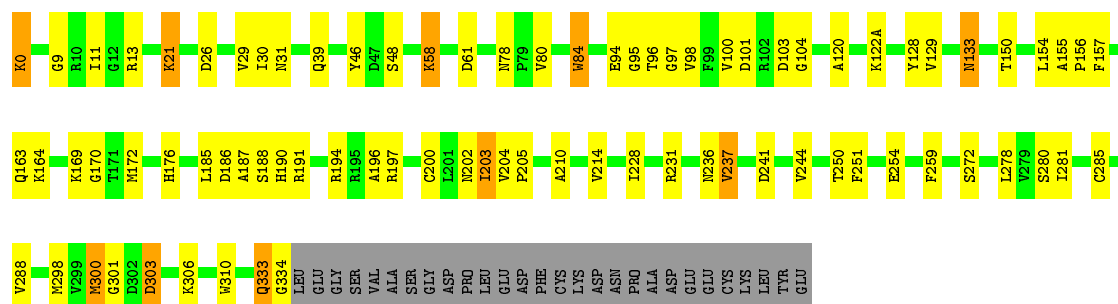
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor

Chain L: 4% 68% 21% 8%



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase Aor

Chain M: 70% 20% 8%



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 105.38Å 217.71Å 114.79Å<br>90.00° 90.04° 90.00°             | Depositor        |
| Resolution (Å)  | 63.22 – 2.40<br>73.14 – 2.40                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 76.5 (63.22-2.40)<br>76.5 (73.14-2.40)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.05  | Depositor        |
| $R_{sym}$   | 0.05  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.70 (at 2.40Å)   | Xtriage          |
| Refinement program  | CNS 1.0   | Depositor        |
| R, $R_{free}$   | 0.249 , 0.258<br>0.241 , 0.250                              | Depositor<br>DCC |
| $R_{free}$ test set   | 7785 reflections (5.06%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 22.0  | Xtriage          |
| Anisotropy  | 0.168   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , -6.3   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction   | 0.478 for h,-k,-l   | Xtriage          |
| $F_o, F_c$ correlation  | 0.90  | EDS              |
| Total number of atoms   | 31248   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 25.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.7836e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: NDP, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$     | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.65         | 3/2583 (0.1%)   | 0.96        | 9/3507 (0.3%)   |
| 1   | B     | 0.74         | 4/2583 (0.2%)   | 0.95        | 11/3507 (0.3%)  |
| 1   | C     | 0.60         | 0/2583          | 0.86        | 4/3507 (0.1%)   |
| 1   | D     | 0.59         | 0/2579          | 0.82        | 3/3502 (0.1%)   |
| 1   | H     | 0.66         | 3/2579 (0.1%)   | 0.97        | 12/3502 (0.3%)  |
| 1   | I     | 0.57         | 0/2583          | 0.81        | 1/3507 (0.0%)   |
| 1   | L     | 0.61         | 1/2579 (0.0%)   | 0.92        | 13/3502 (0.4%)  |
| 1   | M     | 0.57         | 1/2583 (0.0%)   | 0.82        | 3/3507 (0.1%)   |
| 1   | O     | 0.61         | 0/2583          | 0.88        | 4/3507 (0.1%)   |
| 1   | P     | 0.66         | 1/2583 (0.0%)   | 1.04        | 16/3507 (0.5%)  |
| 1   | Q     | 0.59         | 1/2583 (0.0%)   | 0.90        | 8/3507 (0.2%)   |
| 1   | R     | 0.64         | 2/2583 (0.1%)   | 0.99        | 12/3507 (0.3%)  |
| All | All   | 0.63         | 16/30984 (0.1%) | 0.91        | 96/42069 (0.2%) |

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   | A     | 1                   | 7                   |
| 1   | B     | 0                   | 3                   |
| 1   | C     | 0                   | 1                   |
| 1   | H     | 1                   | 5                   |
| 1   | I     | 0                   | 1                   |
| 1   | L     | 0                   | 2                   |
| 1   | M     | 0                   | 2                   |
| 1   | O     | 0                   | 2                   |
| 1   | P     | 1                   | 7                   |
| 1   | Q     | 0                   | 6                   |
| 1   | R     | 0                   | 8                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| All | All   | 3                   | 44                  |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | B     | 210 | ALA  | C-N   | 14.89  | 1.68        | 1.34     |
| 1   | B     | 333 | GLN  | C-N   | -11.20 | 1.12        | 1.33     |
| 1   | A     | 0   | LYS  | C-O   | 10.76  | 1.43        | 1.23     |
| 1   | B     | 205 | PRO  | C-N   | 9.79   | 1.56        | 1.34     |
| 1   | L     | 205 | PRO  | C-N   | -7.87  | 1.16        | 1.34     |
| 1   | H     | 210 | ALA  | C-N   | 7.45   | 1.51        | 1.34     |
| 1   | A     | 206 | THR  | C-N   | -6.90  | 1.18        | 1.34     |
| 1   | P     | 82  | LEU  | C-N   | 6.82   | 1.47        | 1.34     |
| 1   | R     | 62  | SER  | C-N   | 6.75   | 1.49        | 1.34     |
| 1   | R     | 0   | LYS  | N-CA  | 6.60   | 1.59        | 1.46     |
| 1   | M     | 334 | GLY  | N-CA  | -6.25  | 1.36        | 1.46     |
| 1   | H     | 205 | PRO  | C-N   | -5.31  | 1.21        | 1.34     |
| 1   | B     | 334 | GLY  | C-O   | 5.21   | 1.31        | 1.23     |
| 1   | A     | 0   | LYS  | C-N   | -5.19  | 1.22        | 1.34     |
| 1   | Q     | 0   | LYS  | C-N   | 5.17   | 1.46        | 1.34     |
| 1   | H     | 61  | ASP  | CB-CG | 5.02   | 1.62        | 1.51     |

All (96) bond angle outliers are listed below:

| Mol | Chain | Res   | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|--------|-------------|----------|
| 1   | R     | 62    | SER  | O-C-N     | -19.79 | 91.04       | 122.70   |
| 1   | A     | 0     | LYS  | CA-C-O    | -14.38 | 89.89       | 120.10   |
| 1   | C     | 333   | GLN  | C-N-CA    | 13.54  | 150.73      | 122.30   |
| 1   | H     | 206   | THR  | C-N-CA    | 12.83  | 153.76      | 121.70   |
| 1   | A     | 206   | THR  | C-N-CA    | 11.39  | 150.18      | 121.70   |
| 1   | Q     | 0     | LYS  | O-C-N     | -11.07 | 104.98      | 122.70   |
| 1   | L     | 208   | THR  | C-N-CA    | 10.75  | 144.88      | 122.30   |
| 1   | B     | 333   | GLN  | C-N-CA    | 10.72  | 144.82      | 122.30   |
| 1   | A     | 0     | LYS  | CA-C-N    | 10.69  | 140.72      | 117.20   |
| 1   | P     | 0     | LYS  | O-C-N     | 10.61  | 139.68      | 122.70   |
| 1   | Q     | 204   | VAL  | C-N-CD    | 10.56  | 150.57      | 128.40   |
| 1   | R     | 60(A) | GLY  | C-N-CA    | 10.27  | 147.38      | 121.70   |
| 1   | B     | 211   | ALA  | C-N-CA    | 9.87   | 146.37      | 121.70   |
| 1   | B     | 334   | GLY  | CA-C-O    | -9.50  | 103.50      | 120.60   |
| 1   | M     | 303   | ASP  | CB-CG-OD1 | 9.30   | 126.67      | 118.30   |
| 1   | H     | 61    | ASP  | CB-CG-OD1 | 9.26   | 126.64      | 118.30   |
| 1   | H     | 210   | ALA  | O-C-N     | -8.64  | 108.88      | 122.70   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | P     | 206 | THR  | C-N-CA    | 8.62  | 143.25      | 121.70   |
| 1   | P     | 0   | LYS  | CA-C-N    | -8.56 | 98.36       | 117.20   |
| 1   | L     | 61  | ASP  | CB-CG-OD1 | 8.44  | 125.90      | 118.30   |
| 1   | P     | 83  | PRO  | O-C-N     | -8.40 | 109.26      | 122.70   |
| 1   | H     | 61  | ASP  | CB-CA-C   | -8.36 | 93.69       | 110.40   |
| 1   | D     | 0   | LYS  | O-C-N     | -8.21 | 109.57      | 122.70   |
| 1   | P     | 186 | ASP  | CB-CG-OD1 | 8.18  | 125.66      | 118.30   |
| 1   | L     | 61  | ASP  | CB-CA-C   | -8.06 | 94.28       | 110.40   |
| 1   | L     | 86  | ASP  | CB-CG-OD1 | 8.05  | 125.55      | 118.30   |
| 1   | B     | 210 | ALA  | O-C-N     | 8.02  | 135.53      | 122.70   |
| 1   | B     | 206 | THR  | C-N-CA    | 8.01  | 141.73      | 121.70   |
| 1   | Q     | 205 | PRO  | CA-N-CD   | -7.99 | 100.31      | 111.50   |
| 1   | H     | 38  | LYS  | C-N-CA    | 7.80  | 141.21      | 121.70   |
| 1   | R     | 1   | LEU  | CA-C-N    | -7.73 | 100.19      | 117.20   |
| 1   | Q     | 0   | LYS  | C-N-CA    | 7.68  | 140.89      | 121.70   |
| 1   | H     | 205 | PRO  | C-N-CA    | 7.37  | 140.12      | 121.70   |
| 1   | A     | 209 | GLY  | O-C-N     | -7.35 | 110.94      | 122.70   |
| 1   | H     | 86  | ASP  | CB-CG-OD1 | 7.14  | 124.73      | 118.30   |
| 1   | P     | 192 | ASP  | CB-CG-OD1 | 7.10  | 124.69      | 118.30   |
| 1   | H     | 213 | ALA  | O-C-N     | -6.71 | 111.97      | 122.70   |
| 1   | B     | 203 | ILE  | N-CA-C    | -6.69 | 92.95       | 111.00   |
| 1   | P     | 191 | ARG  | O-C-N     | 6.65  | 133.33      | 122.70   |
| 1   | Q     | 203 | ILE  | N-CA-C    | -6.58 | 93.22       | 111.00   |
| 1   | L     | 88  | GLY  | O-C-N     | 6.57  | 133.21      | 122.70   |
| 1   | L     | 84  | TRP  | CA-C-O    | 6.40  | 133.53      | 120.10   |
| 1   | D     | 203 | ILE  | N-CA-C    | -6.34 | 93.89       | 111.00   |
| 1   | P     | 333 | GLN  | C-N-CA    | 6.29  | 135.51      | 122.30   |
| 1   | L     | 88  | GLY  | CA-C-N    | -6.28 | 103.39      | 117.20   |
| 1   | C     | 203 | ILE  | N-CA-C    | -6.26 | 94.10       | 111.00   |
| 1   | L     | 85  | GLY  | CA-C-N    | -6.26 | 103.43      | 117.20   |
| 1   | R     | 203 | ILE  | N-CA-C    | -6.23 | 94.19       | 111.00   |
| 1   | B     | 209 | GLY  | O-C-N     | -6.22 | 112.74      | 122.70   |
| 1   | A     | 203 | ILE  | N-CA-C    | -6.21 | 94.23       | 111.00   |
| 1   | Q     | 208 | THR  | CA-C-N    | -6.21 | 103.78      | 116.20   |
| 1   | P     | 332 | TRP  | C-N-CA    | 6.17  | 137.13      | 121.70   |
| 1   | O     | 287 | ASP  | CB-CG-OD1 | 6.16  | 123.85      | 118.30   |
| 1   | L     | 203 | ILE  | N-CA-C    | -6.10 | 94.53       | 111.00   |
| 1   | M     | 333 | GLN  | C-N-CA    | 6.01  | 134.92      | 122.30   |
| 1   | Q     | 0   | LYS  | CA-C-N    | 5.95  | 130.30      | 117.20   |
| 1   | I     | 203 | ILE  | N-CA-C    | -5.89 | 95.11       | 111.00   |
| 1   | O     | 288 | VAL  | O-C-N     | -5.85 | 113.34      | 122.70   |
| 1   | P     | 208 | THR  | C-N-CA    | 5.79  | 134.47      | 122.30   |

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| Mol | Chain | Res    | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1   | A     | 333    | GLN  | C-N-CA    | 5.77  | 134.42      | 122.30   |
| 1   | P     | 26     | ASP  | CB-CG-OD1 | 5.76  | 123.49      | 118.30   |
| 1   | R     | 0      | LYS  | C-N-CA    | 5.74  | 136.04      | 121.70   |
| 1   | R     | 207    | SER  | CA-C-N    | -5.70 | 104.67      | 117.20   |
| 1   | P     | 26     | ASP  | O-C-N     | -5.68 | 113.61      | 122.70   |
| 1   | Q     | 175    | THR  | N-CA-C    | -5.65 | 95.74       | 111.00   |
| 1   | R     | 61     | ASP  | CA-C-O    | 5.64  | 131.95      | 120.10   |
| 1   | P     | 6      | ASN  | O-C-N     | -5.64 | 113.61      | 123.20   |
| 1   | O     | 203    | ILE  | N-CA-C    | -5.62 | 95.83       | 111.00   |
| 1   | A     | 208    | THR  | N-CA-CB   | 5.62  | 120.97      | 110.30   |
| 1   | H     | 203    | ILE  | N-CA-C    | -5.61 | 95.85       | 111.00   |
| 1   | H     | 61     | ASP  | N-CA-CB   | 5.61  | 120.70      | 110.60   |
| 1   | H     | 38     | LYS  | CA-C-N    | -5.61 | 104.86      | 117.20   |
| 1   | R     | 60     | ALA  | CB-CA-C   | 5.56  | 118.44      | 110.10   |
| 1   | P     | 80     | VAL  | O-C-N     | -5.54 | 113.83      | 122.70   |
| 1   | P     | 122(A) | LYS  | C-N-CA    | -5.45 | 110.85      | 122.30   |
| 1   | B     | 175    | THR  | N-CA-C    | -5.38 | 96.47       | 111.00   |
| 1   | C     | 1      | LEU  | O-C-N     | -5.37 | 114.11      | 122.70   |
| 1   | P     | 187    | ALA  | CA-C-N    | -5.33 | 105.48      | 117.20   |
| 1   | L     | 84     | TRP  | C-N-CA    | -5.33 | 111.11      | 122.30   |
| 1   | B     | 210    | ALA  | C-N-CA    | -5.31 | 108.43      | 121.70   |
| 1   | L     | 245    | GLN  | N-CA-C    | -5.29 | 96.72       | 111.00   |
| 1   | R     | 60(A)  | GLY  | CA-C-O    | -5.28 | 111.10      | 120.60   |
| 1   | H     | 212    | LYS  | N-CA-CB   | 5.28  | 120.10      | 110.60   |
| 1   | M     | 203    | ILE  | N-CA-C    | -5.24 | 96.87       | 111.00   |
| 1   | R     | 175    | THR  | N-CA-C    | -5.19 | 96.99       | 111.00   |
| 1   | A     | 333    | GLN  | N-CA-CB   | 5.12  | 119.81      | 110.60   |
| 1   | R     | 61     | ASP  | N-CA-CB   | 5.11  | 119.79      | 110.60   |
| 1   | B     | 332    | TRP  | C-N-CA    | 5.11  | 134.47      | 121.70   |
| 1   | A     | 206    | THR  | O-C-N     | 5.09  | 130.84      | 122.70   |
| 1   | B     | 210    | ALA  | CA-C-N    | -5.08 | 106.02      | 117.20   |
| 1   | L     | 84     | TRP  | CA-C-N    | -5.08 | 106.05      | 116.20   |
| 1   | C     | 175    | THR  | N-CA-C    | -5.07 | 97.31       | 111.00   |
| 1   | R     | 61     | ASP  | C-N-CA    | -5.06 | 109.04      | 121.70   |
| 1   | O     | 61     | ASP  | CB-CG-OD2 | 5.04  | 122.84      | 118.30   |
| 1   | D     | 0      | LYS  | CA-C-N    | 5.04  | 128.29      | 117.20   |
| 1   | L     | 61     | ASP  | N-CA-CB   | 5.02  | 119.63      | 110.60   |

All (3) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | P     | 208 | THR  | CA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | A     | 208 | THR  | CA   |
| 1   | H     | 212 | LYS  | CA   |

All (44) planarity outliers are listed below:

| Mol | Chain | Res   | Type | Group             |
|-----|-------|-------|------|-------------------|
| 1   | A     | 0     | LYS  | Mainchain,Peptide |
| 1   | A     | 206   | THR  | Peptide           |
| 1   | A     | 208   | THR  | Peptide           |
| 1   | A     | 210   | ALA  | Mainchain         |
| 1   | A     | 211   | ALA  | Mainchain         |
| 1   | A     | 212   | LYS  | Mainchain         |
| 1   | B     | 211   | ALA  | Peptide           |
| 1   | B     | 333   | GLN  | Mainchain,Peptide |
| 1   | C     | 333   | GLN  | Peptide           |
| 1   | H     | 207   | SER  | Peptide           |
| 1   | H     | 210   | ALA  | Mainchain         |
| 1   | H     | 213   | ALA  | Mainchain         |
| 1   | H     | 38    | LYS  | Mainchain         |
| 1   | H     | 85    | GLY  | Mainchain         |
| 1   | I     | 62    | SER  | Mainchain         |
| 1   | L     | 208   | THR  | Mainchain         |
| 1   | L     | 85    | GLY  | Mainchain         |
| 1   | M     | 300   | MET  | Mainchain         |
| 1   | M     | 333   | GLN  | Mainchain         |
| 1   | O     | 285   | CYS  | Mainchain         |
| 1   | O     | 61    | ASP  | Mainchain         |
| 1   | P     | 187   | ALA  | Mainchain         |
| 1   | P     | 203   | ILE  | Mainchain         |
| 1   | P     | 207   | SER  | Mainchain         |
| 1   | P     | 208   | THR  | Mainchain,Peptide |
| 1   | P     | 80    | VAL  | Mainchain         |
| 1   | P     | 83    | PRO  | Mainchain         |
| 1   | Q     | 0     | LYS  | Mainchain         |
| 1   | Q     | 204   | VAL  | Mainchain         |
| 1   | Q     | 207   | SER  | Mainchain,Peptide |
| 1   | Q     | 208   | THR  | Mainchain         |
| 1   | Q     | 213   | ALA  | Mainchain         |
| 1   | R     | 0     | LYS  | Mainchain,Peptide |
| 1   | R     | 206   | THR  | Mainchain         |
| 1   | R     | 333   | GLN  | Mainchain,Peptide |
| 1   | R     | 60(A) | GLY  | Mainchain,Peptide |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | R     | 62  | SER  | Mainchain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2542  | 0        | 2573     | 123     | 0            |
| 1   | B     | 2542  | 0        | 2573     | 132     | 0            |
| 1   | C     | 2542  | 0        | 2576     | 117     | 0            |
| 1   | D     | 2538  | 0        | 2574     | 86      | 0            |
| 1   | H     | 2538  | 0        | 2571     | 96      | 0            |
| 1   | I     | 2542  | 0        | 2577     | 112     | 0            |
| 1   | L     | 2538  | 0        | 2572     | 82      | 1            |
| 1   | M     | 2542  | 0        | 2577     | 94      | 0            |
| 1   | O     | 2542  | 0        | 2577     | 154     | 0            |
| 1   | P     | 2542  | 0        | 2575     | 151     | 0            |
| 1   | Q     | 2542  | 0        | 2577     | 167     | 1            |
| 1   | R     | 2542  | 0        | 2575     | 154     | 0            |
| 2   | A     | 15    | 0        | 0        | 0       | 0            |
| 2   | B     | 15    | 0        | 0        | 2       | 0            |
| 2   | C     | 10    | 0        | 0        | 0       | 0            |
| 2   | D     | 10    | 0        | 0        | 2       | 0            |
| 2   | H     | 15    | 0        | 0        | 4       | 0            |
| 2   | I     | 15    | 0        | 0        | 6       | 0            |
| 2   | L     | 10    | 0        | 0        | 1       | 0            |
| 2   | M     | 15    | 0        | 0        | 3       | 0            |
| 2   | O     | 15    | 0        | 0        | 4       | 0            |
| 2   | P     | 15    | 0        | 0        | 6       | 0            |
| 2   | Q     | 20    | 0        | 0        | 1       | 0            |
| 2   | R     | 15    | 0        | 0        | 3       | 0            |
| 3   | A     | 48    | 0        | 20       | 19      | 0            |
| 3   | B     | 48    | 0        | 21       | 13      | 0            |
| 3   | C     | 48    | 0        | 20       | 16      | 0            |
| 3   | D     | 48    | 0        | 19       | 6       | 0            |
| 3   | H     | 48    | 0        | 20       | 14      | 0            |
| 3   | I     | 48    | 0        | 20       | 10      | 0            |
| 3   | L     | 48    | 0        | 20       | 14      | 0            |
| 3   | M     | 48    | 0        | 20       | 10      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | O     | 48    | 0        | 21       | 15      | 0            |
| 3   | P     | 48    | 0        | 21       | 11      | 0            |
| 3   | Q     | 48    | 0        | 21       | 16      | 0            |
| 3   | R     | 48    | 0        | 20       | 5       | 0            |
| 4   | H     | 2     | 0        | 0        | 0       | 0            |
| 4   | I     | 1     | 0        | 0        | 0       | 0            |
| 4   | L     | 4     | 0        | 0        | 0       | 0            |
| 4   | M     | 2     | 0        | 0        | 1       | 0            |
| 4   | O     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 31248 | 0        | 31140    | 1242    | 1            |

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 20.

All (1242) 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) |
|------------------|-----------------|--------------------------|-------------------|
| 3:D:365:NDP:C3D  | 3:D:365:NDP:C2D | 1.76                     | 1.64              |
| 3:M:381:NDP:C1D  | 3:M:381:NDP:C2D | 1.76                     | 1.62              |
| 3:I:380:NDP:C1D  | 3:I:380:NDP:C2D | 1.77                     | 1.61              |
| 3:C:365:NDP:C2D  | 3:C:365:NDP:C1D | 1.79                     | 1.59              |
| 3:B:378:NDP:C1D  | 3:B:378:NDP:C2D | 1.78                     | 1.55              |
| 3:P:373:NDP:C1D  | 3:P:373:NDP:C2D | 1.80                     | 1.52              |
| 3:Q:375:NDP:C1D  | 3:Q:375:NDP:C2D | 1.82                     | 1.52              |
| 3:L:369:NDP:C2D  | 3:L:369:NDP:C1D | 1.85                     | 1.50              |
| 3:C:365:NDP:O4B  | 3:C:365:NDP:C4B | 1.64                     | 1.46              |
| 3:A:376:NDP:C4B  | 3:A:376:NDP:O4B | 1.63                     | 1.45              |
| 3:B:378:NDP:C4B  | 3:B:378:NDP:O4B | 1.65                     | 1.44              |
| 3:O:372:NDP:O4B  | 3:O:372:NDP:C4B | 1.65                     | 1.44              |
| 3:P:373:NDP:C4B  | 3:P:373:NDP:O4B | 1.64                     | 1.44              |
| 3:R:377:NDP:O4B  | 3:R:377:NDP:C4B | 1.65                     | 1.44              |
| 1:O:163:GLN:NE2  | 1:O:164:LYS:HZ2 | 1.14                     | 1.43              |
| 1:B:210:ALA:C    | 1:B:211:ALA:N   | 1.68                     | 1.43              |
| 3:O:372:NDP:C1D  | 3:O:372:NDP:C2D | 1.96                     | 1.43              |
| 3:Q:375:NDP:C4B  | 3:Q:375:NDP:O4B | 1.64                     | 1.43              |
| 3:D:365:NDP:O4B  | 3:D:365:NDP:C4B | 1.65                     | 1.43              |
| 1:Q:154:LEU:HD11 | 1:Q:242:LEU:CD2 | 1.47                     | 1.43              |
| 3:I:380:NDP:C4B  | 3:I:380:NDP:O4B | 1.64                     | 1.42              |
| 1:R:165:PHE:HA   | 1:R:248:LYS:CD  | 1.47                     | 1.42              |
| 3:A:376:NDP:C1D  | 3:A:376:NDP:O4D | 1.67                     | 1.41              |
| 3:M:381:NDP:C4B  | 3:M:381:NDP:O4B | 1.65                     | 1.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:163:GLN:NE2  | 1:A:164:LYS:NZ   | 1.64                     | 1.39              |
| 1:Q:191:ARG:H    | 1:Q:191:ARG:CD   | 1.10                     | 1.37              |
| 3:L:369:NDP:O4B  | 3:L:369:NDP:C4B  | 1.64                     | 1.36              |
| 1:Q:154:LEU:CD1  | 1:Q:242:LEU:HD23 | 1.53                     | 1.36              |
| 3:H:379:NDP:C4B  | 3:H:379:NDP:O4B  | 1.65                     | 1.35              |
| 3:A:376:NDP:C1D  | 3:A:376:NDP:C2D  | 2.04                     | 1.34              |
| 1:B:165:PHE:HA   | 1:B:248:LYS:CD   | 1.57                     | 1.33              |
| 1:O:163:GLN:HE22 | 1:O:164:LYS:NZ   | 1.25                     | 1.30              |
| 1:I:163:GLN:NE2  | 1:I:164:LYS:HZ2  | 1.30                     | 1.27              |
| 1:O:163:GLN:NE2  | 1:O:164:LYS:NZ   | 1.78                     | 1.27              |
| 1:R:60:ALA:O     | 1:R:60(A):GLY:O  | 1.55                     | 1.22              |
| 1:O:251:PHE:HB2  | 2:O:371:SO4:O2   | 1.42                     | 1.19              |
| 1:O:165:PHE:HD1  | 1:O:248:LYS:HD3  | 1.06                     | 1.18              |
| 1:Q:191:ARG:N    | 1:Q:191:ARG:HD2  | 1.18                     | 1.18              |
| 1:H:210:ALA:O    | 1:H:214:VAL:HG23 | 1.46                     | 1.14              |
| 1:I:163:GLN:HE21 | 1:I:164:LYS:NZ   | 1.45                     | 1.12              |
| 1:O:163:GLN:HE21 | 1:O:164:LYS:HD3  | 1.04                     | 1.11              |
| 1:O:293:ASP:HB3  | 1:O:296:LEU:HD12 | 1.23                     | 1.10              |
| 1:O:163:GLN:HE21 | 1:O:164:LYS:CD   | 1.65                     | 1.10              |
| 1:M:21:LYS:H     | 1:M:21:LYS:HD3   | 1.14                     | 1.08              |
| 1:C:183:ARG:HD2  | 1:C:187:ALA:HB3  | 1.14                     | 1.08              |
| 1:C:159:LYS:O    | 1:C:163:GLN:HG3  | 1.50                     | 1.08              |
| 1:A:202:ASN:HD21 | 1:C:281:ILE:HB   | 1.11                     | 1.07              |
| 1:B:210:ALA:O    | 1:B:211:ALA:O    | 1.71                     | 1.07              |
| 1:I:281:ILE:HB   | 1:M:202:ASN:HD21 | 1.20                     | 1.06              |
| 1:O:281:ILE:HB   | 1:P:202:ASN:HD21 | 1.14                     | 1.06              |
| 1:H:281:ILE:HB   | 1:L:202:ASN:HD21 | 1.21                     | 1.05              |
| 1:O:281:ILE:HB   | 1:P:202:ASN:ND2  | 1.71                     | 1.04              |
| 1:P:27:VAL:HG12  | 1:P:71:ILE:HD11  | 1.07                     | 1.04              |
| 3:A:376:NDP:C4D  | 3:A:376:NDP:C1D  | 2.36                     | 1.04              |
| 1:R:58:LYS:HB3   | 1:R:58:LYS:NZ    | 1.66                     | 1.03              |
| 1:I:163:GLN:NE2  | 1:I:164:LYS:NZ   | 2.01                     | 1.03              |
| 1:P:135:GLU:OE1  | 1:P:135:GLU:N    | 1.90                     | 1.03              |
| 1:B:165:PHE:CA   | 1:B:248:LYS:HD3  | 1.87                     | 1.03              |
| 1:C:80:VAL:HB    | 1:C:110:GLN:OE1  | 1.59                     | 1.02              |
| 1:H:202:ASN:HD21 | 1:L:281:ILE:HB   | 1.23                     | 1.02              |
| 1:H:169:LYS:HD2  | 1:L:301:GLY:HA3  | 1.40                     | 1.02              |
| 1:I:202:ASN:HD21 | 1:M:281:ILE:HB   | 1.25                     | 1.02              |
| 1:M:0:LYS:HD3    | 1:M:26:ASP:HB2   | 1.36                     | 1.00              |
| 1:O:228:ILE:HD12 | 1:P:296:LEU:HD22 | 1.42                     | 0.99              |
| 1:R:165:PHE:CA   | 1:R:248:LYS:HD2  | 1.92                     | 0.99              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:165:PHE:HA   | 1:R:248:LYS:HD2  | 1.04                     | 0.99              |
| 1:R:281:ILE:HB   | 1:Q:202:ASN:HD21 | 1.24                     | 0.98              |
| 3:A:376:NDP:N1N  | 3:A:376:NDP:C2D  | 2.25                     | 0.98              |
| 1:O:165:PHE:CD1  | 1:O:248:LYS:HD3  | 1.97                     | 0.98              |
| 3:Q:375:NDP:C2D  | 3:Q:375:NDP:N1N  | 2.26                     | 0.98              |
| 1:B:281:ILE:HB   | 1:D:202:ASN:HD21 | 1.30                     | 0.97              |
| 1:P:134:GLU:HG2  | 1:P:135:GLU:OE1  | 1.63                     | 0.97              |
| 1:P:208:THR:HG22 | 1:P:228:ILE:HA   | 1.43                     | 0.97              |
| 1:A:188:SER:HB2  | 1:B:39:GLN:OE1   | 1.64                     | 0.97              |
| 1:B:202:ASN:HD21 | 1:D:281:ILE:HB   | 1.26                     | 0.96              |
| 1:O:281:ILE:CB   | 1:P:202:ASN:HD21 | 1.79                     | 0.96              |
| 1:O:228:ILE:HG12 | 1:O:229:ALA:H    | 1.29                     | 0.96              |
| 1:P:203:ILE:HG12 | 1:P:232:VAL:HG12 | 1.47                     | 0.96              |
| 3:O:372:NDP:N1N  | 3:O:372:NDP:C2D  | 2.29                     | 0.95              |
| 3:P:373:NDP:N1N  | 3:P:373:NDP:C2D  | 2.28                     | 0.95              |
| 1:H:301:GLY:HA3  | 1:L:169:LYS:HD2  | 1.47                     | 0.95              |
| 1:B:241:ASP:OD1  | 1:B:306:LYS:HE2  | 1.66                     | 0.95              |
| 3:L:369:NDP:C2D  | 3:L:369:NDP:N1N  | 2.30                     | 0.95              |
| 1:R:165:PHE:HA   | 1:R:248:LYS:CG   | 1.97                     | 0.95              |
| 1:B:202:ASN:ND2  | 1:D:281:ILE:H    | 1.65                     | 0.95              |
| 3:B:378:NDP:N1N  | 3:B:378:NDP:C2D  | 2.29                     | 0.95              |
| 1:P:27:VAL:CG1   | 1:P:71:ILE:HD11  | 1.96                     | 0.94              |
| 1:P:271:LEU:HD13 | 1:P:272:SER:N    | 1.82                     | 0.94              |
| 1:R:165:PHE:CA   | 1:R:248:LYS:CD   | 2.44                     | 0.94              |
| 1:L:158:VAL:CG1  | 1:L:221:LEU:HD11 | 1.97                     | 0.94              |
| 1:P:222:LYS:HD3  | 1:P:223:GLY:N    | 1.83                     | 0.94              |
| 1:P:27:VAL:HG12  | 1:P:71:ILE:CD1   | 1.98                     | 0.94              |
| 3:C:365:NDP:C2D  | 3:C:365:NDP:N1N  | 2.30                     | 0.93              |
| 1:M:0:LYS:CD     | 1:M:26:ASP:HB2   | 1.97                     | 0.93              |
| 1:A:202:ASN:HD21 | 1:C:281:ILE:CB   | 1.81                     | 0.93              |
| 1:O:293:ASP:CB   | 1:O:296:LEU:HD12 | 1.98                     | 0.93              |
| 1:R:202:ASN:HD21 | 1:Q:281:ILE:HB   | 1.32                     | 0.93              |
| 1:O:165:PHE:HD1  | 1:O:248:LYS:CD   | 1.82                     | 0.92              |
| 1:A:169:LYS:HD2  | 1:C:301:GLY:HA3  | 1.48                     | 0.92              |
| 1:O:301:GLY:HA3  | 1:P:169:LYS:HD2  | 1.48                     | 0.92              |
| 1:M:0:LYS:NZ     | 1:M:0:LYS:CB     | 2.32                     | 0.92              |
| 1:O:163:GLN:NE2  | 1:O:164:LYS:CD   | 2.31                     | 0.92              |
| 1:B:165:PHE:HA   | 1:B:248:LYS:HD3  | 0.94                     | 0.92              |
| 1:R:281:ILE:H    | 1:Q:202:ASN:HD22 | 1.15                     | 0.92              |
| 1:A:202:ASN:ND2  | 1:C:281:ILE:HB   | 1.85                     | 0.92              |
| 1:O:183:ARG:NH1  | 1:O:187:ALA:HB1  | 1.84                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:165:PHE:HA   | 1:O:248:LYS:HD2  | 1.50                     | 0.91              |
| 1:I:281:ILE:H    | 1:M:202:ASN:ND2  | 1.68                     | 0.91              |
| 1:O:202:ASN:HD21 | 1:P:281:ILE:HB   | 1.34                     | 0.91              |
| 1:O:165:PHE:HA   | 1:O:248:LYS:HG2  | 1.50                     | 0.91              |
| 1:B:139:HIS:CD2  | 1:B:333:GLN:HB2  | 2.05                     | 0.91              |
| 1:C:77:ARG:NH1   | 3:C:365:NDP:C5A  | 2.34                     | 0.91              |
| 1:C:110:GLN:NE2  | 1:I:106:GLY:HA3  | 1.85                     | 0.91              |
| 1:Q:139:HIS:HE1  | 1:Q:332:TRP:CD2  | 1.89                     | 0.91              |
| 1:O:163:GLN:NE2  | 1:O:164:LYS:CE   | 2.34                     | 0.90              |
| 1:B:202:ASN:HD22 | 1:D:281:ILE:H    | 1.14                     | 0.90              |
| 3:M:381:NDP:N1N  | 3:M:381:NDP:C2D  | 2.33                     | 0.90              |
| 1:R:58:LYS:HB3   | 1:R:58:LYS:HZ3   | 1.35                     | 0.90              |
| 3:A:376:NDP:N1N  | 3:A:376:NDP:O2D  | 2.04                     | 0.90              |
| 1:I:202:ASN:ND2  | 1:M:281:ILE:H    | 1.69                     | 0.90              |
| 1:R:139:HIS:O    | 1:R:139:HIS:HD2  | 1.54                     | 0.90              |
| 3:I:380:NDP:N1N  | 3:I:380:NDP:C2D  | 2.33                     | 0.89              |
| 1:R:139:HIS:HB3  | 1:R:333:GLN:OE1  | 1.73                     | 0.89              |
| 1:B:172:MET:HE1  | 1:B:211:ALA:N    | 1.86                     | 0.89              |
| 1:O:183:ARG:NH1  | 1:O:187:ALA:CB   | 2.35                     | 0.89              |
| 1:B:38:LYS:HD3   | 1:B:59:THR:HG21  | 1.55                     | 0.89              |
| 1:O:163:GLN:NE2  | 1:O:164:LYS:HD3  | 1.85                     | 0.89              |
| 1:Q:191:ARG:H    | 1:Q:191:ARG:HD3  | 1.32                     | 0.89              |
| 1:D:61:ASP:HB2   | 1:H:61:ASP:OD1   | 1.73                     | 0.88              |
| 1:P:208:THR:HG22 | 1:P:228:ILE:CA   | 2.03                     | 0.88              |
| 1:R:281:ILE:H    | 1:Q:202:ASN:ND2  | 1.72                     | 0.88              |
| 1:B:169:LYS:HD2  | 1:D:301:GLY:HA3  | 1.55                     | 0.88              |
| 1:H:281:ILE:HB   | 1:L:202:ASN:ND2  | 1.89                     | 0.88              |
| 1:I:281:ILE:CB   | 1:M:202:ASN:HD21 | 1.87                     | 0.88              |
| 1:C:77:ARG:HH11  | 3:C:365:NDP:C5A  | 1.85                     | 0.88              |
| 1:B:281:ILE:HB   | 1:D:202:ASN:ND2  | 1.87                     | 0.88              |
| 1:O:165:PHE:HA   | 1:O:248:LYS:CG   | 2.02                     | 0.88              |
| 1:P:139:HIS:CD2  | 1:P:333:GLN:HG3  | 2.09                     | 0.88              |
| 1:Q:191:ARG:CD   | 1:Q:191:ARG:N    | 1.92                     | 0.87              |
| 1:A:202:ASN:HD22 | 1:C:281:ILE:H    | 1.20                     | 0.87              |
| 1:O:228:ILE:HG12 | 1:O:229:ALA:N    | 1.87                     | 0.87              |
| 1:R:164:LYS:O    | 1:R:248:LYS:CD   | 2.23                     | 0.87              |
| 1:B:202:ASN:HD21 | 1:D:281:ILE:CB   | 1.88                     | 0.87              |
| 1:O:281:ILE:H    | 1:P:202:ASN:ND2  | 1.73                     | 0.87              |
| 1:C:183:ARG:HD2  | 1:C:187:ALA:CB   | 2.03                     | 0.87              |
| 1:B:183:ARG:HE   | 1:B:187:ALA:HB3  | 1.37                     | 0.86              |
| 1:A:202:ASN:ND2  | 1:C:281:ILE:H    | 1.73                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:202:ASN:HD22 | 1:M:281:ILE:H    | 1.18                     | 0.86              |
| 1:I:281:ILE:HB   | 1:M:202:ASN:ND2  | 1.90                     | 0.86              |
| 1:R:281:ILE:HB   | 1:Q:202:ASN:ND2  | 1.91                     | 0.86              |
| 1:I:202:ASN:HD21 | 1:M:281:ILE:CB   | 1.88                     | 0.86              |
| 1:Q:38:LYS:HD3   | 1:Q:59:THR:HG21  | 1.58                     | 0.86              |
| 1:R:281:ILE:CB   | 1:Q:202:ASN:HD21 | 1.88                     | 0.86              |
| 1:R:165:PHE:O    | 1:R:248:LYS:HG2  | 1.75                     | 0.86              |
| 1:O:298:MET:HE1  | 1:P:226:ASN:OD1  | 1.76                     | 0.85              |
| 1:P:209:GLY:HA3  | 2:P:364:SO4:O1   | 1.76                     | 0.85              |
| 1:H:281:ILE:CB   | 1:L:202:ASN:HD21 | 1.89                     | 0.85              |
| 1:H:77:ARG:NH1   | 3:H:379:NDP:C5A  | 2.40                     | 0.85              |
| 1:O:165:PHE:HA   | 1:O:248:LYS:CD   | 2.07                     | 0.85              |
| 1:I:281:ILE:H    | 1:M:202:ASN:HD22 | 1.20                     | 0.84              |
| 1:Q:154:LEU:HD23 | 1:Q:214:VAL:HG21 | 1.59                     | 0.84              |
| 1:Q:139:HIS:CE1  | 1:Q:332:TRP:HA   | 2.12                     | 0.84              |
| 3:Q:375:NDP:O2D  | 3:Q:375:NDP:N1N  | 2.10                     | 0.84              |
| 1:P:134:GLU:CG   | 1:P:135:GLU:OE1  | 2.25                     | 0.84              |
| 1:D:61:ASP:HB2   | 1:H:61:ASP:CG    | 1.98                     | 0.84              |
| 1:A:2:LYS:HB2    | 1:A:2:LYS:NZ     | 1.91                     | 0.84              |
| 1:R:301:GLY:HA3  | 1:Q:169:LYS:HD2  | 1.58                     | 0.84              |
| 1:A:39:GLN:OE1   | 1:B:188:SER:HB2  | 1.78                     | 0.83              |
| 1:C:110:GLN:HE22 | 1:I:106:GLY:HA3  | 1.41                     | 0.83              |
| 1:I:78:ASN:OD1   | 1:I:80:VAL:HG22  | 1.77                     | 0.83              |
| 1:D:33:THR:HA    | 1:D:75:SER:OG    | 1.78                     | 0.83              |
| 1:H:202:ASN:ND2  | 1:L:281:ILE:HB   | 1.94                     | 0.83              |
| 1:O:202:ASN:ND2  | 1:P:281:ILE:HB   | 1.93                     | 0.83              |
| 3:P:373:NDP:O2D  | 3:P:373:NDP:N1N  | 2.10                     | 0.83              |
| 1:B:202:ASN:ND2  | 1:D:281:ILE:HB   | 1.94                     | 0.83              |
| 1:H:148:SER:HB2  | 2:H:364:SO4:O1   | 1.77                     | 0.83              |
| 1:C:77:ARG:HH12  | 3:C:365:NDP:C8A  | 1.91                     | 0.82              |
| 1:I:202:ASN:ND2  | 1:M:281:ILE:HB   | 1.94                     | 0.82              |
| 1:B:210:ALA:C    | 1:B:211:ALA:O    | 2.17                     | 0.82              |
| 1:Q:164:LYS:O    | 1:Q:248:LYS:HD2  | 1.80                     | 0.81              |
| 1:O:251:PHE:CB   | 2:O:371:SO4:O2   | 2.27                     | 0.81              |
| 1:R:202:ASN:ND2  | 1:Q:281:ILE:HB   | 1.94                     | 0.81              |
| 1:H:202:ASN:HD21 | 1:L:281:ILE:CB   | 1.93                     | 0.81              |
| 1:B:164:LYS:O    | 1:B:248:LYS:HD3  | 1.80                     | 0.81              |
| 1:A:281:ILE:HB   | 1:C:202:ASN:HD21 | 1.44                     | 0.81              |
| 1:D:173:THR:HG23 | 1:D:228:ILE:CD1  | 2.10                     | 0.81              |
| 1:M:0:LYS:CB     | 1:M:0:LYS:HZ3    | 1.91                     | 0.80              |
| 1:C:38:LYS:HD3   | 1:C:59:THR:HG21  | 1.63                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:115:LYS:HE3  | 1:R:332:TRP:CZ3  | 2.16                     | 0.80              |
| 1:O:164:LYS:O    | 1:O:248:LYS:HD2  | 1.82                     | 0.80              |
| 1:O:165:PHE:CD1  | 1:O:248:LYS:CD   | 2.61                     | 0.80              |
| 1:L:38:LYS:HD3   | 1:L:59:THR:HG21  | 1.64                     | 0.80              |
| 1:A:163:GLN:NE2  | 1:A:164:LYS:HZ2  | 1.80                     | 0.79              |
| 1:O:293:ASP:HB3  | 1:O:296:LEU:CD1  | 2.10                     | 0.79              |
| 3:B:378:NDP:O2D  | 3:B:378:NDP:N1N  | 2.16                     | 0.79              |
| 1:A:163:GLN:HE22 | 1:A:164:LYS:NZ   | 1.80                     | 0.79              |
| 1:O:165:PHE:CA   | 1:O:248:LYS:HG2  | 2.13                     | 0.79              |
| 1:R:139:HIS:O    | 1:R:139:HIS:CD2  | 2.34                     | 0.79              |
| 1:H:135:GLU:HA   | 1:H:135:GLU:OE1  | 1.82                     | 0.79              |
| 1:R:115:LYS:NZ   | 1:R:332:TRP:CZ3  | 2.50                     | 0.79              |
| 1:P:187:ALA:O    | 1:Q:43:LEU:HD11  | 1.82                     | 0.79              |
| 1:O:78:ASN:OD1   | 1:O:80:VAL:HG22  | 1.83                     | 0.78              |
| 1:H:276:GLU:OE1  | 1:M:46:TYR:CE2   | 2.37                     | 0.78              |
| 1:M:0:LYS:NZ     | 1:M:0:LYS:HB2    | 1.99                     | 0.78              |
| 1:B:183:ARG:HE   | 1:B:187:ALA:CB   | 1.97                     | 0.78              |
| 1:R:251:PHE:HB2  | 2:R:376:SO4:O2   | 1.83                     | 0.78              |
| 1:Q:120:ALA:HB2  | 3:Q:375:NDP:H2D  | 1.66                     | 0.78              |
| 1:R:1:LEU:CD1    | 1:R:90:ASP:HB2   | 2.14                     | 0.78              |
| 1:A:2:LYS:HG2    | 1:A:89:ILE:HA    | 1.64                     | 0.78              |
| 3:L:369:NDP:O2D  | 3:L:369:NDP:N1N  | 2.16                     | 0.78              |
| 1:B:165:PHE:O    | 1:B:248:LYS:HG3  | 1.82                     | 0.78              |
| 1:P:139:HIS:CG   | 1:P:333:GLN:HG3  | 2.19                     | 0.77              |
| 1:C:77:ARG:NH1   | 3:C:365:NDP:N7A  | 2.32                     | 0.77              |
| 1:O:232:VAL:HG21 | 1:P:203:ILE:HD11 | 1.65                     | 0.77              |
| 1:P:139:HIS:HD2  | 1:P:333:GLN:OE1  | 1.67                     | 0.77              |
| 1:Q:139:HIS:CE1  | 1:Q:332:TRP:CD2  | 2.73                     | 0.77              |
| 1:B:165:PHE:CA   | 1:B:248:LYS:CD   | 2.52                     | 0.77              |
| 1:Q:190:HIS:CE1  | 1:Q:191:ARG:HH11 | 2.02                     | 0.77              |
| 1:Q:165:PHE:HA   | 1:Q:248:LYS:HD2  | 1.64                     | 0.77              |
| 1:A:2:LYS:HD2    | 1:A:88:GLY:O     | 1.85                     | 0.77              |
| 1:B:120:ALA:HB2  | 3:B:378:NDP:H2D  | 1.67                     | 0.77              |
| 1:A:2:LYS:HD3    | 1:A:89:ILE:HD13  | 1.68                     | 0.76              |
| 1:H:202:ASN:HD22 | 1:L:281:ILE:H    | 1.33                     | 0.76              |
| 1:R:58:LYS:CB    | 1:R:58:LYS:NZ    | 2.48                     | 0.76              |
| 1:H:281:ILE:H    | 1:L:202:ASN:HD22 | 1.30                     | 0.76              |
| 1:R:251:PHE:CB   | 2:R:376:SO4:O2   | 2.33                     | 0.76              |
| 1:I:301:GLY:HA3  | 1:M:169:LYS:HD2  | 1.67                     | 0.76              |
| 1:R:58:LYS:HB3   | 1:R:58:LYS:HZ2   | 1.50                     | 0.76              |
| 1:P:150:THR:HB   | 2:P:364:SO4:O3   | 1.85                     | 0.76              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:R:164:LYS:O     | 1:R:248:LYS:HD2  | 1.83                     | 0.76              |
| 1:R:202:ASN:HD21  | 1:Q:281:ILE:CB   | 1.99                     | 0.76              |
| 1:B:165:PHE:HA    | 1:B:248:LYS:CG   | 2.16                     | 0.75              |
| 1:B:281:ILE:CB    | 1:D:202:ASN:HD21 | 1.99                     | 0.75              |
| 1:H:202:ASN:ND2   | 1:L:281:ILE:H    | 1.84                     | 0.75              |
| 1:I:163:GLN:HE21  | 1:I:164:LYS:HZ2  | 0.77                     | 0.75              |
| 1:Q:172:MET:HB2   | 1:Q:242:LEU:HD22 | 1.67                     | 0.75              |
| 1:M:78:ASN:OD1    | 1:M:80:VAL:HG22  | 1.86                     | 0.75              |
| 1:R:18(A):TRP:HH2 | 1:R:69:LYS:NZ    | 1.83                     | 0.75              |
| 1:A:2:LYS:HB2     | 1:A:2:LYS:HZ3    | 1.50                     | 0.75              |
| 1:A:281:ILE:HB    | 1:C:202:ASN:ND2  | 2.00                     | 0.75              |
| 3:I:380:NDP:N1N   | 3:I:380:NDP:O2D  | 2.18                     | 0.75              |
| 1:R:210:ALA:O     | 1:R:214:VAL:HG23 | 1.87                     | 0.75              |
| 1:A:77:ARG:NH2    | 3:A:376:NDP:O1X  | 2.20                     | 0.75              |
| 1:P:20:ARG:HH21   | 1:P:319:GLN:CD   | 1.91                     | 0.74              |
| 1:Q:210:ALA:O     | 1:Q:214:VAL:HG23 | 1.87                     | 0.74              |
| 1:R:18(A):TRP:CH2 | 1:R:69:LYS:NZ    | 2.56                     | 0.74              |
| 1:L:158:VAL:HG11  | 1:L:221:LEU:CD1  | 2.17                     | 0.74              |
| 1:R:60:ALA:O      | 1:R:60(A):GLY:C  | 2.22                     | 0.74              |
| 1:C:183:ARG:CD    | 1:C:187:ALA:HB3  | 2.08                     | 0.74              |
| 3:O:372:NDP:O2D   | 3:O:372:NDP:N1N  | 2.19                     | 0.74              |
| 1:D:38:LYS:HD3    | 1:D:59:THR:HG21  | 1.69                     | 0.73              |
| 1:P:82:LEU:HD13   | 1:P:84:TRP:CZ2   | 2.22                     | 0.73              |
| 1:R:38:LYS:HD3    | 1:R:59:THR:HG21  | 1.70                     | 0.73              |
| 1:Q:191:ARG:H     | 1:Q:191:ARG:HD2  | 0.57                     | 0.73              |
| 1:O:120:ALA:HB2   | 3:O:372:NDP:H2D  | 1.70                     | 0.73              |
| 1:R:173:THR:OG1   | 1:Q:306:LYS:NZ   | 2.21                     | 0.73              |
| 3:M:381:NDP:O2D   | 3:M:381:NDP:N1N  | 2.20                     | 0.73              |
| 1:O:169:LYS:HD2   | 1:P:301:GLY:HA3  | 1.71                     | 0.73              |
| 1:R:115:LYS:CE    | 1:R:332:TRP:CZ3  | 2.71                     | 0.73              |
| 1:O:281:ILE:H     | 1:P:202:ASN:HD22 | 1.34                     | 0.73              |
| 1:Q:165:PHE:HD1   | 1:Q:248:LYS:CD   | 2.01                     | 0.73              |
| 1:Q:328:VAL:CG1   | 1:Q:332:TRP:HZ3  | 2.01                     | 0.73              |
| 1:P:20:ARG:NH2    | 1:P:319:GLN:OE1  | 2.20                     | 0.72              |
| 3:C:365:NDP:N1N   | 3:C:365:NDP:O2D  | 2.20                     | 0.72              |
| 1:C:77:ARG:NH1    | 3:C:365:NDP:C8A  | 2.52                     | 0.72              |
| 1:H:172:MET:HE1   | 1:H:211:ALA:N    | 2.03                     | 0.72              |
| 1:O:281:ILE:N     | 1:P:202:ASN:ND2  | 2.37                     | 0.72              |
| 1:A:77:ARG:NH1    | 3:A:376:NDP:C5A  | 2.52                     | 0.72              |
| 1:A:188:SER:CB    | 1:B:39:GLN:OE1   | 2.38                     | 0.72              |
| 1:O:281:ILE:N     | 1:P:202:ASN:HD22 | 1.87                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:210:ALA:C    | 1:B:211:ALA:C    | 2.47                     | 0.72              |
| 1:H:281:ILE:H    | 1:L:202:ASN:ND2  | 1.88                     | 0.72              |
| 1:R:165:PHE:CA   | 1:R:248:LYS:CG   | 2.67                     | 0.71              |
| 1:I:210:ALA:N    | 2:I:366:SO4:O2   | 2.22                     | 0.71              |
| 1:R:222:LYS:CD   | 1:R:223:GLY:N    | 2.53                     | 0.71              |
| 1:L:158:VAL:CG1  | 1:L:221:LEU:CD1  | 2.69                     | 0.71              |
| 1:O:286:THR:HG22 | 1:O:288:VAL:HG22 | 1.71                     | 0.71              |
| 1:Q:183:ARG:HE   | 1:Q:187:ALA:HB3  | 1.54                     | 0.71              |
| 1:D:78:ASN:OD1   | 1:D:80:VAL:HG22  | 1.90                     | 0.71              |
| 1:P:134:GLU:CD   | 1:P:135:GLU:OE1  | 2.28                     | 0.71              |
| 1:B:332:TRP:CD1  | 1:B:334:GLY:C    | 2.64                     | 0.71              |
| 1:C:159:LYS:HE2  | 1:C:163:GLN:HE22 | 1.55                     | 0.71              |
| 1:O:281:ILE:HG21 | 1:Q:48:SER:HA    | 1.70                     | 0.71              |
| 1:O:165:PHE:CA   | 1:O:248:LYS:CG   | 2.69                     | 0.71              |
| 1:O:232:VAL:CG2  | 1:P:203:ILE:HD11 | 2.20                     | 0.71              |
| 1:L:210:ALA:O    | 1:L:214:VAL:HG23 | 1.91                     | 0.70              |
| 1:L:77:ARG:NH2   | 3:L:369:NDP:O1X  | 2.24                     | 0.70              |
| 1:B:210:ALA:C    | 1:B:211:ALA:CA   | 2.60                     | 0.70              |
| 1:B:210:ALA:O    | 1:B:211:ALA:C    | 2.29                     | 0.70              |
| 1:R:154:LEU:CD2  | 1:R:214:VAL:HG21 | 2.22                     | 0.70              |
| 1:A:77:ARG:HH12  | 3:A:376:NDP:C5A  | 2.03                     | 0.70              |
| 1:B:301:GLY:HA3  | 1:D:169:LYS:HD2  | 1.74                     | 0.70              |
| 1:O:202:ASN:HD21 | 1:P:281:ILE:CB   | 2.04                     | 0.70              |
| 1:Q:171:THR:O    | 1:Q:242:LEU:HD13 | 1.90                     | 0.70              |
| 1:R:154:LEU:HD23 | 1:R:214:VAL:HG21 | 1.73                     | 0.70              |
| 1:A:281:ILE:H    | 1:C:202:ASN:HD22 | 1.38                     | 0.70              |
| 1:R:222:LYS:HD2  | 1:R:223:GLY:N    | 2.05                     | 0.70              |
| 1:R:78:ASN:OD1   | 1:R:80:VAL:HG22  | 1.92                     | 0.70              |
| 1:I:48:SER:HA    | 1:L:281:ILE:HG21 | 1.74                     | 0.70              |
| 1:Q:139:HIS:HE1  | 1:Q:332:TRP:CE3  | 2.09                     | 0.70              |
| 1:R:0:LYS:HB2    | 1:R:24:PRO:O     | 1.92                     | 0.70              |
| 1:C:110:GLN:NE2  | 1:I:106:GLY:CA   | 2.55                     | 0.69              |
| 1:Q:154:LEU:HD13 | 1:Q:240:VAL:HG11 | 1.73                     | 0.69              |
| 1:A:301:GLY:HA3  | 1:C:169:LYS:HD2  | 1.74                     | 0.69              |
| 1:C:57:VAL:C     | 1:C:58:LYS:HG2   | 2.11                     | 0.69              |
| 1:O:293:ASP:CB   | 1:O:296:LEU:CD1  | 2.69                     | 0.69              |
| 1:M:21:LYS:N     | 1:M:21:LYS:HD3   | 1.96                     | 0.69              |
| 1:B:165:PHE:O    | 1:B:248:LYS:CG   | 2.41                     | 0.69              |
| 1:B:29:VAL:HG23  | 1:B:72:LYS:O     | 1.93                     | 0.69              |
| 1:Q:194:ARG:CD   | 1:Q:205:PRO:HD2  | 2.23                     | 0.69              |
| 1:P:184:LEU:O    | 1:P:184:LEU:HD12 | 1.92                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:169:LYS:HD2  | 1:Q:301:GLY:HA3  | 1.75                     | 0.68              |
| 1:Q:241:ASP:OD1  | 1:Q:306:LYS:HE3  | 1.94                     | 0.68              |
| 1:Q:194:ARG:HD2  | 1:Q:205:PRO:HD2  | 1.76                     | 0.68              |
| 1:A:281:ILE:CB   | 1:C:202:ASN:HD21 | 2.06                     | 0.68              |
| 1:O:172:MET:HG2  | 1:O:173:THR:N    | 2.09                     | 0.68              |
| 1:O:202:ASN:HD22 | 1:P:281:ILE:H    | 1.38                     | 0.68              |
| 1:D:139:HIS:CE1  | 1:D:333:GLN:H    | 2.11                     | 0.68              |
| 1:I:154:LEU:HD13 | 1:I:240:VAL:HG21 | 1.75                     | 0.68              |
| 1:O:226:ASN:ND2  | 1:P:300:MET:SD   | 2.67                     | 0.68              |
| 1:B:212:LYS:NZ   | 1:B:226:ASN:CG   | 2.47                     | 0.68              |
| 1:M:0:LYS:HZ3    | 1:M:0:LYS:HB3    | 1.58                     | 0.68              |
| 1:R:139:HIS:CE1  | 1:R:333:GLN:H    | 2.12                     | 0.68              |
| 1:P:208:THR:CG2  | 1:P:228:ILE:CA   | 2.70                     | 0.68              |
| 1:Q:194:ARG:HD2  | 1:Q:205:PRO:O    | 1.94                     | 0.68              |
| 1:H:34:GLY:HA3   | 1:H:39:GLN:OE1   | 1.94                     | 0.68              |
| 1:B:46:TYR:HE2   | 1:C:276:GLU:OE1  | 1.77                     | 0.67              |
| 1:P:39:GLN:OE1   | 1:Q:188:SER:HB2  | 1.94                     | 0.67              |
| 1:P:222:LYS:CD   | 1:P:223:GLY:N    | 2.57                     | 0.67              |
| 1:H:77:ARG:HH11  | 3:H:379:NDP:C5A  | 2.04                     | 0.67              |
| 1:B:48:SER:HA    | 1:C:281:ILE:HG21 | 1.77                     | 0.67              |
| 1:O:293:ASP:CG   | 1:O:296:LEU:HD11 | 2.15                     | 0.67              |
| 1:C:78:ASN:OD1   | 1:C:80:VAL:HG22  | 1.96                     | 0.66              |
| 1:C:77:ARG:NH2   | 3:C:365:NDP:O1X  | 2.27                     | 0.66              |
| 1:L:129:VAL:H    | 1:L:133:ASN:HD21 | 1.43                     | 0.66              |
| 1:L:77:ARG:NH1   | 3:L:369:NDP:C5A  | 2.58                     | 0.66              |
| 1:C:159:LYS:HG2  | 1:C:163:GLN:NE2  | 2.10                     | 0.66              |
| 1:H:24:PRO:HG2   | 1:H:25:LEU:HD23  | 1.76                     | 0.66              |
| 1:O:165:PHE:CA   | 1:O:248:LYS:HD2  | 2.25                     | 0.66              |
| 1:Q:328:VAL:CG1  | 1:Q:332:TRP:CZ3  | 2.78                     | 0.66              |
| 1:R:1:LEU:HD23   | 1:R:329:ALA:HB2  | 1.77                     | 0.66              |
| 1:A:78:ASN:OD1   | 1:A:80:VAL:HG22  | 1.95                     | 0.66              |
| 1:B:210:ALA:CA   | 1:B:211:ALA:N    | 2.59                     | 0.66              |
| 1:C:210:ALA:O    | 1:C:214:VAL:HG23 | 1.95                     | 0.66              |
| 1:P:188:SER:HB2  | 1:Q:39:GLN:OE1   | 1.96                     | 0.66              |
| 1:C:77:ARG:HH22  | 3:C:365:NDP:P2B  | 2.18                     | 0.65              |
| 1:O:310:TRP:HZ2  | 1:P:205:PRO:HG2  | 1.60                     | 0.65              |
| 1:M:0:LYS:HZ3    | 1:M:0:LYS:HB2    | 1.58                     | 0.65              |
| 1:M:155:ALA:HB3  | 1:M:156:PRO:HD3  | 1.77                     | 0.65              |
| 1:H:77:ARG:NH2   | 3:H:379:NDP:O1X  | 2.30                     | 0.65              |
| 1:B:164:LYS:O    | 1:B:248:LYS:CD   | 2.44                     | 0.65              |
| 1:I:281:ILE:HG21 | 1:L:48:SER:HA    | 1.79                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:276:GLU:OE1  | 1:M:46:TYR:HE2   | 1.78                     | 0.65              |
| 1:O:183:ARG:HH12 | 1:O:187:ALA:HB1  | 1.58                     | 0.65              |
| 1:O:183:ARG:HH11 | 1:O:187:ALA:CB   | 2.09                     | 0.65              |
| 1:D:173:THR:HG23 | 1:D:228:ILE:HD11 | 1.78                     | 0.65              |
| 1:R:165:PHE:CD1  | 1:R:248:LYS:HD3  | 2.31                     | 0.65              |
| 1:O:298:MET:CE   | 1:P:226:ASN:OD1  | 2.43                     | 0.64              |
| 1:I:183:ARG:NH1  | 1:I:187:ALA:HB3  | 2.12                     | 0.64              |
| 1:R:227:GLY:HA2  | 1:Q:298:MET:HE1  | 1.77                     | 0.64              |
| 1:M:210:ALA:O    | 1:M:214:VAL:HG23 | 1.97                     | 0.64              |
| 1:H:129:VAL:H    | 1:H:133:ASN:ND2  | 1.95                     | 0.64              |
| 1:L:129:VAL:H    | 1:L:133:ASN:ND2  | 1.96                     | 0.64              |
| 1:M:21:LYS:CD    | 1:M:21:LYS:H     | 2.00                     | 0.64              |
| 1:H:78:ASN:OD1   | 1:H:80:VAL:HG22  | 1.97                     | 0.64              |
| 1:C:106:GLY:HA3  | 1:I:110:GLN:HE22 | 1.63                     | 0.64              |
| 1:O:183:ARG:NH1  | 1:O:187:ALA:HB3  | 2.11                     | 0.64              |
| 1:Q:165:PHE:CD1  | 1:Q:248:LYS:CD   | 2.80                     | 0.64              |
| 1:A:11:ILE:HG13  | 3:A:376:NDP:H1D  | 1.80                     | 0.64              |
| 1:Q:165:PHE:HB3  | 1:Q:248:LYS:HG2  | 1.79                     | 0.64              |
| 1:B:306:LYS:NZ   | 1:D:173:THR:OG1  | 2.20                     | 0.64              |
| 1:R:139:HIS:CB   | 1:R:333:GLN:OE1  | 2.45                     | 0.64              |
| 1:H:25:LEU:HD21  | 1:H:326:ASP:OD1  | 1.98                     | 0.64              |
| 1:R:48:SER:HA    | 1:P:281:ILE:HG21 | 1.80                     | 0.64              |
| 1:P:49:ILE:HD11  | 1:Q:185:LEU:HD22 | 1.80                     | 0.64              |
| 1:D:173:THR:HG23 | 1:D:228:ILE:HD12 | 1.79                     | 0.63              |
| 1:I:208:THR:CB   | 2:I:366:SO4:O3   | 2.46                     | 0.63              |
| 1:P:150:THR:CB   | 2:P:364:SO4:O3   | 2.45                     | 0.63              |
| 1:C:209:GLY:O    | 1:C:212:LYS:HG2  | 1.98                     | 0.63              |
| 1:M:150:THR:OG1  | 2:M:370:SO4:O1   | 2.13                     | 0.63              |
| 1:O:228:ILE:HD12 | 1:P:296:LEU:CD2  | 2.24                     | 0.63              |
| 1:R:164:LYS:O    | 1:R:248:LYS:HD3  | 1.98                     | 0.63              |
| 1:R:1:LEU:CD2    | 1:R:329:ALA:HB2  | 2.29                     | 0.63              |
| 1:H:129:VAL:H    | 1:H:133:ASN:HD21 | 1.45                     | 0.63              |
| 1:O:165:PHE:HB3  | 1:O:248:LYS:HG3  | 1.81                     | 0.63              |
| 1:O:293:ASP:CG   | 1:O:296:LEU:CD1  | 2.67                     | 0.63              |
| 1:P:261:GLU:OE1  | 1:P:261:GLU:C    | 2.36                     | 0.63              |
| 1:L:84:TRP:CE3   | 1:L:84:TRP:HA    | 2.34                     | 0.63              |
| 1:O:226:ASN:C    | 1:O:226:ASN:OD1  | 2.37                     | 0.63              |
| 1:A:281:ILE:CG2  | 1:C:202:ASN:HD21 | 2.12                     | 0.63              |
| 1:P:222:LYS:CD   | 1:P:222:LYS:C    | 2.68                     | 0.63              |
| 1:Q:172:MET:SD   | 1:Q:227:GLY:HA3  | 2.39                     | 0.63              |
| 1:I:203:ILE:HB   | 1:M:280:SER:HB3  | 1.81                     | 0.62              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:P:64:ILE:HG13   | 1:P:71:ILE:HG22  | 1.81                     | 0.62              |
| 1:B:77:ARG:NH2    | 3:B:378:NDP:O1X  | 2.32                     | 0.62              |
| 1:I:172:MET:CG    | 1:I:240:VAL:HG23 | 2.29                     | 0.62              |
| 1:I:183:ARG:NH1   | 1:I:187:ALA:CB   | 2.61                     | 0.62              |
| 1:O:42:HIS:CD2    | 1:R:193:LEU:HD23 | 2.34                     | 0.62              |
| 1:R:1:LEU:HD12    | 1:R:90:ASP:HB2   | 1.81                     | 0.62              |
| 1:Q:128:TYR:HA    | 1:Q:133:ASN:HD21 | 1.64                     | 0.62              |
| 1:Q:190:HIS:C     | 1:Q:191:ARG:HD2  | 2.14                     | 0.62              |
| 1:O:281:ILE:CG2   | 1:Q:48:SER:HA    | 2.29                     | 0.62              |
| 1:D:58:LYS:HB3    | 1:D:58:LYS:NZ    | 2.15                     | 0.62              |
| 1:C:159:LYS:O     | 1:C:163:GLN:CG   | 2.38                     | 0.62              |
| 1:H:276:GLU:CD    | 1:M:46:TYR:OH    | 2.38                     | 0.62              |
| 1:I:280:SER:HB3   | 1:M:203:ILE:HB   | 1.82                     | 0.62              |
| 1:H:48:SER:HA     | 1:M:281:ILE:HG21 | 1.82                     | 0.62              |
| 1:R:195:ARG:NH1   | 2:R:363:SO4:O4   | 2.30                     | 0.62              |
| 1:B:212:LYS:NZ    | 1:B:226:ASN:OD1  | 2.31                     | 0.62              |
| 1:I:155:ALA:HB3   | 1:I:156:PRO:HD3  | 1.82                     | 0.61              |
| 1:I:169:LYS:HD2   | 1:M:301:GLY:HA3  | 1.82                     | 0.61              |
| 1:I:183:ARG:NH2   | 1:I:188:SER:O    | 2.34                     | 0.61              |
| 1:O:310:TRP:HZ2   | 1:P:205:PRO:CG   | 2.12                     | 0.61              |
| 1:R:300:MET:HE1   | 1:Q:226:ASN:HB2  | 1.82                     | 0.61              |
| 1:O:37:VAL:HG21   | 1:O:61:ASP:O     | 2.01                     | 0.61              |
| 1:P:187:ALA:O     | 1:P:196:ALA:HB1  | 2.00                     | 0.61              |
| 1:Q:165:PHE:CD1   | 1:Q:248:LYS:HD2  | 2.36                     | 0.61              |
| 1:O:48:SER:HA     | 1:Q:281:ILE:HG21 | 1.83                     | 0.61              |
| 1:H:276:GLU:CD    | 1:M:46:TYR:HH    | 2.03                     | 0.61              |
| 1:R:227:GLY:C     | 1:R:228:ILE:HG13 | 2.21                     | 0.61              |
| 1:B:205:PRO:HG2   | 1:D:310:TRP:HZ2  | 1.66                     | 0.61              |
| 1:D:139:HIS:CD2   | 1:D:332:TRP:HA   | 2.35                     | 0.61              |
| 1:Q:172:MET:HE1   | 1:Q:211:ALA:N    | 2.15                     | 0.61              |
| 1:R:18(A):TRP:HH2 | 1:R:69:LYS:HZ2   | 1.47                     | 0.61              |
| 1:R:222:LYS:HD3   | 1:R:223:GLY:N    | 2.16                     | 0.61              |
| 1:B:78:ASN:OD1    | 1:B:80:VAL:HG22  | 2.01                     | 0.61              |
| 1:L:84:TRP:HE3    | 1:L:84:TRP:HA    | 1.65                     | 0.61              |
| 1:P:236:ASN:O     | 1:P:237:VAL:HB   | 2.01                     | 0.61              |
| 1:Q:77:ARG:NH2    | 3:Q:375:NDP:O1X  | 2.34                     | 0.61              |
| 1:P:187:ALA:O     | 1:Q:43:LEU:CD1   | 2.49                     | 0.60              |
| 1:L:158:VAL:HG12  | 1:L:221:LEU:HD11 | 1.81                     | 0.60              |
| 1:O:183:ARG:HH11  | 1:O:187:ALA:HB3  | 1.66                     | 0.60              |
| 1:O:42:HIS:CG     | 1:R:193:LEU:CD2  | 2.84                     | 0.60              |
| 1:A:139:HIS:O     | 1:A:139:HIS:CD2  | 2.54                     | 0.60              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:H:221:LEU:HD22 | 1:H:225:LEU:HD11   | 1.84                     | 0.60              |
| 1:R:202:ASN:HD22 | 1:Q:281:ILE:H      | 1.48                     | 0.60              |
| 1:Q:78:ASN:OD1   | 1:Q:80:VAL:HG22    | 2.01                     | 0.60              |
| 1:A:2:LYS:CG     | 1:A:89:ILE:HA      | 2.30                     | 0.60              |
| 1:L:85:GLY:C     | 1:L:87:MET:N       | 2.54                     | 0.59              |
| 1:O:187:ALA:O    | 1:O:196:ALA:HB1    | 2.02                     | 0.59              |
| 1:O:210:ALA:O    | 1:O:214:VAL:HG23   | 2.01                     | 0.59              |
| 1:P:120:ALA:HB2  | 3:P:373:NDP:H2D    | 1.84                     | 0.59              |
| 1:Q:209:GLY:O    | 1:Q:212:LYS:HG2    | 2.02                     | 0.59              |
| 1:R:115:LYS:NZ   | 1:R:332:TRP:CE3    | 2.68                     | 0.59              |
| 1:R:58:LYS:CB    | 1:R:58:LYS:HZ2     | 2.10                     | 0.59              |
| 1:R:37:VAL:HB    | 1:R:61:ASP:OD2     | 2.01                     | 0.59              |
| 1:A:139:HIS:CE1  | 1:A:333:GLN:H      | 2.20                     | 0.59              |
| 1:I:208:THR:HB   | 2:I:366:SO4:O3     | 2.02                     | 0.59              |
| 1:R:194:ARG:HD2  | 1:R:205:PRO:O      | 2.03                     | 0.59              |
| 1:B:46:TYR:CE2   | 1:C:276:GLU:OE1    | 2.55                     | 0.59              |
| 1:A:2:LYS:CD     | 1:A:89:ILE:HA      | 2.33                     | 0.59              |
| 1:H:221:LEU:CD2  | 1:H:225:LEU:HD11   | 2.32                     | 0.59              |
| 1:H:100:VAL:HG23 | 1:H:122(A):LYS:HG2 | 1.85                     | 0.59              |
| 1:C:129:VAL:H    | 1:C:133:ASN:ND2    | 2.01                     | 0.59              |
| 1:A:203:ILE:HB   | 1:C:280:SER:HB3    | 1.83                     | 0.59              |
| 1:C:106:GLY:O    | 1:I:110:GLN:NE2    | 2.36                     | 0.59              |
| 1:L:78:ASN:OD1   | 1:L:80:VAL:HG22    | 2.02                     | 0.59              |
| 1:C:176:HIS:HB3  | 1:C:231:ARG:HD3    | 1.85                     | 0.59              |
| 1:Q:165:PHE:HA   | 1:Q:248:LYS:CD     | 2.30                     | 0.59              |
| 1:I:208:THR:OG1  | 2:I:366:SO4:O3     | 2.21                     | 0.58              |
| 1:B:77:ARG:HH11  | 1:B:77:ARG:HG2     | 1.67                     | 0.58              |
| 1:R:165:PHE:HA   | 1:R:248:LYS:HD3    | 1.70                     | 0.58              |
| 1:A:2:LYS:HD2    | 1:A:88:GLY:C       | 2.21                     | 0.58              |
| 1:B:27:VAL:HG12  | 1:B:71:ILE:HD13    | 1.84                     | 0.58              |
| 1:M:150:THR:CB   | 2:M:370:SO4:O1     | 2.50                     | 0.58              |
| 1:R:281:ILE:CG2  | 1:Q:202:ASN:HD21   | 2.17                     | 0.58              |
| 1:H:84:TRP:HE3   | 1:H:84:TRP:HA      | 1.69                     | 0.58              |
| 1:M:154:LEU:HD23 | 1:M:214:VAL:HG21   | 1.86                     | 0.58              |
| 1:H:276:GLU:OE2  | 1:M:46:TYR:OH      | 2.22                     | 0.58              |
| 1:C:32:ASP:O     | 1:C:75:SER:OG      | 2.21                     | 0.58              |
| 1:B:281:ILE:CG2  | 1:D:202:ASN:HD21   | 2.16                     | 0.58              |
| 1:H:84:TRP:CE3   | 1:H:84:TRP:HA      | 2.39                     | 0.58              |
| 1:C:128:TYR:HA   | 1:C:133:ASN:HD21   | 1.68                     | 0.58              |
| 1:D:139:HIS:NE2  | 1:D:332:TRP:HA     | 2.19                     | 0.58              |
| 1:I:172:MET:HG3  | 1:I:240:VAL:CG2    | 2.34                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:32:ASP:O     | 1:O:75:SER:OG    | 2.22                     | 0.58              |
| 1:Q:129:VAL:H    | 1:Q:133:ASN:ND2  | 2.01                     | 0.58              |
| 1:C:56:ASP:CG    | 1:C:58:LYS:HZ1   | 2.06                     | 0.57              |
| 1:I:172:MET:HG2  | 1:I:173:THR:N    | 2.19                     | 0.57              |
| 1:L:85:GLY:O     | 1:L:86:ASP:C     | 2.39                     | 0.57              |
| 1:M:129:VAL:H    | 1:M:133:ASN:ND2  | 2.00                     | 0.57              |
| 1:O:128:TYR:HA   | 1:O:133:ASN:HD21 | 1.69                     | 0.57              |
| 1:B:281:ILE:H    | 1:D:202:ASN:HD22 | 1.50                     | 0.57              |
| 1:I:210:ALA:O    | 1:I:214:VAL:HG23 | 2.04                     | 0.57              |
| 1:I:58:LYS:NZ    | 1:I:58:LYS:HB3   | 2.18                     | 0.57              |
| 1:R:222:LYS:HD3  | 1:R:223:GLY:H    | 1.69                     | 0.57              |
| 1:A:205:PRO:HG2  | 1:C:310:TRP:HZ2  | 1.69                     | 0.57              |
| 1:A:49:ILE:HD11  | 1:B:185:LEU:HD22 | 1.86                     | 0.57              |
| 1:B:172:MET:HE2  | 1:B:210:ALA:HB3  | 1.85                     | 0.57              |
| 1:B:1:LEU:HD23   | 1:B:3:VAL:CG2    | 2.34                     | 0.57              |
| 1:H:77:ARG:HH12  | 3:H:379:NDP:C5A  | 2.17                     | 0.57              |
| 1:O:278:LEU:O    | 1:P:194:ARG:HD3  | 2.04                     | 0.57              |
| 1:R:222:LYS:C    | 1:R:222:LYS:HD2  | 2.25                     | 0.57              |
| 1:R:228:ILE:HD11 | 1:Q:306:LYS:HE2  | 1.85                     | 0.57              |
| 1:H:33:THR:HG21  | 1:H:77:ARG:HG2   | 1.86                     | 0.57              |
| 1:P:208:THR:HG21 | 1:P:228:ILE:C    | 2.25                     | 0.57              |
| 1:M:129:VAL:H    | 1:M:133:ASN:HD21 | 1.52                     | 0.57              |
| 1:R:202:ASN:HD21 | 1:Q:281:ILE:CG2  | 2.18                     | 0.57              |
| 1:R:115:LYS:HZ2  | 1:R:328:VAL:HG13 | 1.70                     | 0.57              |
| 1:L:77:ARG:HH12  | 3:L:369:NDP:C5A  | 2.17                     | 0.57              |
| 1:O:126:PRO:HG2  | 1:O:144:ILE:HG22 | 1.86                     | 0.57              |
| 1:P:190:HIS:HA   | 1:P:191:ARG:NH1  | 2.19                     | 0.57              |
| 1:R:160:VAL:O    | 1:R:164:LYS:HG2  | 2.05                     | 0.57              |
| 1:C:129:VAL:H    | 1:C:133:ASN:HD21 | 1.53                     | 0.56              |
| 1:M:128:TYR:HA   | 1:M:133:ASN:HD21 | 1.69                     | 0.56              |
| 1:H:281:ILE:HG21 | 1:M:48:SER:HA    | 1.86                     | 0.56              |
| 1:P:64:ILE:CG1   | 1:P:71:ILE:HG22  | 2.35                     | 0.56              |
| 1:L:172:MET:HE1  | 1:L:211:ALA:N    | 2.20                     | 0.56              |
| 1:B:165:PHE:CA   | 1:B:248:LYS:HG3  | 2.35                     | 0.56              |
| 1:C:1:LEU:HD22   | 1:C:329:ALA:HB2  | 1.86                     | 0.56              |
| 1:H:281:ILE:CG2  | 1:L:202:ASN:HD21 | 2.18                     | 0.56              |
| 1:O:165:PHE:O    | 1:O:248:LYS:HG2  | 2.06                     | 0.56              |
| 1:A:42:HIS:CG    | 1:B:193:LEU:HD13 | 2.41                     | 0.56              |
| 1:P:129:VAL:H    | 1:P:133:ASN:ND2  | 2.03                     | 0.56              |
| 1:P:139:HIS:CD2  | 1:P:333:GLN:OE1  | 2.56                     | 0.56              |
| 1:R:310:TRP:HZ2  | 1:Q:205:PRO:HG2  | 1.71                     | 0.56              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:I:208:THR:HG22 | 1:I:228:ILE:HA     | 1.86                     | 0.56              |
| 1:O:282:ASP:OD1  | 1:Q:46:TYR:HB3     | 2.05                     | 0.56              |
| 1:A:236:ASN:O    | 1:A:237:VAL:HB     | 2.06                     | 0.56              |
| 1:B:128:TYR:HA   | 1:B:133:ASN:HD21   | 1.71                     | 0.56              |
| 1:A:194:ARG:HD3  | 1:C:278:LEU:O      | 2.06                     | 0.56              |
| 1:M:58:LYS:HB3   | 1:M:58:LYS:NZ      | 2.20                     | 0.56              |
| 1:R:222:LYS:CD   | 1:R:222:LYS:C      | 2.74                     | 0.56              |
| 1:A:2:LYS:CD     | 1:A:89:ILE:HD13    | 2.36                     | 0.56              |
| 1:H:148:SER:CB   | 2:H:364:SO4:O1     | 2.53                     | 0.56              |
| 1:P:184:LEU:HD11 | 1:Q:178:TYR:CE1    | 2.41                     | 0.56              |
| 1:L:187:ALA:O    | 1:L:196:ALA:HB1    | 2.06                     | 0.56              |
| 1:C:77:ARG:NH1   | 3:C:365:NDP:C4A    | 2.68                     | 0.56              |
| 1:P:221:LEU:HD22 | 1:P:225:LEU:HD11   | 1.87                     | 0.56              |
| 3:P:373:NDP:O2D  | 3:P:373:NDP:C1D    | 2.35                     | 0.56              |
| 1:A:155:ALA:HB3  | 1:A:156:PRO:HD3    | 1.87                     | 0.55              |
| 1:H:172:MET:HE1  | 1:H:211:ALA:H      | 1.70                     | 0.55              |
| 1:M:97:GLY:HA3   | 3:M:381:NDP:O3D    | 2.06                     | 0.55              |
| 1:P:188:SER:CB   | 1:Q:39:GLN:OE1     | 2.54                     | 0.55              |
| 1:A:197:ARG:HH21 | 1:B:48:SER:N       | 2.04                     | 0.55              |
| 1:P:98:VAL:HG23  | 1:P:99:PHE:CD2     | 2.41                     | 0.55              |
| 1:R:115:LYS:NZ   | 1:R:328:VAL:HG13   | 2.21                     | 0.55              |
| 1:Q:139:HIS:ND1  | 1:Q:332:TRP:HA     | 2.21                     | 0.55              |
| 1:H:77:ARG:HH12  | 3:H:379:NDP:C4A    | 2.19                     | 0.55              |
| 1:L:194:ARG:HD2  | 1:L:205:PRO:O      | 2.07                     | 0.55              |
| 1:L:97:GLY:HA3   | 3:L:369:NDP:O3D    | 2.06                     | 0.55              |
| 1:I:129:VAL:H    | 1:I:133:ASN:HD21   | 1.55                     | 0.55              |
| 1:R:155:ALA:HB3  | 1:R:156:PRO:HD3    | 1.87                     | 0.55              |
| 1:R:165:PHE:HB3  | 1:R:248:LYS:HG3    | 1.89                     | 0.55              |
| 1:O:97:GLY:HA3   | 3:O:372:NDP:O3D    | 2.07                     | 0.55              |
| 1:B:209:GLY:O    | 1:B:213:ALA:HB3    | 2.07                     | 0.55              |
| 1:P:185:LEU:HD22 | 1:Q:49:ILE:HD11    | 1.89                     | 0.55              |
| 1:R:228:ILE:CD1  | 1:Q:306:LYS:NZ     | 2.70                     | 0.55              |
| 1:B:251:PHE:CZ   | 1:B:254:GLU:HB2    | 2.42                     | 0.55              |
| 1:I:183:ARG:CZ   | 1:I:188:SER:O      | 2.55                     | 0.55              |
| 1:O:165:PHE:CD1  | 1:O:248:LYS:HD2    | 2.41                     | 0.54              |
| 1:O:208:THR:HG22 | 1:O:228:ILE:HA     | 1.88                     | 0.54              |
| 1:R:115:LYS:HE3  | 1:R:332:TRP:CH2    | 2.42                     | 0.54              |
| 1:B:202:ASN:ND2  | 1:D:281:ILE:N      | 2.47                     | 0.54              |
| 1:H:276:GLU:OE1  | 1:M:46:TYR:OH      | 2.25                     | 0.54              |
| 1:R:100:VAL:HG23 | 1:R:122(A):LYS:HG2 | 1.89                     | 0.54              |
| 1:L:33:THR:HA    | 1:L:75:SER:OG      | 2.08                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:117:LEU:HD23 | 1:O:117:LEU:C    | 2.28                     | 0.54              |
| 1:O:42:HIS:CG    | 1:R:193:LEU:HD22 | 2.43                     | 0.54              |
| 1:O:97:GLY:CA    | 3:O:372:NDP:O3D  | 2.56                     | 0.54              |
| 1:A:2:LYS:HB2    | 1:A:2:LYS:HZ2    | 1.71                     | 0.54              |
| 1:B:148:SER:HB2  | 2:B:364:SO4:O4   | 2.07                     | 0.54              |
| 1:C:155:ALA:HB3  | 1:C:156:PRO:HD3  | 1.88                     | 0.54              |
| 1:B:281:ILE:HG21 | 1:C:48:SER:HA    | 1.90                     | 0.54              |
| 1:I:209:GLY:O    | 1:I:212:LYS:HG2  | 2.08                     | 0.54              |
| 1:O:202:ASN:ND2  | 1:P:281:ILE:H    | 2.04                     | 0.54              |
| 1:B:332:TRP:HD1  | 1:B:334:GLY:C    | 2.11                     | 0.54              |
| 1:M:0:LYS:NZ     | 1:M:0:LYS:HB3    | 2.15                     | 0.54              |
| 1:Q:251:PHE:CZ   | 1:Q:254:GLU:HB2  | 2.42                     | 0.54              |
| 1:R:0:LYS:HD2    | 1:R:23:SER:O     | 2.07                     | 0.54              |
| 1:D:82:LEU:HD13  | 1:D:84:TRP:CZ2   | 2.42                     | 0.54              |
| 1:P:129:VAL:H    | 1:P:133:ASN:HD21 | 1.54                     | 0.54              |
| 1:B:46:TYR:OH    | 1:C:276:GLU:OE2  | 2.25                     | 0.54              |
| 1:I:163:GLN:HE21 | 1:I:164:LYS:CE   | 2.19                     | 0.54              |
| 1:I:202:ASN:HD21 | 1:M:281:ILE:CG2  | 2.20                     | 0.54              |
| 1:Q:242:LEU:HD12 | 1:Q:243:VAL:N    | 2.23                     | 0.54              |
| 1:A:117:LEU:HD23 | 1:A:117:LEU:C    | 2.28                     | 0.54              |
| 1:A:281:ILE:H    | 1:C:202:ASN:ND2  | 2.05                     | 0.54              |
| 1:C:9:GLY:O      | 1:C:13:ARG:HG3   | 2.08                     | 0.54              |
| 1:C:110:GLN:HE21 | 1:I:106:GLY:C    | 2.11                     | 0.54              |
| 1:L:155:ALA:HB3  | 1:L:156:PRO:HD3  | 1.88                     | 0.54              |
| 1:R:281:ILE:HG21 | 1:P:48:SER:HA    | 1.89                     | 0.54              |
| 1:B:151:THR:OG1  | 1:B:209:GLY:O    | 2.26                     | 0.54              |
| 1:B:31:ASN:ND2   | 3:B:378:NDP:H2A  | 2.23                     | 0.54              |
| 1:L:1:LEU:HD22   | 1:L:329:ALA:HB2  | 1.90                     | 0.54              |
| 1:O:82:LEU:HD13  | 1:O:84:TRP:CZ2   | 2.43                     | 0.54              |
| 1:O:310:TRP:CZ2  | 1:P:205:PRO:CG   | 2.91                     | 0.53              |
| 1:B:202:ASN:HD21 | 1:D:281:ILE:CG2  | 2.21                     | 0.53              |
| 1:L:228:ILE:C    | 1:L:228:ILE:HD12 | 2.29                     | 0.53              |
| 1:R:303:ASP:OD1  | 1:Q:169:LYS:HE3  | 2.07                     | 0.53              |
| 1:B:129:VAL:H    | 1:B:133:ASN:ND2  | 2.06                     | 0.53              |
| 1:A:129:VAL:H    | 1:A:133:ASN:ND2  | 2.06                     | 0.53              |
| 1:A:208:THR:O    | 1:A:210:ALA:N    | 2.41                     | 0.53              |
| 1:A:98:VAL:HG23  | 1:A:99:PHE:CD2   | 2.43                     | 0.53              |
| 1:C:80:VAL:CB    | 1:C:110:GLN:OE1  | 2.47                     | 0.53              |
| 1:H:24:PRO:HG2   | 1:H:25:LEU:CD2   | 2.38                     | 0.53              |
| 1:I:236:ASN:O    | 1:I:237:VAL:HB   | 2.09                     | 0.53              |
| 1:R:202:ASN:ND2  | 1:Q:281:ILE:H    | 2.06                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:209:GLY:HA3  | 1:C:212:LYS:HE2  | 1.90                     | 0.53              |
| 1:C:272:SER:OG   | 1:C:288:VAL:HG11 | 2.09                     | 0.53              |
| 1:I:172:MET:HG3  | 1:I:240:VAL:HG23 | 1.89                     | 0.53              |
| 1:A:48:SER:HA    | 1:D:281:ILE:HG21 | 1.88                     | 0.53              |
| 1:I:129:VAL:H    | 1:I:133:ASN:ND2  | 2.06                     | 0.53              |
| 1:I:97:GLY:HA3   | 3:I:380:NDP:O3D  | 2.09                     | 0.53              |
| 1:L:58:LYS:NZ    | 1:L:58:LYS:HB3   | 2.24                     | 0.53              |
| 1:I:169:LYS:NZ   | 1:M:303:ASP:OD1  | 2.37                     | 0.53              |
| 1:R:228:ILE:HD12 | 1:Q:306:LYS:NZ   | 2.24                     | 0.53              |
| 1:D:103:ASP:OD1  | 1:D:103:ASP:N    | 2.42                     | 0.53              |
| 1:D:129:VAL:H    | 1:D:133:ASN:HD21 | 1.56                     | 0.53              |
| 1:D:228:ILE:HD12 | 1:D:228:ILE:C    | 2.30                     | 0.53              |
| 1:P:139:HIS:CD2  | 1:P:333:GLN:CG   | 2.88                     | 0.53              |
| 1:A:281:ILE:HG21 | 1:D:48:SER:HA    | 1.91                     | 0.53              |
| 1:B:97:GLY:HA3   | 3:B:378:NDP:O3D  | 2.09                     | 0.53              |
| 1:D:148:SER:HB2  | 2:D:364:SO4:O3   | 2.08                     | 0.53              |
| 1:D:272:SER:OG   | 1:D:288:VAL:HG11 | 2.09                     | 0.53              |
| 1:H:176:HIS:HB3  | 1:H:231:ARG:HD3  | 1.89                     | 0.53              |
| 1:P:0:LYS:HB3    | 1:P:24:PRO:O     | 2.09                     | 0.53              |
| 1:R:279:VAL:HG12 | 1:Q:205:PRO:HD3  | 1.91                     | 0.53              |
| 1:A:0:LYS:HD3    | 1:A:1:LEU:N      | 2.22                     | 0.52              |
| 1:I:202:ASN:ND2  | 1:M:281:ILE:N    | 2.50                     | 0.52              |
| 1:O:277:PRO:O    | 1:P:194:ARG:HG2  | 2.09                     | 0.52              |
| 1:Q:154:LEU:CD1  | 1:Q:242:LEU:CD2  | 2.41                     | 0.52              |
| 1:B:28:VAL:C     | 1:B:71:ILE:HG23  | 2.30                     | 0.52              |
| 1:B:77:ARG:HG2   | 1:B:77:ARG:NH1   | 2.24                     | 0.52              |
| 1:H:272:SER:OG   | 1:H:288:VAL:HG11 | 2.09                     | 0.52              |
| 1:H:58:LYS:HB3   | 1:H:58:LYS:NZ    | 2.24                     | 0.52              |
| 1:P:9:GLY:O      | 1:P:13:ARG:HG3   | 2.10                     | 0.52              |
| 1:R:227:GLY:HA2  | 1:Q:298:MET:CE   | 2.38                     | 0.52              |
| 1:A:129:VAL:H    | 1:A:133:ASN:HD21 | 1.56                     | 0.52              |
| 1:C:204:VAL:HB   | 1:C:231:ARG:HB2  | 1.92                     | 0.52              |
| 1:D:148:SER:CB   | 2:D:364:SO4:O3   | 2.57                     | 0.52              |
| 1:M:150:THR:HB   | 2:M:370:SO4:O1   | 2.09                     | 0.52              |
| 1:D:210:ALA:O    | 1:D:214:VAL:HG23 | 2.09                     | 0.52              |
| 1:B:203:ILE:HB   | 1:D:280:SER:HB3  | 1.91                     | 0.52              |
| 1:H:128:TYR:HA   | 1:H:133:ASN:HD21 | 1.75                     | 0.52              |
| 1:H:135:GLU:OE1  | 1:H:135:GLU:CA   | 2.56                     | 0.52              |
| 1:M:97:GLY:CA    | 3:M:381:NDP:O3D  | 2.58                     | 0.52              |
| 1:P:222:LYS:HD3  | 1:P:223:GLY:H    | 1.70                     | 0.52              |
| 1:Q:248:LYS:O    | 1:Q:248:LYS:HG3  | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:96:THR:OG1   | 1:C:98:VAL:HG22  | 2.09                     | 0.52              |
| 1:I:281:ILE:N    | 1:M:202:ASN:HD22 | 2.00                     | 0.52              |
| 1:O:125:ILE:HG23 | 1:O:126:PRO:HD2  | 1.91                     | 0.52              |
| 1:Q:176:HIS:HB3  | 1:Q:231:ARG:HD3  | 1.91                     | 0.52              |
| 1:D:11:ILE:HD11  | 3:D:365:NDP:H42N | 1.92                     | 0.52              |
| 1:C:106:GLY:C    | 1:I:110:GLN:NE2  | 2.62                     | 0.52              |
| 1:I:11:ILE:HD11  | 3:I:380:NDP:H42N | 1.91                     | 0.52              |
| 1:L:95:GLY:O     | 3:L:369:NDP:H51A | 2.09                     | 0.52              |
| 1:I:281:ILE:N    | 1:M:202:ASN:ND2  | 2.49                     | 0.52              |
| 1:O:281:ILE:CG2  | 1:P:202:ASN:HD21 | 2.22                     | 0.52              |
| 1:D:172:MET:HE3  | 1:D:211:ALA:HB2  | 1.91                     | 0.52              |
| 1:O:148:SER:HB2  | 2:O:364:SO4:O1   | 2.10                     | 0.52              |
| 1:A:202:ASN:ND2  | 1:C:281:ILE:N    | 2.53                     | 0.52              |
| 1:M:241:ASP:OD1  | 1:M:306:LYS:HE2  | 2.10                     | 0.52              |
| 1:I:205:PRO:HG2  | 1:M:310:TRP:HZ2  | 1.74                     | 0.52              |
| 1:H:276:GLU:OE1  | 1:M:46:TYR:CZ    | 2.62                     | 0.52              |
| 1:O:282:ASP:CG   | 1:P:197:ARG:HH12 | 2.12                     | 0.52              |
| 1:R:172:MET:HE1  | 1:R:211:ALA:N    | 2.25                     | 0.52              |
| 1:R:97:GLY:HA3   | 3:R:377:NDP:O3D  | 2.10                     | 0.52              |
| 1:O:129:VAL:H    | 1:O:133:ASN:ND2  | 2.08                     | 0.52              |
| 1:O:155:ALA:HB3  | 1:O:156:PRO:HD3  | 1.91                     | 0.52              |
| 1:O:165:PHE:CA   | 1:O:248:LYS:CD   | 2.85                     | 0.52              |
| 1:Q:149:CYS:HB3  | 3:Q:375:NDP:H41N | 1.91                     | 0.52              |
| 1:A:2:LYS:NZ     | 1:A:2:LYS:CB     | 2.67                     | 0.51              |
| 1:B:210:ALA:N    | 1:B:211:ALA:N    | 2.58                     | 0.51              |
| 1:B:245:GLN:HE22 | 1:D:245:GLN:HE22 | 1.58                     | 0.51              |
| 1:A:210:ALA:C    | 1:A:212:LYS:N    | 2.63                     | 0.51              |
| 1:D:155:ALA:HB3  | 1:D:156:PRO:HD3  | 1.90                     | 0.51              |
| 1:D:97:GLY:HA3   | 3:D:365:NDP:O3D  | 2.10                     | 0.51              |
| 1:Q:95:GLY:O     | 3:Q:375:NDP:H51A | 2.10                     | 0.51              |
| 1:R:310:TRP:HZ2  | 1:Q:205:PRO:CG   | 2.22                     | 0.51              |
| 1:B:159:LYS:O    | 1:B:163:GLN:HG3  | 2.08                     | 0.51              |
| 1:H:58:LYS:HB3   | 1:H:58:LYS:HZ2   | 1.75                     | 0.51              |
| 1:A:2:LYS:CG     | 1:A:89:ILE:HD13  | 2.40                     | 0.51              |
| 1:C:97:GLY:HA3   | 3:C:365:NDP:O3D  | 2.11                     | 0.51              |
| 1:M:0:LYS:HB2    | 1:M:0:LYS:HZ2    | 1.72                     | 0.51              |
| 1:O:281:ILE:CB   | 1:P:202:ASN:ND2  | 2.50                     | 0.51              |
| 1:P:195:ARG:NH1  | 2:P:363:SO4:O4   | 2.40                     | 0.51              |
| 1:L:133:ASN:HD22 | 1:L:133:ASN:H    | 1.59                     | 0.51              |
| 1:C:159:LYS:CG   | 1:C:163:GLN:NE2  | 2.73                     | 0.51              |
| 1:C:57:VAL:N     | 1:C:58:LYS:HZ2   | 2.08                     | 0.51              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:P:208:THR:CG2  | 1:P:228:ILE:C      | 2.79                     | 0.51              |
| 1:B:280:SER:HB3  | 1:D:203:ILE:HB     | 1.93                     | 0.51              |
| 1:D:129:VAL:H    | 1:D:133:ASN:ND2    | 2.09                     | 0.51              |
| 1:H:33:THR:HA    | 1:H:75:SER:OG      | 2.10                     | 0.51              |
| 1:M:0:LYS:CB     | 1:M:0:LYS:HZ2      | 2.18                     | 0.51              |
| 1:R:300:MET:SD   | 1:Q:226:ASN:HB3    | 2.51                     | 0.51              |
| 1:C:117:LEU:HD23 | 1:C:117:LEU:C      | 2.30                     | 0.51              |
| 1:O:42:HIS:CB    | 1:R:193:LEU:CD2    | 2.88                     | 0.51              |
| 1:A:194:ARG:HD2  | 1:A:205:PRO:O      | 2.11                     | 0.51              |
| 1:C:228:ILE:HD12 | 1:C:228:ILE:C      | 2.31                     | 0.51              |
| 1:H:172:MET:HE1  | 1:H:210:ALA:HB3    | 1.93                     | 0.51              |
| 1:C:110:GLN:HE21 | 1:I:106:GLY:CA     | 2.24                     | 0.51              |
| 1:Q:228:ILE:HD12 | 1:Q:228:ILE:C      | 2.32                     | 0.51              |
| 1:P:188:SER:OG   | 3:Q:375:NDP:O3X    | 2.28                     | 0.51              |
| 1:A:185:LEU:HD22 | 1:B:49:ILE:HD11    | 1.92                     | 0.51              |
| 1:A:77:ARG:NH1   | 3:A:376:NDP:N7A    | 2.59                     | 0.51              |
| 1:B:205:PRO:CG   | 1:D:310:TRP:HZ2    | 2.23                     | 0.51              |
| 1:I:281:ILE:CG2  | 1:M:202:ASN:HD21   | 2.23                     | 0.51              |
| 1:P:96:THR:OG1   | 1:P:98:VAL:HG22    | 2.11                     | 0.51              |
| 1:C:159:LYS:HE2  | 1:C:163:GLN:NE2    | 2.25                     | 0.50              |
| 1:D:128:TYR:HA   | 1:D:133:ASN:HD21   | 1.76                     | 0.50              |
| 1:I:103:ASP:N    | 1:I:103:ASP:OD1    | 2.43                     | 0.50              |
| 1:R:278:LEU:O    | 1:Q:194:ARG:HD3    | 2.10                     | 0.50              |
| 1:Q:253:GLU:HA   | 1:Q:253:GLU:OE1    | 2.06                     | 0.50              |
| 1:R:129:VAL:H    | 1:R:133:ASN:HD21   | 1.58                     | 0.50              |
| 1:H:149:CYS:HB3  | 3:H:379:NDP:H41N   | 1.93                     | 0.50              |
| 1:P:271:LEU:C    | 1:P:271:LEU:HD13   | 2.31                     | 0.50              |
| 1:R:0:LYS:HG3    | 1:R:24:PRO:C       | 2.31                     | 0.50              |
| 1:B:98:VAL:HG23  | 1:B:99:PHE:CD2     | 2.46                     | 0.50              |
| 1:H:77:ARG:HH12  | 3:H:379:NDP:C8A    | 2.23                     | 0.50              |
| 1:O:202:ASN:HD21 | 1:P:281:ILE:CG2    | 2.24                     | 0.50              |
| 1:B:29:VAL:HA    | 1:B:72:LYS:O       | 2.11                     | 0.50              |
| 1:A:184:LEU:HD21 | 1:B:199:ALA:HB3    | 1.93                     | 0.50              |
| 1:L:100:VAL:HG23 | 1:L:122(A):LYS:HG2 | 1.93                     | 0.50              |
| 1:P:117:LEU:C    | 1:P:117:LEU:HD23   | 2.31                     | 0.50              |
| 1:D:154:LEU:HD23 | 1:D:214:VAL:HG21   | 1.93                     | 0.50              |
| 1:P:157:PHE:HB2  | 1:P:259:PHE:CE1    | 2.47                     | 0.50              |
| 1:R:233:PRO:HB2  | 1:Q:233:PRO:HB2    | 1.92                     | 0.50              |
| 1:C:236:ASN:O    | 1:C:237:VAL:HB     | 2.12                     | 0.50              |
| 1:M:103:ASP:OD1  | 1:M:104:GLY:N      | 2.45                     | 0.50              |
| 1:R:128:TYR:HA   | 1:R:133:ASN:HD21   | 1.76                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:129:VAL:H    | 1:R:133:ASN:ND2  | 2.10                     | 0.50              |
| 1:Q:139:HIS:CE1  | 1:Q:332:TRP:CG   | 3.00                     | 0.50              |
| 1:Q:187:ALA:O    | 1:Q:196:ALA:HB1  | 2.11                     | 0.50              |
| 1:R:203:ILE:HB   | 1:Q:280:SER:HB3  | 1.94                     | 0.50              |
| 1:R:280:SER:HB3  | 1:Q:203:ILE:HB   | 1.93                     | 0.50              |
| 1:C:80:VAL:HG13  | 1:C:107:LYS:HZ2  | 1.77                     | 0.50              |
| 1:H:236:ASN:O    | 1:H:237:VAL:HB   | 2.12                     | 0.50              |
| 1:H:77:ARG:NH1   | 3:H:379:NDP:N7A  | 2.59                     | 0.50              |
| 1:L:33:THR:HG21  | 1:L:77:ARG:HG2   | 1.92                     | 0.50              |
| 1:M:236:ASN:O    | 1:M:237:VAL:HB   | 2.12                     | 0.50              |
| 1:P:155:ALA:HB3  | 1:P:156:PRO:HD3  | 1.93                     | 0.50              |
| 1:Q:11:ILE:HD11  | 3:Q:375:NDP:H42N | 1.93                     | 0.50              |
| 1:A:202:ASN:HD21 | 1:C:281:ILE:CG2  | 2.23                     | 0.49              |
| 1:O:1:LEU:HD22   | 1:O:329:ALA:HB2  | 1.93                     | 0.49              |
| 1:A:133:ASN:HD22 | 1:A:133:ASN:N    | 2.09                     | 0.49              |
| 1:D:58:LYS:HZ3   | 1:D:58:LYS:HB3   | 1.77                     | 0.49              |
| 1:I:168:ILE:HD12 | 1:I:245:GLN:HG2  | 1.93                     | 0.49              |
| 1:O:281:ILE:HD11 | 1:O:284:ARG:HD2  | 1.94                     | 0.49              |
| 1:P:218:LEU:HB3  | 1:P:221:LEU:HD12 | 1.95                     | 0.49              |
| 1:Q:129:VAL:H    | 1:Q:133:ASN:HD21 | 1.59                     | 0.49              |
| 1:A:128:TYR:HA   | 1:A:133:ASN:HD21 | 1.77                     | 0.49              |
| 1:C:209:GLY:CA   | 1:C:212:LYS:HE2  | 2.42                     | 0.49              |
| 1:L:58:LYS:HZ2   | 1:L:58:LYS:HB3   | 1.77                     | 0.49              |
| 1:O:129:VAL:H    | 1:O:133:ASN:HD21 | 1.60                     | 0.49              |
| 1:Q:298:MET:HE2  | 1:Q:306:LYS:HD3  | 1.93                     | 0.49              |
| 1:P:190:HIS:O    | 1:Q:39:GLN:NE2   | 2.44                     | 0.49              |
| 1:R:226:ASN:HB3  | 1:Q:300:MET:SD   | 2.52                     | 0.49              |
| 1:H:157:PHE:HB2  | 1:H:259:PHE:CE1  | 2.47                     | 0.49              |
| 1:O:272:SER:OG   | 1:O:288:VAL:HG11 | 2.12                     | 0.49              |
| 1:P:58:LYS:HB3   | 1:P:58:LYS:NZ    | 2.27                     | 0.49              |
| 1:C:172:MET:C    | 1:C:172:MET:HE2  | 2.33                     | 0.49              |
| 1:H:228:ILE:C    | 1:H:228:ILE:HD12 | 2.33                     | 0.49              |
| 1:H:310:TRP:HZ2  | 1:L:205:PRO:HG2  | 1.77                     | 0.49              |
| 1:L:240:VAL:HG13 | 1:L:311:TYR:CE1  | 2.47                     | 0.49              |
| 1:Q:194:ARG:HD3  | 1:Q:205:PRO:HD2  | 1.91                     | 0.49              |
| 1:A:9:GLY:HA3    | 3:A:376:NDP:O5B  | 2.12                     | 0.49              |
| 1:I:241:ASP:OD1  | 1:I:306:LYS:HE2  | 2.12                     | 0.49              |
| 1:O:176:HIS:HB3  | 1:O:231:ARG:HD3  | 1.93                     | 0.49              |
| 1:A:154:LEU:HD21 | 1:A:172:MET:HE2  | 1.95                     | 0.49              |
| 1:A:188:SER:CA   | 1:B:39:GLN:OE1   | 2.60                     | 0.49              |
| 1:B:1:LEU:HD23   | 1:B:3:VAL:HG22   | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:159:LYS:O    | 1:Q:163:GLN:HG3  | 2.13                     | 0.49              |
| 1:A:82:LEU:HD13  | 1:A:84:TRP:CZ2   | 2.48                     | 0.49              |
| 1:A:193:LEU:HB3  | 1:B:42:HIS:CD2   | 2.48                     | 0.49              |
| 1:L:272:SER:OG   | 1:L:288:VAL:HG11 | 2.13                     | 0.49              |
| 1:O:154:LEU:HD12 | 1:O:157:PHE:CZ   | 2.48                     | 0.49              |
| 1:Q:165:PHE:CB   | 1:Q:248:LYS:HG2  | 2.42                     | 0.49              |
| 1:B:172:MET:SD   | 1:B:227:GLY:HA3  | 2.52                     | 0.49              |
| 1:Q:181:ASP:OD2  | 1:Q:195:ARG:NH1  | 2.43                     | 0.49              |
| 1:A:97:GLY:CA    | 3:A:376:NDP:O3D  | 2.61                     | 0.48              |
| 1:O:165:PHE:HB3  | 1:O:248:LYS:CG   | 2.42                     | 0.48              |
| 1:O:165:PHE:C    | 1:O:248:LYS:HG2  | 2.33                     | 0.48              |
| 1:P:184:LEU:C    | 1:P:184:LEU:HD12 | 2.33                     | 0.48              |
| 1:P:98:VAL:HG23  | 1:P:99:PHE:CE2   | 2.47                     | 0.48              |
| 1:R:236:ASN:O    | 1:R:237:VAL:HB   | 2.12                     | 0.48              |
| 1:A:133:ASN:HD22 | 1:A:133:ASN:H    | 1.62                     | 0.48              |
| 1:B:129:VAL:H    | 1:B:133:ASN:HD21 | 1.60                     | 0.48              |
| 1:L:176:HIS:HB3  | 1:L:231:ARG:HD3  | 1.94                     | 0.48              |
| 1:P:176:HIS:HB3  | 1:P:231:ARG:HD3  | 1.95                     | 0.48              |
| 1:A:272:SER:OG   | 1:A:288:VAL:HG11 | 2.13                     | 0.48              |
| 1:H:278:LEU:O    | 1:L:194:ARG:HD3  | 2.13                     | 0.48              |
| 1:I:172:MET:HE2  | 1:I:172:MET:HB3  | 1.66                     | 0.48              |
| 1:I:208:THR:OG1  | 2:I:366:SO4:O2   | 2.23                     | 0.48              |
| 1:I:278:LEU:O    | 1:M:194:ARG:HD3  | 2.14                     | 0.48              |
| 1:Q:212:LYS:O    | 1:Q:215:ALA:HB3  | 2.12                     | 0.48              |
| 1:R:149:CYS:HB3  | 3:R:377:NDP:H41N | 1.96                     | 0.48              |
| 1:C:187:ALA:O    | 1:C:196:ALA:HB1  | 2.14                     | 0.48              |
| 1:C:39:GLN:HG3   | 1:D:193:LEU:CD2  | 2.44                     | 0.48              |
| 1:H:154:LEU:HD23 | 1:H:214:VAL:HG21 | 1.95                     | 0.48              |
| 1:I:128:TYR:HA   | 1:I:133:ASN:HD21 | 1.79                     | 0.48              |
| 1:Q:248:LYS:CG   | 1:Q:248:LYS:O    | 2.61                     | 0.48              |
| 1:Q:328:VAL:HG12 | 1:Q:332:TRP:CZ3  | 2.47                     | 0.48              |
| 1:R:228:ILE:HD11 | 1:Q:306:LYS:CE   | 2.44                     | 0.48              |
| 1:H:172:MET:CE   | 1:H:210:ALA:HB3  | 2.44                     | 0.48              |
| 1:H:77:ARG:HH22  | 3:H:379:NDP:P2B  | 2.36                     | 0.48              |
| 1:A:205:PRO:HG2  | 1:C:310:TRP:CZ2  | 2.48                     | 0.48              |
| 1:L:149:CYS:HB3  | 3:L:369:NDP:H41N | 1.96                     | 0.48              |
| 1:A:276:GLU:OE1  | 1:D:46:TYR:OH    | 2.20                     | 0.48              |
| 1:B:187:ALA:O    | 1:B:196:ALA:HB1  | 2.13                     | 0.48              |
| 1:M:29:VAL:HG22  | 1:M:30:ILE:N     | 2.29                     | 0.48              |
| 1:B:165:PHE:C    | 1:B:248:LYS:HG3  | 2.34                     | 0.48              |
| 1:C:56:ASP:CG    | 1:C:58:LYS:NZ    | 2.67                     | 0.48              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:P:236:ASN:O    | 1:P:237:VAL:CB     | 2.62                     | 0.48              |
| 1:R:248:LYS:HE2  | 1:R:248:LYS:HB3    | 1.67                     | 0.48              |
| 1:L:77:ARG:HH12  | 3:L:369:NDP:C4A    | 2.26                     | 0.48              |
| 1:M:272:SER:OG   | 1:M:288:VAL:HG11   | 2.14                     | 0.48              |
| 1:P:128:TYR:HA   | 1:P:133:ASN:HD21   | 1.78                     | 0.48              |
| 1:R:228:ILE:CD1  | 1:Q:306:LYS:HZ3    | 2.27                     | 0.48              |
| 1:I:97:GLY:CA    | 3:I:380:NDP:O3D    | 2.62                     | 0.48              |
| 1:I:310:TRP:HZ2  | 1:M:205:PRO:HG2    | 1.78                     | 0.48              |
| 1:B:0:LYS:HE3    | 1:B:23:SER:O       | 2.14                     | 0.47              |
| 1:L:188:SER:HB2  | 1:M:39:GLN:OE1     | 2.14                     | 0.47              |
| 1:L:82:LEU:HD13  | 1:L:84:TRP:CZ2     | 2.49                     | 0.47              |
| 1:P:228:ILE:C    | 1:P:228:ILE:HD12   | 2.35                     | 0.47              |
| 1:Q:157:PHE:HB2  | 1:Q:259:PHE:CE1    | 2.49                     | 0.47              |
| 1:Q:82:LEU:HD13  | 1:Q:84:TRP:CZ2     | 2.49                     | 0.47              |
| 1:R:84:TRP:CE3   | 1:R:84:TRP:HA      | 2.49                     | 0.47              |
| 1:R:2:LYS:N      | 1:R:90:ASP:OD2     | 2.47                     | 0.47              |
| 1:D:157:PHE:HB2  | 1:D:259:PHE:CE1    | 2.48                     | 0.47              |
| 1:H:281:ILE:CB   | 1:L:202:ASN:ND2    | 2.64                     | 0.47              |
| 1:I:253:GLU:HA   | 2:I:379:SO4:O2     | 2.15                     | 0.47              |
| 1:P:210:ALA:O    | 1:P:213:ALA:HB3    | 2.14                     | 0.47              |
| 1:Q:164:LYS:O    | 1:Q:248:LYS:CD     | 2.59                     | 0.47              |
| 1:A:210:ALA:HA   | 1:A:213:ALA:HB3    | 1.96                     | 0.47              |
| 1:D:209:GLY:O    | 1:D:212:LYS:HG2    | 2.15                     | 0.47              |
| 1:H:209:GLY:O    | 1:H:213:ALA:CB     | 2.62                     | 0.47              |
| 1:I:95:GLY:O     | 3:I:380:NDP:H51A   | 2.15                     | 0.47              |
| 1:Q:154:LEU:HD21 | 1:Q:242:LEU:HD21   | 1.95                     | 0.47              |
| 1:H:97:GLY:HA3   | 3:H:379:NDP:O3D    | 2.14                     | 0.47              |
| 1:Q:165:PHE:HD1  | 1:Q:248:LYS:CG     | 2.27                     | 0.47              |
| 1:Q:261:GLU:OE1  | 1:Q:261:GLU:CA     | 2.62                     | 0.47              |
| 1:C:82:LEU:HD13  | 1:C:84:TRP:CZ2     | 2.49                     | 0.47              |
| 1:H:201:LEU:HD21 | 1:I:235:PRO:HG3    | 1.94                     | 0.47              |
| 1:M:176:HIS:HB3  | 1:M:231:ARG:HD3    | 1.96                     | 0.47              |
| 1:O:236:ASN:O    | 1:O:237:VAL:HB     | 2.13                     | 0.47              |
| 1:Q:170:GLY:HA3  | 1:Q:244:VAL:HG12   | 1.96                     | 0.47              |
| 1:O:42:HIS:HB3   | 1:R:193:LEU:CD2    | 2.45                     | 0.47              |
| 1:A:184:LEU:O    | 1:A:184:LEU:HD12   | 2.15                     | 0.47              |
| 1:A:97:GLY:HA3   | 3:A:376:NDP:O3D    | 2.15                     | 0.47              |
| 1:B:228:ILE:C    | 1:B:228:ILE:HD12   | 2.35                     | 0.47              |
| 1:C:33:THR:HG21  | 1:C:77:ARG:HG2     | 1.96                     | 0.47              |
| 1:M:100:VAL:HG23 | 1:M:122(A):LYS:HG2 | 1.97                     | 0.47              |
| 1:R:139:HIS:CG   | 1:R:333:GLN:OE1    | 2.68                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:84:TRP:HE3   | 1:R:84:TRP:HA    | 1.80                     | 0.47              |
| 1:B:155:ALA:HB3  | 1:B:156:PRO:HD3  | 1.96                     | 0.47              |
| 1:A:202:ASN:ND2  | 1:C:281:ILE:CB   | 2.60                     | 0.47              |
| 1:D:238:SER:HB2  | 1:D:311:TYR:CZ   | 2.49                     | 0.47              |
| 1:H:133:ASN:HD22 | 1:H:133:ASN:H    | 1.61                     | 0.47              |
| 1:L:133:ASN:HD22 | 1:L:133:ASN:N    | 2.10                     | 0.47              |
| 1:L:154:LEU:HD23 | 1:L:214:VAL:HG21 | 1.96                     | 0.47              |
| 1:L:236:ASN:O    | 1:L:237:VAL:HB   | 2.15                     | 0.47              |
| 1:P:133:ASN:H    | 1:P:133:ASN:HD22 | 1.63                     | 0.47              |
| 1:A:187:ALA:O    | 1:A:196:ALA:HB1  | 2.15                     | 0.47              |
| 1:A:11:ILE:HD11  | 3:A:376:NDP:H42N | 1.95                     | 0.47              |
| 1:B:176:HIS:HB3  | 1:B:231:ARG:HD3  | 1.96                     | 0.47              |
| 1:B:33:THR:HA    | 1:B:75:SER:OG    | 2.15                     | 0.47              |
| 1:H:77:ARG:NH1   | 3:H:379:NDP:C4A  | 2.77                     | 0.47              |
| 1:O:84:TRP:CE3   | 1:O:84:TRP:HA    | 2.50                     | 0.47              |
| 1:P:11:ILE:HG13  | 3:P:373:NDP:H1D  | 1.96                     | 0.47              |
| 1:P:77:ARG:O     | 1:P:79:PRO:HD3   | 2.15                     | 0.47              |
| 1:A:202:ASN:HD22 | 1:C:281:ILE:N    | 2.00                     | 0.47              |
| 1:B:169:LYS:NZ   | 1:D:303:ASP:OD1  | 2.47                     | 0.47              |
| 1:D:84:TRP:CE3   | 1:D:84:TRP:HA    | 2.50                     | 0.47              |
| 1:L:128:TYR:HA   | 1:L:133:ASN:HD21 | 1.80                     | 0.47              |
| 1:L:126:PRO:HD2  | 1:L:143:ILE:O    | 2.15                     | 0.47              |
| 1:O:240:VAL:HG13 | 1:O:311:TYR:CE1  | 2.50                     | 0.47              |
| 1:Q:96:THR:OG1   | 1:Q:98:VAL:HG22  | 2.15                     | 0.47              |
| 1:B:149:CYS:HB3  | 3:B:378:NDP:H41N | 1.96                     | 0.46              |
| 1:H:207:SER:O    | 1:H:208:THR:HB   | 2.14                     | 0.46              |
| 1:B:96:THR:OG1   | 1:B:98:VAL:HG22  | 2.15                     | 0.46              |
| 1:C:97:GLY:CA    | 3:C:365:NDP:O3D  | 2.64                     | 0.46              |
| 1:Q:190:HIS:CD2  | 1:Q:191:ARG:NH1  | 2.83                     | 0.46              |
| 1:A:204:VAL:HB   | 1:A:231:ARG:HB2  | 1.98                     | 0.46              |
| 1:C:154:LEU:HD12 | 1:C:157:PHE:CZ   | 2.50                     | 0.46              |
| 1:O:42:HIS:CD2   | 1:R:193:LEU:CD2  | 2.97                     | 0.46              |
| 1:P:271:LEU:HD13 | 1:P:272:SER:H    | 1.76                     | 0.46              |
| 1:H:202:ASN:HD21 | 1:L:281:ILE:CG2  | 2.28                     | 0.46              |
| 1:I:154:LEU:HD23 | 1:I:214:VAL:HG21 | 1.98                     | 0.46              |
| 1:M:11:ILE:HD11  | 3:M:381:NDP:H42N | 1.97                     | 0.46              |
| 1:Q:155:ALA:HB3  | 1:Q:156:PRO:HD3  | 1.97                     | 0.46              |
| 1:Q:190:HIS:HB3  | 1:Q:196:ALA:HB2  | 1.97                     | 0.46              |
| 1:R:228:ILE:HG13 | 1:Q:298:MET:HE1  | 1.96                     | 0.46              |
| 1:A:205:PRO:CG   | 1:C:310:TRP:HZ2  | 2.28                     | 0.46              |
| 1:I:163:GLN:NE2  | 1:I:164:LYS:HZ3  | 2.07                     | 0.46              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:I:16:LEU:HD23  | 1:I:16:LEU:O       | 2.15                     | 0.46              |
| 1:P:194:ARG:HD2  | 1:P:205:PRO:O      | 2.15                     | 0.46              |
| 1:Q:173:THR:HG23 | 1:Q:228:ILE:CD1    | 2.46                     | 0.46              |
| 1:Q:183:ARG:HE   | 1:Q:187:ALA:CB     | 2.27                     | 0.46              |
| 1:Q:98:VAL:HG23  | 1:Q:99:PHE:CD2     | 2.50                     | 0.46              |
| 1:H:151:THR:OG1  | 1:H:210:ALA:HA     | 2.15                     | 0.46              |
| 1:H:155:ALA:HB3  | 1:H:156:PRO:HD3    | 1.97                     | 0.46              |
| 1:B:236:ASN:O    | 1:B:237:VAL:HB     | 2.15                     | 0.46              |
| 1:L:65:SER:HA    | 1:L:69:LYS:O       | 2.15                     | 0.46              |
| 1:L:83:PRO:O     | 1:L:87:MET:HG3     | 2.15                     | 0.46              |
| 1:L:97:GLY:CA    | 3:L:369:NDP:O3D    | 2.63                     | 0.46              |
| 1:O:209:GLY:O    | 1:O:212:LYS:HG2    | 2.16                     | 0.46              |
| 1:P:97:GLY:HA3   | 3:P:373:NDP:O3D    | 2.16                     | 0.46              |
| 1:R:272:SER:OG   | 1:R:288:VAL:HG11   | 2.16                     | 0.46              |
| 1:A:320:ARG:NE   | 1:A:320:ARG:HA     | 2.31                     | 0.46              |
| 1:D:149:CYS:HB3  | 3:D:365:NDP:H41N   | 1.98                     | 0.46              |
| 1:R:165:PHE:C    | 1:R:248:LYS:HG2    | 2.36                     | 0.46              |
| 1:B:191:ARG:HB3  | 1:B:191:ARG:NH1    | 2.31                     | 0.46              |
| 1:H:250:THR:OG1  | 1:H:251:PHE:N      | 2.49                     | 0.46              |
| 1:I:80:VAL:HB    | 1:I:110:GLN:OE1    | 2.15                     | 0.46              |
| 1:P:133:ASN:N    | 1:P:133:ASN:HD22   | 2.13                     | 0.46              |
| 1:Q:165:PHE:CA   | 1:Q:248:LYS:HD2    | 2.41                     | 0.46              |
| 1:I:157:PHE:HB2  | 1:I:259:PHE:CE1    | 2.51                     | 0.45              |
| 1:I:163:GLN:HG2  | 1:I:164:LYS:HD3    | 1.98                     | 0.45              |
| 1:R:137:TYR:CE2  | 1:R:331:LYS:HG3    | 2.51                     | 0.45              |
| 1:R:139:HIS:CD2  | 1:R:139:HIS:C      | 2.89                     | 0.45              |
| 1:R:250:THR:OG1  | 1:R:251:PHE:N      | 2.50                     | 0.45              |
| 1:A:208:THR:HG22 | 1:A:228:ILE:CA     | 2.46                     | 0.45              |
| 1:H:183:ARG:HE   | 1:H:187:ALA:HB3    | 1.82                     | 0.45              |
| 1:O:100:VAL:HG23 | 1:O:122(A):LYS:HG2 | 1.98                     | 0.45              |
| 1:O:148:SER:CB   | 2:O:364:SO4:O1     | 2.63                     | 0.45              |
| 1:O:96:THR:OG1   | 1:O:98:VAL:HG22    | 2.16                     | 0.45              |
| 1:I:183:ARG:NH1  | 1:I:187:ALA:HB1    | 2.31                     | 0.45              |
| 1:M:95:GLY:O     | 3:M:381:NDP:H51A   | 2.16                     | 0.45              |
| 1:M:96:THR:OG1   | 1:M:98:VAL:HG22    | 2.15                     | 0.45              |
| 1:O:190:HIS:HB3  | 1:O:196:ALA:HB2    | 1.98                     | 0.45              |
| 1:O:84:TRP:HE3   | 1:O:84:TRP:HA      | 1.81                     | 0.45              |
| 1:P:211:ALA:HB1  | 1:P:226:ASN:HA     | 1.98                     | 0.45              |
| 1:R:126:PRO:HD2  | 1:R:143:ILE:O      | 2.16                     | 0.45              |
| 1:A:84:TRP:CE3   | 1:A:84:TRP:HA      | 2.51                     | 0.45              |
| 1:B:281:ILE:H    | 1:D:202:ASN:ND2    | 2.14                     | 0.45              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:B:97:GLY:CA    | 3:B:378:NDP:O3D    | 2.65                     | 0.45              |
| 1:A:96:THR:OG1   | 1:A:98:VAL:HG22    | 2.17                     | 0.45              |
| 1:B:181:ASP:OD2  | 1:B:195:ARG:NH1    | 2.46                     | 0.45              |
| 1:O:11:ILE:HG13  | 3:O:372:NDP:H1D    | 1.98                     | 0.45              |
| 1:Q:172:MET:CB   | 1:Q:242:LEU:HD22   | 2.40                     | 0.45              |
| 1:B:165:PHE:CA   | 1:B:248:LYS:CG     | 2.85                     | 0.45              |
| 1:C:153:CYS:HA   | 1:C:290:SER:HB2    | 1.99                     | 0.45              |
| 1:H:96:THR:OG1   | 1:H:98:VAL:HG22    | 2.16                     | 0.45              |
| 1:Q:190:HIS:NE2  | 1:Q:191:ARG:NH1    | 2.65                     | 0.45              |
| 1:R:29:VAL:HG22  | 1:R:30:ILE:N       | 2.32                     | 0.45              |
| 1:P:184:LEU:CD1  | 1:Q:178:TYR:CE1    | 2.99                     | 0.45              |
| 1:D:84:TRP:HE3   | 1:D:84:TRP:HA      | 1.80                     | 0.45              |
| 1:I:272:SER:OG   | 1:I:288:VAL:HG11   | 2.17                     | 0.45              |
| 1:M:58:LYS:HB3   | 1:M:58:LYS:HZ3     | 1.82                     | 0.45              |
| 1:A:84:TRP:HE3   | 1:A:84:TRP:HA      | 1.81                     | 0.45              |
| 1:I:100:VAL:HG23 | 1:I:122(A):LYS:HG2 | 1.99                     | 0.45              |
| 1:I:163:GLN:HG2  | 1:I:164:LYS:N      | 2.32                     | 0.45              |
| 1:L:170:GLY:HA3  | 1:L:244:VAL:HG12   | 1.99                     | 0.45              |
| 1:O:204:VAL:HB   | 1:O:231:ARG:HB2    | 1.99                     | 0.45              |
| 1:P:298:MET:CE   | 1:P:306:LYS:HD2    | 2.46                     | 0.45              |
| 1:A:228:ILE:HD12 | 1:A:228:ILE:C      | 2.38                     | 0.45              |
| 1:H:221:LEU:HD22 | 1:H:225:LEU:CD1    | 2.47                     | 0.45              |
| 1:O:281:ILE:HD13 | 1:O:281:ILE:O      | 2.16                     | 0.45              |
| 1:O:300:MET:SD   | 1:P:226:ASN:HB2    | 2.57                     | 0.45              |
| 1:R:157:PHE:HB2  | 1:R:259:PHE:CE1    | 2.51                     | 0.45              |
| 1:B:212:LYS:HZ3  | 1:B:226:ASN:CG     | 2.08                     | 0.44              |
| 1:C:157:PHE:HB2  | 1:C:259:PHE:CE1    | 2.53                     | 0.44              |
| 1:D:176:HIS:HB3  | 1:D:231:ARG:HD3    | 1.98                     | 0.44              |
| 1:P:154:LEU:HD23 | 1:P:214:VAL:HG21   | 1.99                     | 0.44              |
| 1:P:222:LYS:HD2  | 1:P:222:LYS:C      | 2.37                     | 0.44              |
| 1:I:250:THR:OG1  | 1:I:251:PHE:N      | 2.49                     | 0.44              |
| 1:O:126:PRO:HD2  | 1:O:143:ILE:O      | 2.17                     | 0.44              |
| 1:Q:211:ALA:CB   | 1:Q:226:ASN:HA     | 2.46                     | 0.44              |
| 1:Q:327:ILE:O    | 1:Q:331:LYS:HG2    | 2.17                     | 0.44              |
| 1:A:194:ARG:HG2  | 1:C:277:PRO:O      | 2.18                     | 0.44              |
| 1:O:11:ILE:HD11  | 3:O:372:NDP:H42N   | 1.98                     | 0.44              |
| 1:P:34:GLY:HA3   | 1:P:39:GLN:OE1     | 2.17                     | 0.44              |
| 1:Q:33:THR:HA    | 1:Q:75:SER:OG      | 2.18                     | 0.44              |
| 1:A:266:GLU:HG2  | 1:A:267:LEU:HG     | 1.99                     | 0.44              |
| 1:B:170:GLY:HA3  | 1:B:244:VAL:HG12   | 1.99                     | 0.44              |
| 1:C:84:TRP:CE3   | 1:C:84:TRP:HA      | 2.53                     | 0.44              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:B:227:GLY:O    | 1:D:298:MET:HE1    | 2.17                     | 0.44              |
| 1:I:58:LYS:HZ3   | 1:I:58:LYS:HB3     | 1.82                     | 0.44              |
| 1:A:103:ASP:OD1  | 1:A:103:ASP:O      | 2.35                     | 0.44              |
| 1:B:172:MET:CE   | 1:B:211:ALA:N      | 2.72                     | 0.44              |
| 1:I:84:TRP:CE3   | 1:I:84:TRP:HA      | 2.53                     | 0.44              |
| 1:R:117:LEU:HD23 | 1:R:117:LEU:C      | 2.38                     | 0.44              |
| 1:R:99:PHE:HZ    | 3:R:377:NDP:N6A    | 2.14                     | 0.44              |
| 1:A:176:HIS:HB3  | 1:A:231:ARG:HD3    | 1.99                     | 0.44              |
| 1:B:100:VAL:HG23 | 1:B:122(A):LYS:HG2 | 1.99                     | 0.44              |
| 1:I:194:ARG:HD3  | 1:M:278:LEU:O      | 2.18                     | 0.44              |
| 1:O:165:PHE:CB   | 1:O:248:LYS:CG     | 2.95                     | 0.44              |
| 1:O:300:MET:HE2  | 1:P:224:LYS:O      | 2.18                     | 0.44              |
| 1:Q:120:ALA:CB   | 3:Q:375:NDP:H2D    | 2.40                     | 0.44              |
| 1:A:18:CYS:SG    | 1:A:319:GLN:HG2    | 2.58                     | 0.44              |
| 1:H:77:ARG:HH11  | 3:H:379:NDP:C6A    | 2.30                     | 0.44              |
| 1:P:204:VAL:HB   | 1:P:231:ARG:HB2    | 2.00                     | 0.44              |
| 1:P:261:GLU:OE1  | 1:P:262:SER:N      | 2.50                     | 0.44              |
| 1:A:0:LYS:HD3    | 1:A:0:LYS:C        | 2.37                     | 0.44              |
| 1:B:9:GLY:HA3    | 3:B:378:NDP:O5B    | 2.18                     | 0.44              |
| 1:B:281:ILE:CB   | 1:D:202:ASN:ND2    | 2.65                     | 0.44              |
| 1:C:201:LEU:HD21 | 1:D:235:PRO:HG3    | 1.99                     | 0.44              |
| 1:D:236:ASN:O    | 1:D:237:VAL:HB     | 2.18                     | 0.44              |
| 1:O:191:ARG:HA   | 1:O:191:ARG:HD2    | 1.80                     | 0.44              |
| 1:O:300:MET:HG3  | 1:P:170:GLY:O      | 2.18                     | 0.44              |
| 1:P:84:TRP:HA    | 1:P:84:TRP:HE3     | 1.83                     | 0.44              |
| 1:Q:320:ARG:NE   | 1:Q:320:ARG:HA     | 2.33                     | 0.44              |
| 1:A:205:PRO:CG   | 1:C:310:TRP:CZ2    | 3.01                     | 0.44              |
| 1:H:82:LEU:HD13  | 1:H:84:TRP:CZ2     | 2.53                     | 0.44              |
| 1:B:204:VAL:HB   | 1:B:231:ARG:HB2    | 2.00                     | 0.43              |
| 1:B:29:VAL:HG22  | 1:B:30:ILE:N       | 2.32                     | 0.43              |
| 1:C:2:LYS:HD2    | 1:C:28:VAL:HG11    | 1.99                     | 0.43              |
| 1:M:200:CYS:HB2  | 4:M:383:HOH:O      | 2.17                     | 0.43              |
| 1:O:120:ALA:CB   | 3:O:372:NDP:H2D    | 2.44                     | 0.43              |
| 1:Q:242:LEU:HD13 | 1:Q:242:LEU:HA     | 1.73                     | 0.43              |
| 1:Q:31:ASN:ND2   | 3:Q:375:NDP:H2A    | 2.33                     | 0.43              |
| 1:R:187:ALA:O    | 1:R:196:ALA:HB1    | 2.19                     | 0.43              |
| 1:H:95:GLY:O     | 3:H:379:NDP:H51A   | 2.18                     | 0.43              |
| 1:I:31:ASN:ND2   | 3:I:380:NDP:H2A    | 2.34                     | 0.43              |
| 1:L:11:ILE:HD11  | 3:L:369:NDP:H42N   | 2.00                     | 0.43              |
| 1:M:187:ALA:O    | 1:M:196:ALA:HB1    | 2.18                     | 0.43              |
| 1:P:197:ARG:HH21 | 1:Q:48:SER:N       | 2.16                     | 0.43              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:R:160:VAL:HG13 | 1:R:164:LYS:HZ2    | 1.83                     | 0.43              |
| 1:A:153:CYS:SG   | 1:A:240:VAL:CG2    | 3.06                     | 0.43              |
| 1:D:172:MET:CE   | 1:D:211:ALA:HB2    | 2.47                     | 0.43              |
| 1:I:187:ALA:O    | 1:I:196:ALA:HB1    | 2.18                     | 0.43              |
| 1:I:170:GLY:HA3  | 1:I:244:VAL:HG12   | 1.99                     | 0.43              |
| 1:M:185:LEU:O    | 1:M:186:ASP:C      | 2.57                     | 0.43              |
| 1:O:203:ILE:HB   | 1:P:280:SER:HB3    | 2.01                     | 0.43              |
| 1:O:228:ILE:CG1  | 1:O:229:ALA:H      | 2.14                     | 0.43              |
| 1:P:25:LEU:HD11  | 1:P:325:ALA:HB3    | 2.00                     | 0.43              |
| 1:R:238:SER:HB2  | 1:R:311:TYR:CZ     | 2.53                     | 0.43              |
| 1:A:98:VAL:HG23  | 1:A:99:PHE:CE2     | 2.52                     | 0.43              |
| 1:B:154:LEU:HD23 | 1:B:214:VAL:HG21   | 1.99                     | 0.43              |
| 1:D:172:MET:SD   | 1:D:227:GLY:HA3    | 2.58                     | 0.43              |
| 1:L:179:THR:OG1  | 2:L:367:SO4:O4     | 2.22                     | 0.43              |
| 1:M:251:PHE:CZ   | 1:M:254:GLU:HB2    | 2.53                     | 0.43              |
| 1:P:135:GLU:N    | 1:P:135:GLU:CD     | 2.67                     | 0.43              |
| 1:P:84:TRP:HA    | 1:P:84:TRP:CE3     | 2.53                     | 0.43              |
| 1:Q:11:ILE:HG13  | 3:Q:375:NDP:H1D    | 2.01                     | 0.43              |
| 1:R:178:TYR:HA   | 1:R:182:GLN:OE1    | 2.18                     | 0.43              |
| 1:H:133:ASN:HD22 | 1:H:133:ASN:N      | 2.14                     | 0.43              |
| 1:H:231:ARG:NH2  | 2:H:363:SO4:O2     | 2.36                     | 0.43              |
| 1:M:170:GLY:HA3  | 1:M:244:VAL:HG12   | 2.00                     | 0.43              |
| 1:Q:97:GLY:HA3   | 3:Q:375:NDP:O3D    | 2.18                     | 0.43              |
| 1:R:1:LEU:HD23   | 1:R:25:LEU:HD23    | 2.00                     | 0.43              |
| 1:R:165:PHE:CB   | 1:R:248:LYS:HG3    | 2.48                     | 0.43              |
| 1:I:236:ASN:O    | 1:I:237:VAL:CB     | 2.66                     | 0.43              |
| 1:M:120:ALA:HB2  | 3:M:381:NDP:C2D    | 2.49                     | 0.43              |
| 1:B:117:LEU:C    | 1:B:117:LEU:HD23   | 2.39                     | 0.43              |
| 1:B:241:ASP:OD1  | 1:B:306:LYS:CE     | 2.53                     | 0.43              |
| 1:C:100:VAL:HG23 | 1:C:122(A):LYS:HG2 | 2.01                     | 0.43              |
| 1:D:33:THR:HA    | 1:D:75:SER:HG      | 1.79                     | 0.43              |
| 1:M:204:VAL:HB   | 1:M:231:ARG:HB2    | 2.00                     | 0.43              |
| 1:O:248:LYS:HE2  | 1:O:248:LYS:HB2    | 1.64                     | 0.43              |
| 1:P:33:THR:HA    | 1:P:75:SER:OG      | 2.18                     | 0.43              |
| 1:P:149:CYS:HB3  | 3:P:373:NDP:H41N   | 2.01                     | 0.43              |
| 1:A:289:SER:OG   | 1:A:320:ARG:HD2    | 2.18                     | 0.43              |
| 1:L:9:GLY:O      | 1:L:13:ARG:HG3     | 2.19                     | 0.43              |
| 1:M:31:ASN:ND2   | 3:M:381:NDP:H2A    | 2.33                     | 0.43              |
| 1:O:281:ILE:CD1  | 1:O:284:ARG:HD2    | 2.49                     | 0.43              |
| 1:R:169:LYS:NZ   | 1:Q:303:ASP:OD1    | 2.50                     | 0.43              |
| 1:R:228:ILE:HD11 | 1:Q:306:LYS:NZ     | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:243:VAL:HG11 | 1:C:243:VAL:HG11 | 2.01                     | 0.43              |
| 1:A:31:ASN:ND2   | 3:A:376:NDP:H2A  | 2.33                     | 0.43              |
| 1:A:54:ASP:O     | 1:A:54:ASP:OD1   | 2.37                     | 0.43              |
| 1:C:9:GLY:HA3    | 3:C:365:NDP:O5B  | 2.19                     | 0.43              |
| 1:D:187:ALA:O    | 1:D:196:ALA:HB1  | 2.19                     | 0.43              |
| 1:I:84:TRP:CD1   | 1:I:113:ALA:HB2  | 2.54                     | 0.43              |
| 1:R:133:ASN:N    | 1:R:133:ASN:HD22 | 2.17                     | 0.43              |
| 1:B:197:ARG:HH12 | 1:D:282:ASP:CG   | 2.22                     | 0.43              |
| 1:I:172:MET:HG2  | 1:I:173:THR:H    | 1.83                     | 0.43              |
| 1:I:9:GLY:HA3    | 3:I:380:NDP:O5B  | 2.19                     | 0.43              |
| 1:L:157:PHE:HB2  | 1:L:259:PHE:CE1  | 2.54                     | 0.43              |
| 1:P:186:ASP:OD1  | 1:Q:48:SER:HB2   | 2.19                     | 0.43              |
| 1:Q:222:LYS:HD2  | 1:Q:222:LYS:HA   | 1.67                     | 0.43              |
| 1:A:95:GLY:O     | 3:A:376:NDP:H51A | 2.19                     | 0.42              |
| 1:M:250:THR:OG1  | 1:M:251:PHE:N    | 2.51                     | 0.42              |
| 1:P:97:GLY:CA    | 3:P:373:NDP:O3D  | 2.67                     | 0.42              |
| 1:R:245:GLN:HE22 | 1:Q:245:GLN:HE22 | 1.65                     | 0.42              |
| 1:R:202:ASN:ND2  | 1:Q:281:ILE:CB   | 2.70                     | 0.42              |
| 1:B:98:VAL:HG23  | 1:B:99:PHE:CE2   | 2.54                     | 0.42              |
| 1:C:106:GLY:HA3  | 1:I:110:GLN:NE2  | 2.33                     | 0.42              |
| 1:A:224:LYS:O    | 1:C:300:MET:HE2  | 2.19                     | 0.42              |
| 1:C:235:PRO:HG3  | 1:D:201:LEU:HD21 | 2.01                     | 0.42              |
| 1:H:98:VAL:HG23  | 1:H:99:PHE:CD2   | 2.54                     | 0.42              |
| 1:L:289:SER:OG   | 1:L:320:ARG:HD2  | 2.19                     | 0.42              |
| 1:O:310:TRP:CZ2  | 1:P:205:PRO:HG2  | 2.49                     | 0.42              |
| 1:A:163:GLN:HG2  | 1:A:164:LYS:N    | 2.35                     | 0.42              |
| 1:A:188:SER:HA   | 1:B:39:GLN:OE1   | 2.19                     | 0.42              |
| 1:C:106:GLY:CA   | 1:I:110:GLN:NE2  | 2.82                     | 0.42              |
| 1:B:120:ALA:CB   | 3:B:378:NDP:H2D  | 2.43                     | 0.42              |
| 1:D:0:LYS:HA     | 1:D:0:LYS:HD2    | 1.95                     | 0.42              |
| 1:L:84:TRP:CA    | 1:L:84:TRP:CE3   | 3.02                     | 0.42              |
| 1:O:95:GLY:O     | 3:O:372:NDP:H51A | 2.19                     | 0.42              |
| 1:R:300:MET:CE   | 1:Q:226:ASN:HB2  | 2.47                     | 0.42              |
| 1:Q:45:LYS:HB3   | 2:Q:373:SO4:O1   | 2.19                     | 0.42              |
| 1:R:106:GLY:O    | 1:R:109:LEU:N    | 2.48                     | 0.42              |
| 1:R:137:TYR:HE2  | 1:R:331:LYS:HB2  | 1.84                     | 0.42              |
| 1:A:157:PHE:HB2  | 1:A:259:PHE:CE1  | 2.55                     | 0.42              |
| 1:A:194:ARG:CZ   | 1:C:277:PRO:HA   | 2.49                     | 0.42              |
| 1:C:56:ASP:CA    | 1:C:58:LYS:HZ1   | 2.33                     | 0.42              |
| 1:I:281:ILE:CB   | 1:M:202:ASN:ND2  | 2.65                     | 0.42              |
| 1:I:202:ASN:ND2  | 1:M:281:ILE:CB   | 2.66                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:163:GLN:NE2  | 1:O:164:LYS:HZ3  | 2.02                     | 0.42              |
| 1:O:281:ILE:HG21 | 1:Q:48:SER:CA    | 2.44                     | 0.42              |
| 1:Q:236:ASN:O    | 1:Q:237:VAL:HB   | 2.18                     | 0.42              |
| 1:R:327:ILE:O    | 1:R:331:LYS:HG2  | 2.20                     | 0.42              |
| 1:A:163:GLN:CG   | 1:A:164:LYS:N    | 2.82                     | 0.42              |
| 1:A:236:ASN:O    | 1:A:237:VAL:CB   | 2.67                     | 0.42              |
| 1:B:320:ARG:NE   | 1:B:320:ARG:HA   | 2.35                     | 0.42              |
| 1:I:48:SER:CA    | 1:L:281:ILE:HG21 | 2.48                     | 0.42              |
| 1:I:226:ASN:ND2  | 1:M:298:MET:CE   | 2.82                     | 0.42              |
| 1:P:208:THR:HG21 | 1:P:228:ILE:O    | 2.18                     | 0.42              |
| 1:P:95:GLY:O     | 3:P:373:NDP:H51A | 2.19                     | 0.42              |
| 1:A:212:LYS:C    | 1:A:214:VAL:N    | 2.73                     | 0.42              |
| 1:A:149:CYS:HB3  | 3:A:376:NDP:H41N | 2.01                     | 0.42              |
| 1:D:106:GLY:O    | 1:D:109:LEU:N    | 2.49                     | 0.42              |
| 1:O:202:ASN:ND2  | 1:P:281:ILE:CB   | 2.71                     | 0.42              |
| 1:O:282:ASP:OD2  | 1:P:197:ARG:NH1  | 2.52                     | 0.42              |
| 1:P:29:VAL:HG22  | 1:P:30:ILE:N     | 2.35                     | 0.42              |
| 3:O:372:NDP:O3X  | 1:R:188:SER:HB2  | 2.19                     | 0.42              |
| 1:R:164:LYS:C    | 1:R:248:LYS:HD2  | 2.39                     | 0.42              |
| 1:A:154:LEU:HD23 | 1:A:214:VAL:HG21 | 2.02                     | 0.42              |
| 1:B:213:ALA:O    | 1:B:216:LEU:HB2  | 2.19                     | 0.42              |
| 1:D:115:LYS:NZ   | 1:D:141:ASP:O    | 2.50                     | 0.42              |
| 1:L:10:ARG:HH11  | 1:L:13:ARG:NH2   | 2.18                     | 0.42              |
| 1:L:48:SER:N     | 1:M:197:ARG:HH21 | 2.17                     | 0.42              |
| 1:O:9:GLY:HA3    | 3:O:372:NDP:O5B  | 2.20                     | 0.42              |
| 1:Q:240:VAL:HG23 | 1:Q:311:TYR:CE1  | 2.55                     | 0.42              |
| 1:A:154:LEU:HD12 | 1:A:157:PHE:CZ   | 2.55                     | 0.42              |
| 1:H:194:ARG:HD3  | 1:L:278:LEU:O    | 2.20                     | 0.42              |
| 1:I:191:ARG:HB3  | 1:I:191:ARG:NH1  | 2.34                     | 0.42              |
| 1:I:1:LEU:HD22   | 1:I:329:ALA:HB2  | 2.02                     | 0.42              |
| 1:M:190:HIS:HB3  | 1:M:196:ALA:HB2  | 2.02                     | 0.42              |
| 1:O:303:ASP:OD1  | 1:P:169:LYS:NZ   | 2.51                     | 0.42              |
| 1:P:42:HIS:CG    | 1:Q:193:LEU:HD13 | 2.54                     | 0.42              |
| 1:Q:97:GLY:CA    | 3:Q:375:NDP:O3D  | 2.68                     | 0.42              |
| 1:B:11:ILE:HG13  | 3:B:378:NDP:H1D  | 2.02                     | 0.42              |
| 1:C:84:TRP:HE3   | 1:C:84:TRP:HA    | 1.84                     | 0.42              |
| 1:D:133:ASN:HD22 | 1:D:133:ASN:N    | 2.18                     | 0.42              |
| 1:D:240:VAL:HG13 | 1:D:311:TYR:CE1  | 2.55                     | 0.42              |
| 1:M:236:ASN:O    | 1:M:237:VAL:CB   | 2.68                     | 0.42              |
| 1:O:9:GLY:O      | 1:O:13:ARG:HG3   | 2.20                     | 0.42              |
| 1:Q:248:LYS:HB2  | 1:Q:248:LYS:HE2  | 1.66                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:106:GLY:CA   | 1:I:110:GLN:HE22 | 2.30                     | 0.41              |
| 1:L:158:VAL:HG11 | 1:L:221:LEU:HD13 | 1.99                     | 0.41              |
| 1:Q:37:VAL:HG21  | 1:Q:62:SER:HA    | 2.02                     | 0.41              |
| 1:A:33:THR:HA    | 1:A:75:SER:OG    | 2.20                     | 0.41              |
| 1:D:117:LEU:HD23 | 1:D:117:LEU:C    | 2.40                     | 0.41              |
| 1:H:79:PRO:HA    | 1:H:82:LEU:CD1   | 2.51                     | 0.41              |
| 1:O:149:CYS:HB3  | 3:O:372:NDP:H41N | 2.01                     | 0.41              |
| 1:P:168:ILE:HG22 | 1:P:169:LYS:HD3  | 2.01                     | 0.41              |
| 1:C:320:ARG:HA   | 1:C:320:ARG:NE   | 2.35                     | 0.41              |
| 1:C:39:GLN:HG3   | 1:D:193:LEU:HD21 | 2.02                     | 0.41              |
| 1:L:96:THR:OG1   | 1:L:98:VAL:HG22  | 2.19                     | 0.41              |
| 1:Q:9:GLY:HA3    | 3:Q:375:NDP:O5B  | 2.20                     | 0.41              |
| 1:B:30:ILE:HG13  | 1:B:71:ILE:HG21  | 2.02                     | 0.41              |
| 1:C:80:VAL:HG13  | 1:C:107:LYS:NZ   | 2.34                     | 0.41              |
| 1:H:289:SER:OG   | 1:H:320:ARG:HD2  | 2.20                     | 0.41              |
| 1:I:168:ILE:HG22 | 1:I:169:LYS:HD3  | 2.01                     | 0.41              |
| 1:M:191:ARG:NH1  | 1:M:191:ARG:HB3  | 2.35                     | 0.41              |
| 1:O:228:ILE:CG1  | 1:O:229:ALA:N    | 2.68                     | 0.41              |
| 1:O:320:ARG:NE   | 1:O:320:ARG:HA   | 2.36                     | 0.41              |
| 1:O:97:GLY:HA2   | 3:O:372:NDP:O3D  | 2.20                     | 0.41              |
| 1:O:300:MET:CG   | 1:P:171:THR:HG22 | 2.50                     | 0.41              |
| 1:P:148:SER:OG   | 2:P:364:SO4:O3   | 2.38                     | 0.41              |
| 1:D:133:ASN:ND2  | 1:D:133:ASN:C    | 2.73                     | 0.41              |
| 1:D:133:ASN:HD22 | 1:D:133:ASN:H    | 1.67                     | 0.41              |
| 1:H:252:ALA:N    | 2:H:378:SO4:O3   | 2.28                     | 0.41              |
| 1:I:204:VAL:HB   | 1:I:231:ARG:HB2  | 2.02                     | 0.41              |
| 1:I:9:GLY:O      | 1:I:13:ARG:HG3   | 2.20                     | 0.41              |
| 1:H:280:SER:HB3  | 1:L:203:ILE:HB   | 2.01                     | 0.41              |
| 1:M:157:PHE:HB2  | 1:M:259:PHE:CE1  | 2.55                     | 0.41              |
| 1:O:220:ASN:N    | 1:O:220:ASN:OD1  | 2.54                     | 0.41              |
| 1:O:63:ALA:HB1   | 1:O:71:ILE:O     | 2.20                     | 0.41              |
| 1:Q:61:ASP:OD1   | 1:Q:61:ASP:C     | 2.58                     | 0.41              |
| 1:B:185:LEU:O    | 1:B:186:ASP:C    | 2.57                     | 0.41              |
| 1:I:183:ARG:HH12 | 1:I:187:ALA:HB1  | 1.85                     | 0.41              |
| 1:P:208:THR:CG2  | 1:P:228:ILE:N    | 2.83                     | 0.41              |
| 1:Q:120:ALA:HB1  | 1:Q:121:PRO:CD   | 2.51                     | 0.41              |
| 1:R:253:GLU:OE1  | 1:R:253:GLU:HA   | 2.19                     | 0.41              |
| 1:A:39:GLN:OE1   | 1:B:188:SER:CB   | 2.57                     | 0.41              |
| 1:D:34:GLY:HA3   | 1:D:39:GLN:OE1   | 2.20                     | 0.41              |
| 1:O:153:CYS:HA   | 1:O:290:SER:HB2  | 2.03                     | 0.41              |
| 1:O:300:MET:HG3  | 1:P:171:THR:HG22 | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:256:ASN:OD1  | 2:P:372:SO4:O1   | 2.39                     | 0.41              |
| 1:P:39:GLN:OE1   | 1:Q:188:SER:CB   | 2.67                     | 0.41              |
| 1:R:281:ILE:N    | 1:Q:202:ASN:ND2  | 2.53                     | 0.41              |
| 1:R:191:ARG:HB3  | 1:R:191:ARG:NH1  | 2.35                     | 0.41              |
| 1:R:213:ALA:O    | 1:R:216:LEU:HB2  | 2.20                     | 0.41              |
| 1:R:95:GLY:O     | 3:R:377:NDP:H51A | 2.21                     | 0.41              |
| 1:A:163:GLN:NE2  | 1:A:164:LYS:CE   | 2.71                     | 0.41              |
| 1:A:197:ARG:HH12 | 1:C:282:ASP:CG   | 2.24                     | 0.41              |
| 1:C:126:PRO:HD2  | 1:C:143:ILE:O    | 2.21                     | 0.41              |
| 1:A:281:ILE:CB   | 1:C:202:ASN:ND2  | 2.72                     | 0.41              |
| 1:D:159:LYS:O    | 1:D:163:GLN:HG3  | 2.19                     | 0.41              |
| 1:D:208:THR:HG22 | 1:D:228:ILE:HA   | 2.02                     | 0.41              |
| 1:H:209:GLY:O    | 1:H:213:ALA:HB2  | 2.20                     | 0.41              |
| 1:I:228:ILE:HD12 | 1:I:228:ILE:C    | 2.41                     | 0.41              |
| 1:I:232:VAL:HA   | 1:I:233:PRO:HD3  | 1.86                     | 0.41              |
| 1:I:84:TRP:HA    | 1:I:84:TRP:HE3   | 1.85                     | 0.41              |
| 1:P:184:LEU:HD21 | 1:Q:199:ALA:HB3  | 2.03                     | 0.41              |
| 1:P:241:ASP:OD1  | 1:P:306:LYS:HE2  | 2.20                     | 0.41              |
| 1:R:310:TRP:CZ2  | 1:Q:205:PRO:HG3  | 2.56                     | 0.41              |
| 1:R:80:VAL:HG23  | 1:R:81:ASN:ND2   | 2.36                     | 0.41              |
| 1:A:9:GLY:HA3    | 3:A:376:NDP:C5B  | 2.51                     | 0.41              |
| 1:B:1:LEU:HD21   | 1:B:91:LEU:HB3   | 2.02                     | 0.41              |
| 1:C:213:ALA:O    | 1:C:216:LEU:HB2  | 2.21                     | 0.41              |
| 1:I:133:ASN:N    | 1:I:133:ASN:HD22 | 2.19                     | 0.41              |
| 1:L:193:LEU:CD2  | 1:M:39:GLN:HG3   | 2.50                     | 0.41              |
| 1:O:1:LEU:HA     | 1:O:1:LEU:HD12   | 1.70                     | 0.41              |
| 1:O:298:MET:CE   | 1:P:226:ASN:CG   | 2.89                     | 0.41              |
| 1:P:154:LEU:HD12 | 1:P:157:PHE:CZ   | 2.56                     | 0.41              |
| 1:P:332:TRP:CD1  | 1:P:334:GLY:HA3  | 2.56                     | 0.41              |
| 1:Q:261:GLU:HA   | 1:Q:261:GLU:OE1  | 2.20                     | 0.41              |
| 1:R:205:PRO:HG2  | 1:Q:310:TRP:HZ2  | 1.85                     | 0.41              |
| 1:D:95:GLY:O     | 3:D:365:NDP:H51A | 2.21                     | 0.41              |
| 1:I:226:ASN:HB2  | 1:M:300:MET:SD   | 2.61                     | 0.41              |
| 1:P:27:VAL:CG1   | 1:P:71:ILE:CD1   | 2.79                     | 0.41              |
| 1:R:172:MET:SD   | 1:R:227:GLY:HA3  | 2.61                     | 0.41              |
| 1:A:56:ASP:OD1   | 1:A:58:LYS:HE2   | 2.21                     | 0.41              |
| 1:A:80:VAL:HG23  | 1:A:81:ASN:ND2   | 2.36                     | 0.41              |
| 1:B:194:ARG:HD3  | 1:D:278:LEU:O    | 2.21                     | 0.41              |
| 1:C:154:LEU:HD23 | 1:C:214:VAL:HG21 | 2.03                     | 0.41              |
| 1:C:186:ASP:HA   | 1:C:196:ALA:O    | 2.21                     | 0.41              |
| 1:L:185:LEU:O    | 1:L:186:ASP:C    | 2.59                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:185:LEU:O    | 1:Q:186:ASP:C    | 2.59                     | 0.41              |
| 1:B:150:THR:HB   | 2:B:364:SO4:O2   | 2.21                     | 0.40              |
| 1:B:165:PHE:C    | 1:B:248:LYS:CG   | 2.90                     | 0.40              |
| 1:C:77:ARG:HA    | 3:C:365:NDP:N1A  | 2.36                     | 0.40              |
| 1:B:16:LEU:HD23  | 1:B:16:LEU:O     | 2.22                     | 0.40              |
| 1:C:80:VAL:HG23  | 1:C:81:ASN:ND2   | 2.36                     | 0.40              |
| 1:D:126:PRO:HD2  | 1:D:143:ILE:O    | 2.20                     | 0.40              |
| 1:H:281:ILE:HG12 | 1:M:48:SER:HA    | 2.04                     | 0.40              |
| 1:I:208:THR:CG2  | 1:I:228:ILE:HA   | 2.51                     | 0.40              |
| 1:L:120:ALA:HB2  | 3:L:369:NDP:C2D  | 2.51                     | 0.40              |
| 1:L:34:GLY:HA3   | 1:L:39:GLN:OE1   | 2.22                     | 0.40              |
| 1:O:154:LEU:HD23 | 1:O:214:VAL:HG21 | 2.03                     | 0.40              |
| 1:Q:117:LEU:HD23 | 1:Q:117:LEU:C    | 2.41                     | 0.40              |
| 1:R:236:ASN:O    | 1:R:237:VAL:CB   | 2.69                     | 0.40              |
| 1:B:190:HIS:HB3  | 1:B:196:ALA:HB2  | 2.03                     | 0.40              |
| 1:H:159:LYS:O    | 1:H:163:GLN:HG3  | 2.22                     | 0.40              |
| 1:M:84:TRP:HA    | 1:M:84:TRP:CE3   | 2.57                     | 0.40              |
| 1:Q:261:GLU:O    | 1:Q:261:GLU:OE1  | 2.40                     | 0.40              |
| 1:A:103:ASP:OD1  | 1:A:103:ASP:C    | 2.60                     | 0.40              |
| 1:C:190:HIS:HB3  | 1:C:196:ALA:HB2  | 2.03                     | 0.40              |
| 1:O:232:VAL:HA   | 1:O:233:PRO:HD3  | 1.82                     | 0.40              |
| 1:A:193:LEU:HD13 | 1:B:42:HIS:CG    | 2.56                     | 0.40              |
| 1:H:10:ARG:HH11  | 1:H:13:ARG:NH2   | 2.19                     | 0.40              |
| 1:M:101:ASP:CG   | 1:M:103:ASP:OD1  | 2.59                     | 0.40              |
| 1:M:9:GLY:O      | 1:M:13:ARG:HG3   | 2.22                     | 0.40              |
| 1:P:37:VAL:HG21  | 1:P:62:SER:HA    | 2.03                     | 0.40              |
| 1:P:82:LEU:HD13  | 1:P:84:TRP:CE2   | 2.54                     | 0.40              |
| 1:R:282:ASP:CG   | 1:Q:197:ARG:HH12 | 2.23                     | 0.40              |
| 1:Q:61:ASP:CG    | 1:Q:61:ASP:O     | 2.59                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|------------------------|--------------------------|-------------------|
| 1:Q:62:SER:OG | 1:L:253:GLU:OE2[2_555] | 2.19                     | 0.01              |

## 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     | 335/365 (92%)   | 308 (92%)  | 23 (7%)  | 4 (1%)   | 13          | 19 |
| 1   | B     | 335/365 (92%)   | 313 (93%)  | 17 (5%)  | 5 (2%)   | 10          | 14 |
| 1   | C     | 335/365 (92%)   | 315 (94%)  | 19 (6%)  | 1 (0%)   | 41          | 55 |
| 1   | D     | 334/365 (92%)   | 318 (95%)  | 13 (4%)  | 3 (1%)   | 17          | 25 |
| 1   | H     | 334/365 (92%)   | 314 (94%)  | 17 (5%)  | 3 (1%)   | 17          | 25 |
| 1   | I     | 335/365 (92%)   | 316 (94%)  | 16 (5%)  | 3 (1%)   | 17          | 25 |
| 1   | L     | 334/365 (92%)   | 315 (94%)  | 15 (4%)  | 4 (1%)   | 13          | 19 |
| 1   | M     | 335/365 (92%)   | 312 (93%)  | 22 (7%)  | 1 (0%)   | 41          | 55 |
| 1   | O     | 335/365 (92%)   | 317 (95%)  | 16 (5%)  | 2 (1%)   | 25          | 36 |
| 1   | P     | 335/365 (92%)   | 312 (93%)  | 21 (6%)  | 2 (1%)   | 25          | 36 |
| 1   | Q     | 335/365 (92%)   | 309 (92%)  | 25 (8%)  | 1 (0%)   | 41          | 55 |
| 1   | R     | 335/365 (92%)   | 312 (93%)  | 19 (6%)  | 4 (1%)   | 13          | 19 |
| All | All   | 4017/4380 (92%) | 3761 (94%) | 223 (6%) | 33 (1%)  | 19          | 29 |

All (33) Ramachandran outliers are listed below:

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | R     | 1     | LEU  |
| 1   | R     | 60(A) | GLY  |
| 1   | P     | 209   | GLY  |
| 1   | A     | 209   | GLY  |
| 1   | A     | 211   | ALA  |
| 1   | B     | 207   | SER  |
| 1   | B     | 211   | ALA  |
| 1   | B     | 212   | LYS  |
| 1   | R     | 237   | VAL  |
| 1   | P     | 237   | VAL  |
| 1   | Q     | 237   | VAL  |
| 1   | A     | 237   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 237 | VAL  |
| 1   | C     | 237 | VAL  |
| 1   | D     | 237 | VAL  |
| 1   | H     | 208 | THR  |
| 1   | H     | 237 | VAL  |
| 1   | I     | 237 | VAL  |
| 1   | L     | 237 | VAL  |
| 1   | M     | 237 | VAL  |
| 1   | O     | 237 | VAL  |
| 1   | I     | 62  | SER  |
| 1   | L     | 86  | ASP  |
| 1   | L     | 302 | ASP  |
| 1   | D     | 198 | ALA  |
| 1   | H     | 302 | ASP  |
| 1   | A     | 166 | GLY  |
| 1   | B     | 166 | GLY  |
| 1   | D     | 166 | GLY  |
| 1   | L     | 166 | GLY  |
| 1   | R     | 166 | GLY  |
| 1   | O     | 166 | GLY  |
| 1   | I     | 166 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 279/303 (92%) | 262 (94%) | 17 (6%)  | 18          | 30 |
| 1   | B     | 279/303 (92%) | 269 (96%) | 10 (4%)  | 35          | 54 |
| 1   | C     | 279/303 (92%) | 267 (96%) | 12 (4%)  | 29          | 46 |
| 1   | D     | 279/303 (92%) | 269 (96%) | 10 (4%)  | 35          | 54 |
| 1   | H     | 279/303 (92%) | 264 (95%) | 15 (5%)  | 22          | 36 |
| 1   | I     | 279/303 (92%) | 267 (96%) | 12 (4%)  | 29          | 46 |
| 1   | L     | 279/303 (92%) | 269 (96%) | 10 (4%)  | 35          | 54 |
| 1   | M     | 279/303 (92%) | 266 (95%) | 13 (5%)  | 26          | 42 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | O     | 279/303 (92%)   | 262 (94%)  | 17 (6%)  | 18          | 30 |
| 1   | P     | 279/303 (92%)   | 256 (92%)  | 23 (8%)  | 11          | 17 |
| 1   | Q     | 279/303 (92%)   | 265 (95%)  | 14 (5%)  | 24          | 40 |
| 1   | R     | 279/303 (92%)   | 262 (94%)  | 17 (6%)  | 18          | 30 |
| All | All   | 3348/3636 (92%) | 3178 (95%) | 170 (5%) | 24          | 39 |

All (170) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 0   | LYS  |
| 1   | O     | 53  | PHE  |
| 1   | O     | 61  | ASP  |
| 1   | O     | 75  | SER  |
| 1   | O     | 83  | PRO  |
| 1   | O     | 84  | TRP  |
| 1   | O     | 94  | GLU  |
| 1   | O     | 133 | ASN  |
| 1   | O     | 164 | LYS  |
| 1   | O     | 172 | MET  |
| 1   | O     | 191 | ARG  |
| 1   | O     | 208 | THR  |
| 1   | O     | 220 | ASN  |
| 1   | O     | 248 | LYS  |
| 1   | O     | 276 | GLU  |
| 1   | O     | 281 | ILE  |
| 1   | O     | 285 | CYS  |
| 1   | R     | 0   | LYS  |
| 1   | R     | 33  | THR  |
| 1   | R     | 58  | LYS  |
| 1   | R     | 62  | SER  |
| 1   | R     | 84  | TRP  |
| 1   | R     | 133 | ASN  |
| 1   | R     | 154 | LEU  |
| 1   | R     | 171 | THR  |
| 1   | R     | 172 | MET  |
| 1   | R     | 183 | ARG  |
| 1   | R     | 193 | LEU  |
| 1   | R     | 222 | LYS  |
| 1   | R     | 228 | ILE  |
| 1   | R     | 248 | LYS  |
| 1   | R     | 253 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 261 | GLU  |
| 1   | R     | 285 | CYS  |
| 1   | P     | 0   | LYS  |
| 1   | P     | 58  | LYS  |
| 1   | P     | 84  | TRP  |
| 1   | P     | 94  | GLU  |
| 1   | P     | 133 | ASN  |
| 1   | P     | 135 | GLU  |
| 1   | P     | 138 | THR  |
| 1   | P     | 164 | LYS  |
| 1   | P     | 172 | MET  |
| 1   | P     | 184 | LEU  |
| 1   | P     | 190 | HIS  |
| 1   | P     | 191 | ARG  |
| 1   | P     | 193 | LEU  |
| 1   | P     | 208 | THR  |
| 1   | P     | 221 | LEU  |
| 1   | P     | 222 | LYS  |
| 1   | P     | 261 | GLU  |
| 1   | P     | 266 | GLU  |
| 1   | P     | 272 | SER  |
| 1   | P     | 276 | GLU  |
| 1   | P     | 281 | ILE  |
| 1   | P     | 285 | CYS  |
| 1   | P     | 333 | GLN  |
| 1   | Q     | 61  | ASP  |
| 1   | Q     | 84  | TRP  |
| 1   | Q     | 94  | GLU  |
| 1   | Q     | 133 | ASN  |
| 1   | Q     | 164 | LYS  |
| 1   | Q     | 169 | LYS  |
| 1   | Q     | 172 | MET  |
| 1   | Q     | 191 | ARG  |
| 1   | Q     | 242 | LEU  |
| 1   | Q     | 248 | LYS  |
| 1   | Q     | 253 | GLU  |
| 1   | Q     | 261 | GLU  |
| 1   | Q     | 285 | CYS  |
| 1   | Q     | 333 | GLN  |
| 1   | A     | 2   | LYS  |
| 1   | A     | 38  | LYS  |
| 1   | A     | 84  | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 94  | GLU  |
| 1   | A     | 133 | ASN  |
| 1   | A     | 163 | GLN  |
| 1   | A     | 164 | LYS  |
| 1   | A     | 172 | MET  |
| 1   | A     | 184 | LEU  |
| 1   | A     | 191 | ARG  |
| 1   | A     | 207 | SER  |
| 1   | A     | 208 | THR  |
| 1   | A     | 240 | VAL  |
| 1   | A     | 266 | GLU  |
| 1   | A     | 276 | GLU  |
| 1   | A     | 285 | CYS  |
| 1   | A     | 333 | GLN  |
| 1   | B     | 0   | LYS  |
| 1   | B     | 1   | LEU  |
| 1   | B     | 2   | LYS  |
| 1   | B     | 84  | TRP  |
| 1   | B     | 133 | ASN  |
| 1   | B     | 164 | LYS  |
| 1   | B     | 172 | MET  |
| 1   | B     | 188 | SER  |
| 1   | B     | 248 | LYS  |
| 1   | B     | 285 | CYS  |
| 1   | C     | 0   | LYS  |
| 1   | C     | 21  | LYS  |
| 1   | C     | 56  | ASP  |
| 1   | C     | 58  | LYS  |
| 1   | C     | 83  | PRO  |
| 1   | C     | 84  | TRP  |
| 1   | C     | 94  | GLU  |
| 1   | C     | 133 | ASN  |
| 1   | C     | 164 | LYS  |
| 1   | C     | 172 | MET  |
| 1   | C     | 253 | GLU  |
| 1   | C     | 285 | CYS  |
| 1   | D     | 58  | LYS  |
| 1   | D     | 75  | SER  |
| 1   | D     | 83  | PRO  |
| 1   | D     | 84  | TRP  |
| 1   | D     | 94  | GLU  |
| 1   | D     | 103 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 133 | ASN  |
| 1   | D     | 164 | LYS  |
| 1   | D     | 172 | MET  |
| 1   | D     | 285 | CYS  |
| 1   | H     | 25  | LEU  |
| 1   | H     | 58  | LYS  |
| 1   | H     | 76  | ASP  |
| 1   | H     | 84  | TRP  |
| 1   | H     | 94  | GLU  |
| 1   | H     | 133 | ASN  |
| 1   | H     | 135 | GLU  |
| 1   | H     | 164 | LYS  |
| 1   | H     | 172 | MET  |
| 1   | H     | 206 | THR  |
| 1   | H     | 207 | SER  |
| 1   | H     | 212 | LYS  |
| 1   | H     | 221 | LEU  |
| 1   | H     | 247 | SER  |
| 1   | H     | 285 | CYS  |
| 1   | I     | 38  | LYS  |
| 1   | I     | 58  | LYS  |
| 1   | I     | 61  | ASP  |
| 1   | I     | 83  | PRO  |
| 1   | I     | 84  | TRP  |
| 1   | I     | 94  | GLU  |
| 1   | I     | 103 | ASP  |
| 1   | I     | 133 | ASN  |
| 1   | I     | 164 | LYS  |
| 1   | I     | 172 | MET  |
| 1   | I     | 208 | THR  |
| 1   | I     | 285 | CYS  |
| 1   | L     | 58  | LYS  |
| 1   | L     | 84  | TRP  |
| 1   | L     | 94  | GLU  |
| 1   | L     | 133 | ASN  |
| 1   | L     | 164 | LYS  |
| 1   | L     | 169 | LYS  |
| 1   | L     | 172 | MET  |
| 1   | L     | 188 | SER  |
| 1   | L     | 191 | ARG  |
| 1   | L     | 285 | CYS  |
| 1   | M     | 0   | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 21  | LYS  |
| 1   | M     | 58  | LYS  |
| 1   | M     | 61  | ASP  |
| 1   | M     | 84  | TRP  |
| 1   | M     | 94  | GLU  |
| 1   | M     | 133 | ASN  |
| 1   | M     | 163 | GLN  |
| 1   | M     | 164 | LYS  |
| 1   | M     | 172 | MET  |
| 1   | M     | 188 | SER  |
| 1   | M     | 228 | ILE  |
| 1   | M     | 285 | CYS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 42  | HIS  |
| 1   | O     | 81  | ASN  |
| 1   | O     | 133 | ASN  |
| 1   | O     | 152 | ASN  |
| 1   | O     | 163 | GLN  |
| 1   | O     | 202 | ASN  |
| 1   | O     | 256 | ASN  |
| 1   | O     | 330 | ASN  |
| 1   | R     | 81  | ASN  |
| 1   | R     | 133 | ASN  |
| 1   | R     | 139 | HIS  |
| 1   | R     | 152 | ASN  |
| 1   | R     | 202 | ASN  |
| 1   | R     | 245 | GLN  |
| 1   | R     | 256 | ASN  |
| 1   | R     | 330 | ASN  |
| 1   | P     | 42  | HIS  |
| 1   | P     | 133 | ASN  |
| 1   | P     | 139 | HIS  |
| 1   | P     | 152 | ASN  |
| 1   | P     | 202 | ASN  |
| 1   | P     | 256 | ASN  |
| 1   | P     | 330 | ASN  |
| 1   | Q     | 81  | ASN  |
| 1   | Q     | 133 | ASN  |
| 1   | Q     | 139 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Q     | 202 | ASN  |
| 1   | Q     | 256 | ASN  |
| 1   | Q     | 330 | ASN  |
| 1   | A     | 42  | HIS  |
| 1   | A     | 81  | ASN  |
| 1   | A     | 133 | ASN  |
| 1   | A     | 152 | ASN  |
| 1   | A     | 202 | ASN  |
| 1   | A     | 256 | ASN  |
| 1   | A     | 330 | ASN  |
| 1   | B     | 81  | ASN  |
| 1   | B     | 133 | ASN  |
| 1   | B     | 139 | HIS  |
| 1   | B     | 152 | ASN  |
| 1   | B     | 202 | ASN  |
| 1   | B     | 256 | ASN  |
| 1   | B     | 330 | ASN  |
| 1   | C     | 42  | HIS  |
| 1   | C     | 81  | ASN  |
| 1   | C     | 110 | GLN  |
| 1   | C     | 133 | ASN  |
| 1   | C     | 152 | ASN  |
| 1   | C     | 163 | GLN  |
| 1   | C     | 202 | ASN  |
| 1   | C     | 245 | GLN  |
| 1   | C     | 256 | ASN  |
| 1   | C     | 330 | ASN  |
| 1   | D     | 81  | ASN  |
| 1   | D     | 133 | ASN  |
| 1   | D     | 152 | ASN  |
| 1   | D     | 202 | ASN  |
| 1   | D     | 245 | GLN  |
| 1   | D     | 256 | ASN  |
| 1   | D     | 330 | ASN  |
| 1   | H     | 81  | ASN  |
| 1   | H     | 133 | ASN  |
| 1   | H     | 152 | ASN  |
| 1   | H     | 202 | ASN  |
| 1   | H     | 256 | ASN  |
| 1   | H     | 330 | ASN  |
| 1   | I     | 81  | ASN  |
| 1   | I     | 110 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 133 | ASN  |
| 1   | I     | 152 | ASN  |
| 1   | I     | 163 | GLN  |
| 1   | I     | 202 | ASN  |
| 1   | I     | 256 | ASN  |
| 1   | I     | 330 | ASN  |
| 1   | L     | 81  | ASN  |
| 1   | L     | 133 | ASN  |
| 1   | L     | 152 | ASN  |
| 1   | L     | 202 | ASN  |
| 1   | L     | 256 | ASN  |
| 1   | L     | 330 | ASN  |
| 1   | M     | 81  | ASN  |
| 1   | M     | 110 | GLN  |
| 1   | M     | 133 | ASN  |
| 1   | M     | 152 | ASN  |
| 1   | M     | 202 | ASN  |
| 1   | M     | 256 | ASN  |
| 1   | M     | 330 | 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

46 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 | $\# Z  > 2$ |
| 3   | NDP  | B     | 378 | -    | 45,52,52     | 4.07 | 24 (53%)    | 53,80,80    | 6.26 | 33 (62%)    |
| 2   | SO4  | A     | 363 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | D     | 363 | -    | 4,4,4        | 0.26 | 0           | 6,6,6       | 0.09 | 0           |
| 3   | NDP  | O     | 372 | -    | 45,52,52     | 4.48 | 24 (53%)    | 53,80,80    | 5.86 | 28 (52%)    |
| 3   | NDP  | M     | 381 | -    | 45,52,52     | 4.02 | 22 (48%)    | 53,80,80    | 6.15 | 32 (60%)    |
| 2   | SO4  | R     | 363 | -    | 4,4,4        | 0.25 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | Q     | 374 | -    | 4,4,4        | 0.33 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | L     | 368 | -    | 4,4,4        | 0.32 | 0           | 6,6,6       | 0.09 | 0           |
| 3   | NDP  | I     | 380 | -    | 45,52,52     | 4.03 | 23 (51%)    | 53,80,80    | 6.25 | 31 (58%)    |
| 2   | SO4  | H     | 364 | -    | 4,4,4        | 0.34 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | O     | 371 | -    | 4,4,4        | 0.31 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | H     | 378 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.10 | 0           |
| 2   | SO4  | P     | 364 | -    | 4,4,4        | 0.31 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | A     | 364 | -    | 4,4,4        | 0.32 | 0           | 6,6,6       | 0.09 | 0           |
| 3   | NDP  | R     | 377 | -    | 45,52,52     | 4.21 | 23 (51%)    | 53,80,80    | 6.10 | 31 (58%)    |
| 2   | SO4  | I     | 365 | -    | 4,4,4        | 0.23 | 0           | 6,6,6       | 0.08 | 0           |
| 3   | NDP  | A     | 376 | -    | 45,52,52     | 4.79 | 25 (55%)    | 53,80,80    | 5.80 | 35 (66%)    |
| 2   | SO4  | Q     | 373 | -    | 4,4,4        | 0.23 | 0           | 6,6,6       | 0.08 | 0           |
| 2   | SO4  | B     | 364 | -    | 4,4,4        | 0.30 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | R     | 376 | -    | 4,4,4        | 0.31 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | B     | 363 | -    | 4,4,4        | 0.21 | 0           | 6,6,6       | 0.08 | 0           |
| 2   | SO4  | D     | 364 | -    | 4,4,4        | 0.34 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | L     | 367 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | O     | 363 | -    | 4,4,4        | 0.23 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | C     | 364 | -    | 4,4,4        | 0.33 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | C     | 363 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | R     | 364 | -    | 4,4,4        | 0.31 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | O     | 364 | -    | 4,4,4        | 0.31 | 0           | 6,6,6       | 0.08 | 0           |
| 2   | SO4  | Q     | 363 | -    | 4,4,4        | 0.23 | 0           | 6,6,6       | 0.08 | 0           |
| 2   | SO4  | P     | 363 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | A     | 375 | -    | 4,4,4        | 0.25 | 0           | 6,6,6       | 0.09 | 0           |
| 3   | NDP  | L     | 369 | -    | 45,52,52     | 4.23 | 22 (48%)    | 53,80,80    | 5.79 | 34 (64%)    |
| 3   | NDP  | D     | 365 | -    | 45,52,52     | 4.14 | 22 (48%)    | 53,80,80    | 6.22 | 31 (58%)    |
| 2   | SO4  | I     | 366 | -    | 4,4,4        | 0.32 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | P     | 372 | -    | 4,4,4        | 0.31 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | M     | 380 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | H     | 363 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.09 | 0           |
| 3   | NDP  | H     | 379 | -    | 45,52,52     | 4.10 | 22 (48%)    | 53,80,80    | 6.14 | 32 (60%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | SO4  | M     | 370 | -    | 4,4,4        | 0.30 | 0        | 6,6,6       | 0.08 | 0        |
| 2   | SO4  | I     | 379 | -    | 4,4,4        | 0.32 | 0        | 6,6,6       | 0.09 | 0        |
| 3   | NDP  | Q     | 375 | -    | 45,52,52     | 4.01 | 23 (51%) | 53,80,80    | 6.10 | 34 (64%) |
| 3   | NDP  | P     | 373 | -    | 45,52,52     | 4.14 | 25 (55%) | 53,80,80    | 5.74 | 33 (62%) |
| 3   | NDP  | C     | 365 | -    | 45,52,52     | 4.04 | 23 (51%) | 53,80,80    | 6.09 | 34 (64%) |
| 2   | SO4  | B     | 377 | -    | 4,4,4        | 0.20 | 0        | 6,6,6       | 0.08 | 0        |
| 2   | SO4  | Q     | 364 | -    | 4,4,4        | 0.33 | 0        | 6,6,6       | 0.09 | 0        |
| 2   | SO4  | M     | 369 | -    | 4,4,4        | 0.25 | 0        | 6,6,6       | 0.09 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals   | Torsions    | Rings   |
|-----|------|-------|-----|------|-----------|-------------|---------|
| 3   | NDP  | B     | 378 | -    | 7/7/14/17 | 17/30/77/77 | 0/4/5/5 |
| 3   | NDP  | Q     | 375 | -    | 7/7/14/17 | 16/30/77/77 | 0/4/5/5 |
| 3   | NDP  | O     | 372 | -    | 7/7/14/17 | 18/30/77/77 | 0/4/5/5 |
| 3   | NDP  | C     | 365 | -    | 7/7/14/17 | 15/30/77/77 | 0/4/5/5 |
| 3   | NDP  | M     | 381 | -    | 7/7/14/17 | 15/30/77/77 | 0/4/5/5 |
| 3   | NDP  | H     | 379 | -    | 7/7/14/17 | 18/30/77/77 | 0/4/5/5 |
| 3   | NDP  | P     | 373 | -    | 7/7/14/17 | 16/30/77/77 | 0/4/5/5 |
| 3   | NDP  | R     | 377 | -    | 7/7/14/17 | 16/30/77/77 | 0/4/5/5 |
| 3   | NDP  | L     | 369 | -    | 7/7/14/17 | 15/30/77/77 | 0/4/5/5 |
| 3   | NDP  | D     | 365 | -    | 7/7/14/17 | 14/30/77/77 | 0/4/5/5 |
| 3   | NDP  | I     | 380 | -    | 7/7/14/17 | 17/30/77/77 | 0/4/5/5 |
| 3   | NDP  | A     | 376 | -    | 7/7/14/17 | 17/30/77/77 | 0/4/5/5 |

All (278) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 3   | A     | 376 | NDP  | C2D-C1D | 15.81  | 2.04        | 1.53     |
| 3   | R     | 377 | NDP  | O2D-C2D | -14.02 | 1.10        | 1.43     |
| 3   | H     | 379 | NDP  | O2D-C2D | -13.48 | 1.11        | 1.43     |
| 3   | O     | 372 | NDP  | C2D-C1D | 13.46  | 1.96        | 1.53     |
| 3   | D     | 365 | NDP  | O2D-C2D | -13.28 | 1.11        | 1.43     |
| 3   | C     | 365 | NDP  | O2D-C2D | -13.27 | 1.11        | 1.43     |
| 3   | B     | 378 | NDP  | O2D-C2D | -13.17 | 1.12        | 1.43     |
| 3   | P     | 373 | NDP  | O2D-C2D | -13.13 | 1.12        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 3   | I     | 380 | NDP  | O2D-C2D | -12.83 | 1.12        | 1.43     |
| 3   | M     | 381 | NDP  | O2D-C2D | -12.72 | 1.13        | 1.43     |
| 3   | L     | 369 | NDP  | O2D-C2D | -12.70 | 1.13        | 1.43     |
| 3   | A     | 376 | NDP  | O2D-C2D | -12.59 | 1.13        | 1.43     |
| 3   | Q     | 375 | NDP  | O2D-C2D | -12.33 | 1.13        | 1.43     |
| 3   | O     | 372 | NDP  | O2D-C2D | -12.26 | 1.14        | 1.43     |
| 3   | A     | 376 | NDP  | O4D-C1D | 10.67  | 1.67        | 1.42     |
| 3   | L     | 369 | NDP  | C2D-C1D | 10.10  | 1.85        | 1.53     |
| 3   | O     | 372 | NDP  | C2A-N3A | 9.34   | 1.47        | 1.32     |
| 3   | R     | 377 | NDP  | O4B-C4B | 9.32   | 1.65        | 1.45     |
| 3   | D     | 365 | NDP  | O4B-C4B | 9.29   | 1.65        | 1.45     |
| 3   | M     | 381 | NDP  | O4B-C4B | 9.11   | 1.65        | 1.45     |
| 3   | Q     | 375 | NDP  | C2D-C1D | 9.00   | 1.82        | 1.53     |
| 3   | O     | 372 | NDP  | O4B-C4B | 8.94   | 1.65        | 1.45     |
| 3   | H     | 379 | NDP  | O4B-C4B | 8.94   | 1.65        | 1.45     |
| 3   | B     | 378 | NDP  | O4B-C4B | 8.93   | 1.65        | 1.45     |
| 3   | Q     | 375 | NDP  | O4B-C4B | 8.88   | 1.64        | 1.45     |
| 3   | I     | 380 | NDP  | O4B-C4B | 8.76   | 1.64        | 1.45     |
| 3   | P     | 373 | NDP  | O4B-C4B | 8.75   | 1.64        | 1.45     |
| 3   | L     | 369 | NDP  | O4B-C4B | 8.72   | 1.64        | 1.45     |
| 3   | C     | 365 | NDP  | O4B-C4B | 8.71   | 1.64        | 1.45     |
| 3   | P     | 373 | NDP  | C2D-C1D | 8.52   | 1.80        | 1.53     |
| 3   | A     | 376 | NDP  | O4B-C4B | 8.47   | 1.63        | 1.45     |
| 3   | D     | 365 | NDP  | C2D-C3D | 8.47   | 1.76        | 1.53     |
| 3   | R     | 377 | NDP  | C2A-N3A | 8.37   | 1.45        | 1.32     |
| 3   | D     | 365 | NDP  | C2A-N3A | 8.27   | 1.45        | 1.32     |
| 3   | C     | 365 | NDP  | C2D-C1D | 8.21   | 1.79        | 1.53     |
| 3   | B     | 378 | NDP  | C2D-C1D | 7.83   | 1.78        | 1.53     |
| 3   | H     | 379 | NDP  | C2A-N3A | 7.73   | 1.44        | 1.32     |
| 3   | M     | 381 | NDP  | C2A-N3A | 7.68   | 1.44        | 1.32     |
| 3   | Q     | 375 | NDP  | C2A-N3A | 7.62   | 1.44        | 1.32     |
| 3   | I     | 380 | NDP  | C2D-C3D | 7.59   | 1.74        | 1.53     |
| 3   | A     | 376 | NDP  | C2A-N3A | 7.58   | 1.44        | 1.32     |
| 3   | I     | 380 | NDP  | C2D-C1D | 7.58   | 1.77        | 1.53     |
| 3   | P     | 373 | NDP  | C2A-N3A | 7.54   | 1.44        | 1.32     |
| 3   | L     | 369 | NDP  | C2A-N3A | 7.51   | 1.44        | 1.32     |
| 3   | C     | 365 | NDP  | C2A-N3A | 7.49   | 1.44        | 1.32     |
| 3   | B     | 378 | NDP  | C2A-N3A | 7.47   | 1.44        | 1.32     |
| 3   | Q     | 375 | NDP  | C2D-C3D | 7.37   | 1.73        | 1.53     |
| 3   | I     | 380 | NDP  | C2A-N3A | 7.33   | 1.43        | 1.32     |
| 3   | O     | 372 | NDP  | C2D-C3D | 7.28   | 1.73        | 1.53     |
| 3   | M     | 381 | NDP  | C2D-C3D | 7.28   | 1.73        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | L     | 369 | NDP  | C2D-C3D | 7.21  | 1.73        | 1.53     |
| 3   | C     | 365 | NDP  | C2D-C3D | 7.21  | 1.73        | 1.53     |
| 3   | M     | 381 | NDP  | C2D-C1D | 7.09  | 1.76        | 1.53     |
| 3   | A     | 376 | NDP  | C2D-C3D | 6.83  | 1.72        | 1.53     |
| 3   | H     | 379 | NDP  | C2D-C3D | 6.82  | 1.72        | 1.53     |
| 3   | O     | 372 | NDP  | PA-O5B  | 6.80  | 1.86        | 1.59     |
| 3   | R     | 377 | NDP  | C2D-C3D | 6.74  | 1.71        | 1.53     |
| 3   | P     | 373 | NDP  | C2D-C3D | 6.59  | 1.71        | 1.53     |
| 3   | M     | 381 | NDP  | O4B-C1B | -6.58 | 1.31        | 1.41     |
| 3   | R     | 377 | NDP  | O3B-C3B | 6.53  | 1.58        | 1.43     |
| 3   | L     | 369 | NDP  | C4A-N3A | 6.48  | 1.44        | 1.35     |
| 3   | H     | 379 | NDP  | C4A-N3A | 6.41  | 1.44        | 1.35     |
| 3   | R     | 377 | NDP  | O4B-C1B | -6.39 | 1.32        | 1.41     |
| 3   | A     | 376 | NDP  | C8A-N7A | -6.26 | 1.23        | 1.34     |
| 3   | B     | 378 | NDP  | C2D-C3D | 6.24  | 1.70        | 1.53     |
| 3   | O     | 372 | NDP  | C8A-N7A | -6.22 | 1.23        | 1.34     |
| 3   | B     | 378 | NDP  | C8A-N7A | -6.20 | 1.23        | 1.34     |
| 3   | I     | 380 | NDP  | C8A-N7A | -6.18 | 1.23        | 1.34     |
| 3   | C     | 365 | NDP  | C3B-C4B | 6.18  | 1.68        | 1.53     |
| 3   | C     | 365 | NDP  | C8A-N7A | -6.11 | 1.23        | 1.34     |
| 3   | Q     | 375 | NDP  | C8A-N7A | -6.02 | 1.24        | 1.34     |
| 3   | L     | 369 | NDP  | PA-O5B  | 6.02  | 1.83        | 1.59     |
| 3   | D     | 365 | NDP  | O3B-C3B | 6.01  | 1.57        | 1.43     |
| 3   | A     | 376 | NDP  | C3D-C4D | -6.00 | 1.37        | 1.53     |
| 3   | M     | 381 | NDP  | C8A-N7A | -5.89 | 1.24        | 1.34     |
| 3   | D     | 365 | NDP  | C8A-N7A | -5.85 | 1.24        | 1.34     |
| 3   | H     | 379 | NDP  | C2D-C1D | 5.81  | 1.72        | 1.53     |
| 3   | P     | 373 | NDP  | C3B-C4B | 5.77  | 1.67        | 1.53     |
| 3   | R     | 377 | NDP  | C3B-C2B | 5.76  | 1.65        | 1.52     |
| 3   | D     | 365 | NDP  | C3B-C4B | 5.66  | 1.67        | 1.53     |
| 3   | R     | 377 | NDP  | C8A-N7A | -5.66 | 1.24        | 1.34     |
| 3   | Q     | 375 | NDP  | C3B-C4B | 5.66  | 1.67        | 1.53     |
| 3   | P     | 373 | NDP  | O3B-C3B | 5.59  | 1.56        | 1.43     |
| 3   | H     | 379 | NDP  | C3B-C4B | 5.59  | 1.67        | 1.53     |
| 3   | O     | 372 | NDP  | C3B-C4B | 5.59  | 1.67        | 1.53     |
| 3   | C     | 365 | NDP  | PA-O5B  | 5.59  | 1.81        | 1.59     |
| 3   | H     | 379 | NDP  | O4B-C1B | -5.58 | 1.33        | 1.41     |
| 3   | B     | 378 | NDP  | O3B-C3B | 5.56  | 1.56        | 1.43     |
| 3   | I     | 380 | NDP  | C3D-C4D | -5.53 | 1.38        | 1.53     |
| 3   | P     | 373 | NDP  | C8A-N7A | -5.53 | 1.24        | 1.34     |
| 3   | H     | 379 | NDP  | C8A-N7A | -5.50 | 1.24        | 1.34     |
| 3   | B     | 378 | NDP  | PA-O5B  | 5.50  | 1.81        | 1.59     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | B     | 378 | NDP  | C4A-N3A | 5.48  | 1.43        | 1.35     |
| 3   | O     | 372 | NDP  | C4A-N3A | 5.46  | 1.43        | 1.35     |
| 3   | L     | 369 | NDP  | C3D-C4D | -5.40 | 1.39        | 1.53     |
| 3   | A     | 376 | NDP  | PA-O5B  | 5.34  | 1.80        | 1.59     |
| 3   | H     | 379 | NDP  | PA-O5B  | 5.32  | 1.80        | 1.59     |
| 3   | L     | 369 | NDP  | C3B-C4B | 5.30  | 1.66        | 1.53     |
| 3   | C     | 365 | NDP  | C3D-C4D | -5.29 | 1.39        | 1.53     |
| 3   | P     | 373 | NDP  | PA-O5B  | 5.26  | 1.80        | 1.59     |
| 3   | Q     | 375 | NDP  | PA-O5B  | 5.22  | 1.80        | 1.59     |
| 3   | L     | 369 | NDP  | C8A-N7A | -5.22 | 1.25        | 1.34     |
| 3   | M     | 381 | NDP  | C3B-C4B | 5.21  | 1.66        | 1.53     |
| 3   | I     | 380 | NDP  | C3B-C4B | 5.16  | 1.66        | 1.53     |
| 3   | L     | 369 | NDP  | O3B-C3B | 5.15  | 1.55        | 1.43     |
| 3   | D     | 365 | NDP  | O4B-C1B | -5.14 | 1.33        | 1.41     |
| 3   | H     | 379 | NDP  | O3B-C3B | 5.13  | 1.55        | 1.43     |
| 3   | C     | 365 | NDP  | O3B-C3B | 5.12  | 1.55        | 1.43     |
| 3   | I     | 380 | NDP  | O4B-C1B | -5.10 | 1.34        | 1.41     |
| 3   | I     | 380 | NDP  | C5D-C4D | -5.09 | 1.35        | 1.51     |
| 3   | C     | 365 | NDP  | C5D-C4D | -5.08 | 1.35        | 1.51     |
| 3   | M     | 381 | NDP  | PA-O5B  | 5.08  | 1.79        | 1.59     |
| 3   | R     | 377 | NDP  | C2D-C1D | 5.06  | 1.69        | 1.53     |
| 3   | I     | 380 | NDP  | PA-O5B  | 5.05  | 1.79        | 1.59     |
| 3   | D     | 365 | NDP  | C2D-C1D | 5.02  | 1.69        | 1.53     |
| 3   | M     | 381 | NDP  | C5D-C4D | -5.02 | 1.36        | 1.51     |
| 3   | R     | 377 | NDP  | C3B-C4B | 5.01  | 1.65        | 1.53     |
| 3   | A     | 376 | NDP  | C3B-C4B | 5.01  | 1.65        | 1.53     |
| 3   | B     | 378 | NDP  | C3B-C4B | 4.98  | 1.65        | 1.53     |
| 3   | P     | 373 | NDP  | C5D-C4D | -4.97 | 1.36        | 1.51     |
| 3   | L     | 369 | NDP  | O4D-C1D | 4.93  | 1.53        | 1.42     |
| 3   | O     | 372 | NDP  | O3B-C3B | 4.91  | 1.54        | 1.43     |
| 3   | R     | 377 | NDP  | PA-O5B  | 4.88  | 1.79        | 1.59     |
| 3   | O     | 372 | NDP  | C3D-C4D | -4.88 | 1.40        | 1.53     |
| 3   | L     | 369 | NDP  | C5D-C4D | -4.86 | 1.36        | 1.51     |
| 3   | D     | 365 | NDP  | C3D-C4D | -4.85 | 1.40        | 1.53     |
| 3   | Q     | 375 | NDP  | C5D-C4D | -4.83 | 1.36        | 1.51     |
| 3   | P     | 373 | NDP  | O4D-C1D | 4.82  | 1.53        | 1.42     |
| 3   | M     | 381 | NDP  | O3B-C3B | 4.82  | 1.54        | 1.43     |
| 3   | H     | 379 | NDP  | C5D-C4D | -4.80 | 1.36        | 1.51     |
| 3   | Q     | 375 | NDP  | O3B-C3B | 4.77  | 1.54        | 1.43     |
| 3   | D     | 365 | NDP  | PA-O5B  | 4.74  | 1.78        | 1.59     |
| 3   | B     | 378 | NDP  | C5D-C4D | -4.72 | 1.36        | 1.51     |
| 3   | Q     | 375 | NDP  | C4A-N3A | 4.67  | 1.42        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | R     | 377 | NDP  | C4A-N3A | 4.65  | 1.42        | 1.35     |
| 3   | P     | 373 | NDP  | C4A-N3A | 4.63  | 1.42        | 1.35     |
| 3   | D     | 365 | NDP  | C3B-C2B | 4.55  | 1.63        | 1.52     |
| 3   | A     | 376 | NDP  | O3B-C3B | 4.54  | 1.53        | 1.43     |
| 3   | B     | 378 | NDP  | C3B-C2B | 4.53  | 1.63        | 1.52     |
| 3   | H     | 379 | NDP  | C3D-C4D | -4.52 | 1.41        | 1.53     |
| 3   | M     | 381 | NDP  | C3D-C4D | -4.48 | 1.41        | 1.53     |
| 3   | D     | 365 | NDP  | C4A-N3A | 4.38  | 1.41        | 1.35     |
| 3   | R     | 377 | NDP  | C5D-C4D | -4.37 | 1.38        | 1.51     |
| 3   | D     | 365 | NDP  | C5D-C4D | -4.25 | 1.38        | 1.51     |
| 3   | I     | 380 | NDP  | O3B-C3B | 4.20  | 1.52        | 1.43     |
| 3   | O     | 372 | NDP  | O4B-C1B | -4.19 | 1.35        | 1.41     |
| 3   | B     | 378 | NDP  | O4B-C1B | -4.17 | 1.35        | 1.41     |
| 3   | A     | 376 | NDP  | C5D-C4D | -4.17 | 1.38        | 1.51     |
| 3   | L     | 369 | NDP  | PN-O5D  | 4.10  | 1.75        | 1.59     |
| 3   | P     | 373 | NDP  | C3B-C2B | 4.09  | 1.62        | 1.52     |
| 3   | Q     | 375 | NDP  | C3D-C4D | -4.09 | 1.42        | 1.53     |
| 3   | A     | 376 | NDP  | C7N-N7N | 4.06  | 1.44        | 1.33     |
| 3   | I     | 380 | NDP  | C3B-C2B | 4.05  | 1.62        | 1.52     |
| 3   | O     | 372 | NDP  | C5D-C4D | -4.03 | 1.39        | 1.51     |
| 3   | H     | 379 | NDP  | PN-O5D  | 4.02  | 1.75        | 1.59     |
| 3   | M     | 381 | NDP  | C3B-C2B | 4.02  | 1.61        | 1.52     |
| 3   | A     | 376 | NDP  | C4A-N3A | 3.89  | 1.41        | 1.35     |
| 3   | R     | 377 | NDP  | C3D-C4D | -3.87 | 1.43        | 1.53     |
| 3   | Q     | 375 | NDP  | PN-O5D  | 3.83  | 1.74        | 1.59     |
| 3   | L     | 369 | NDP  | C3B-C2B | 3.82  | 1.61        | 1.52     |
| 3   | C     | 365 | NDP  | C4A-N3A | 3.80  | 1.40        | 1.35     |
| 3   | P     | 373 | NDP  | C3D-C4D | -3.80 | 1.43        | 1.53     |
| 3   | H     | 379 | NDP  | O4D-C1D | 3.78  | 1.51        | 1.42     |
| 3   | Q     | 375 | NDP  | C7N-N7N | 3.77  | 1.43        | 1.33     |
| 3   | H     | 379 | NDP  | C7N-N7N | 3.76  | 1.43        | 1.33     |
| 3   | R     | 377 | NDP  | C7N-N7N | 3.74  | 1.43        | 1.33     |
| 3   | A     | 376 | NDP  | PN-O5D  | 3.70  | 1.74        | 1.59     |
| 3   | B     | 378 | NDP  | C3D-C4D | -3.69 | 1.43        | 1.53     |
| 3   | A     | 376 | NDP  | C3B-C2B | 3.68  | 1.61        | 1.52     |
| 3   | M     | 381 | NDP  | C7N-N7N | 3.67  | 1.43        | 1.33     |
| 3   | L     | 369 | NDP  | C7N-N7N | 3.65  | 1.43        | 1.33     |
| 3   | D     | 365 | NDP  | PN-O5D  | 3.65  | 1.74        | 1.59     |
| 3   | C     | 365 | NDP  | C7N-N7N | 3.63  | 1.43        | 1.33     |
| 3   | M     | 381 | NDP  | PN-O5D  | 3.60  | 1.73        | 1.59     |
| 3   | P     | 373 | NDP  | C7N-N7N | 3.58  | 1.42        | 1.33     |
| 3   | B     | 378 | NDP  | C7N-N7N | 3.57  | 1.42        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | R     | 377 | NDP  | PN-O5D  | 3.56  | 1.73        | 1.59     |
| 3   | C     | 365 | NDP  | C3B-C2B | 3.55  | 1.60        | 1.52     |
| 3   | O     | 372 | NDP  | C7N-N7N | 3.54  | 1.42        | 1.33     |
| 3   | H     | 379 | NDP  | O5D-C5D | 3.54  | 1.58        | 1.44     |
| 3   | O     | 372 | NDP  | C3B-C2B | 3.54  | 1.60        | 1.52     |
| 3   | P     | 373 | NDP  | P2B-O2B | 3.51  | 1.65        | 1.59     |
| 3   | H     | 379 | NDP  | C3B-C2B | 3.51  | 1.60        | 1.52     |
| 3   | B     | 378 | NDP  | PN-O5D  | 3.50  | 1.73        | 1.59     |
| 3   | L     | 369 | NDP  | O4B-C1B | -3.50 | 1.36        | 1.41     |
| 3   | P     | 373 | NDP  | O4B-C1B | -3.50 | 1.36        | 1.41     |
| 3   | A     | 376 | NDP  | O4B-C1B | -3.46 | 1.36        | 1.41     |
| 3   | D     | 365 | NDP  | O4D-C1D | 3.46  | 1.50        | 1.42     |
| 3   | O     | 372 | NDP  | O4D-C1D | 3.45  | 1.50        | 1.42     |
| 3   | D     | 365 | NDP  | C7N-N7N | 3.44  | 1.42        | 1.33     |
| 3   | A     | 376 | NDP  | P2B-O2B | 3.44  | 1.65        | 1.59     |
| 3   | I     | 380 | NDP  | C7N-N7N | 3.43  | 1.42        | 1.33     |
| 3   | I     | 380 | NDP  | PN-O5D  | 3.41  | 1.73        | 1.59     |
| 3   | R     | 377 | NDP  | O4D-C1D | 3.40  | 1.50        | 1.42     |
| 3   | A     | 376 | NDP  | O5D-C5D | 3.35  | 1.57        | 1.44     |
| 3   | P     | 373 | NDP  | PN-O5D  | 3.33  | 1.72        | 1.59     |
| 3   | D     | 365 | NDP  | C6A-N1A | 3.32  | 1.51        | 1.37     |
| 3   | Q     | 375 | NDP  | O5D-C5D | 3.29  | 1.57        | 1.44     |
| 3   | I     | 380 | NDP  | C4A-N3A | 3.28  | 1.40        | 1.35     |
| 3   | A     | 376 | NDP  | C2N-C3N | 3.27  | 1.44        | 1.34     |
| 3   | O     | 372 | NDP  | C6A-N1A | 3.25  | 1.51        | 1.37     |
| 3   | P     | 373 | NDP  | O5D-C5D | 3.21  | 1.57        | 1.44     |
| 3   | P     | 373 | NDP  | C6N-N1N | -3.21 | 1.29        | 1.37     |
| 3   | M     | 381 | NDP  | O4D-C1D | 3.20  | 1.49        | 1.42     |
| 3   | R     | 377 | NDP  | C6A-N1A | 3.19  | 1.51        | 1.37     |
| 3   | D     | 365 | NDP  | O5D-C5D | 3.18  | 1.57        | 1.44     |
| 3   | B     | 378 | NDP  | O5D-C5D | 3.17  | 1.57        | 1.44     |
| 3   | I     | 380 | NDP  | O4D-C1D | 3.14  | 1.49        | 1.42     |
| 3   | I     | 380 | NDP  | O5D-C5D | 3.14  | 1.56        | 1.44     |
| 3   | M     | 381 | NDP  | O5D-C5D | 3.13  | 1.56        | 1.44     |
| 3   | R     | 377 | NDP  | O5D-C5D | 3.13  | 1.56        | 1.44     |
| 3   | C     | 365 | NDP  | C5B-C4B | -3.10 | 1.41        | 1.51     |
| 3   | A     | 376 | NDP  | O4D-C4D | -3.10 | 1.38        | 1.45     |
| 3   | O     | 372 | NDP  | PN-O5D  | 3.07  | 1.71        | 1.59     |
| 3   | L     | 369 | NDP  | O5D-C5D | 3.05  | 1.56        | 1.44     |
| 3   | Q     | 375 | NDP  | C3B-C2B | 3.03  | 1.59        | 1.52     |
| 3   | I     | 380 | NDP  | O4D-C4D | -3.00 | 1.38        | 1.45     |
| 3   | R     | 377 | NDP  | C4N-C5N | 3.00  | 1.56        | 1.48     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | O     | 372 | NDP  | C5B-C4B | -2.95 | 1.42        | 1.51     |
| 3   | B     | 378 | NDP  | C5B-C4B | -2.94 | 1.42        | 1.51     |
| 3   | O     | 372 | NDP  | C4N-C3N | 2.83  | 1.55        | 1.49     |
| 3   | B     | 378 | NDP  | C6A-N1A | 2.83  | 1.49        | 1.37     |
| 3   | Q     | 375 | NDP  | P2B-O3X | 2.82  | 1.65        | 1.54     |
| 3   | B     | 378 | NDP  | P2B-O3X | 2.81  | 1.65        | 1.54     |
| 3   | O     | 372 | NDP  | O3D-C3D | 2.81  | 1.49        | 1.43     |
| 3   | P     | 373 | NDP  | C6A-N1A | 2.79  | 1.49        | 1.37     |
| 3   | H     | 379 | NDP  | C5B-C4B | -2.76 | 1.43        | 1.51     |
| 3   | Q     | 375 | NDP  | C6A-N1A | 2.76  | 1.49        | 1.37     |
| 3   | B     | 378 | NDP  | O4D-C1D | 2.75  | 1.48        | 1.42     |
| 3   | M     | 381 | NDP  | C5B-C4B | -2.75 | 1.43        | 1.51     |
| 3   | B     | 378 | NDP  | C4N-C5N | 2.74  | 1.56        | 1.48     |
| 3   | R     | 377 | NDP  | P2B-O2B | 2.74  | 1.64        | 1.59     |
| 3   | L     | 369 | NDP  | C6A-N1A | 2.74  | 1.49        | 1.37     |
| 3   | A     | 376 | NDP  | C6A-N1A | 2.74  | 1.49        | 1.37     |
| 3   | C     | 365 | NDP  | C6A-N1A | 2.74  | 1.49        | 1.37     |
| 3   | H     | 379 | NDP  | C6A-N1A | 2.74  | 1.49        | 1.37     |
| 3   | O     | 372 | NDP  | P2B-O3X | 2.73  | 1.65        | 1.54     |
| 3   | L     | 369 | NDP  | C5B-C4B | -2.72 | 1.43        | 1.51     |
| 3   | A     | 376 | NDP  | C5B-C4B | -2.71 | 1.43        | 1.51     |
| 3   | H     | 379 | NDP  | C5A-C4A | 2.70  | 1.48        | 1.40     |
| 3   | I     | 380 | NDP  | C6A-N1A | 2.68  | 1.48        | 1.37     |
| 3   | A     | 376 | NDP  | P2B-O3X | 2.67  | 1.65        | 1.54     |
| 3   | R     | 377 | NDP  | P2B-O3X | 2.64  | 1.65        | 1.54     |
| 3   | C     | 365 | NDP  | PN-O5D  | 2.64  | 1.70        | 1.59     |
| 3   | D     | 365 | NDP  | P2B-O3X | 2.61  | 1.64        | 1.54     |
| 3   | R     | 377 | NDP  | C5B-C4B | -2.60 | 1.43        | 1.51     |
| 3   | A     | 376 | NDP  | C4N-C5N | 2.60  | 1.55        | 1.48     |
| 3   | B     | 378 | NDP  | P2B-O2B | 2.59  | 1.64        | 1.59     |
| 3   | M     | 381 | NDP  | C4A-N3A | 2.58  | 1.39        | 1.35     |
| 3   | I     | 380 | NDP  | C5B-C4B | -2.56 | 1.43        | 1.51     |
| 3   | I     | 380 | NDP  | P2B-O3X | 2.56  | 1.64        | 1.54     |
| 3   | C     | 365 | NDP  | C4N-C5N | 2.53  | 1.55        | 1.48     |
| 3   | P     | 373 | NDP  | C4N-C5N | 2.53  | 1.55        | 1.48     |
| 3   | Q     | 375 | NDP  | C4N-C5N | 2.52  | 1.55        | 1.48     |
| 3   | C     | 365 | NDP  | O5D-C5D | 2.51  | 1.54        | 1.44     |
| 3   | Q     | 375 | NDP  | O4D-C1D | 2.50  | 1.47        | 1.42     |
| 3   | M     | 381 | NDP  | C6A-N1A | 2.48  | 1.48        | 1.37     |
| 3   | H     | 379 | NDP  | P2B-O3X | 2.47  | 1.64        | 1.54     |
| 3   | P     | 373 | NDP  | P2B-O3X | 2.46  | 1.64        | 1.54     |
| 3   | L     | 369 | NDP  | C5A-C4A | 2.44  | 1.47        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | L     | 369 | NDP  | P2B-O3X | 2.42  | 1.64        | 1.54     |
| 3   | D     | 365 | NDP  | C4N-C5N | 2.42  | 1.55        | 1.48     |
| 3   | C     | 365 | NDP  | P2B-O3X | 2.42  | 1.64        | 1.54     |
| 3   | I     | 380 | NDP  | C4N-C5N | 2.41  | 1.55        | 1.48     |
| 3   | M     | 381 | NDP  | P2B-O3X | 2.39  | 1.64        | 1.54     |
| 3   | C     | 365 | NDP  | P2B-O2B | 2.38  | 1.63        | 1.59     |
| 3   | Q     | 375 | NDP  | C5B-C4B | -2.37 | 1.44        | 1.51     |
| 3   | C     | 365 | NDP  | O4B-C1B | -2.36 | 1.37        | 1.41     |
| 3   | P     | 373 | NDP  | C5B-C4B | -2.34 | 1.44        | 1.51     |
| 3   | O     | 372 | NDP  | O5D-C5D | 2.33  | 1.53        | 1.44     |
| 3   | D     | 365 | NDP  | P2B-O2B | 2.31  | 1.63        | 1.59     |
| 3   | Q     | 375 | NDP  | O4B-C1B | -2.31 | 1.37        | 1.41     |
| 3   | C     | 365 | NDP  | O4D-C1D | 2.18  | 1.47        | 1.42     |
| 3   | M     | 381 | NDP  | C4N-C5N | 2.17  | 1.54        | 1.48     |
| 3   | Q     | 375 | NDP  | P2B-O2B | 2.15  | 1.63        | 1.59     |
| 3   | O     | 372 | NDP  | C6N-C5N | -2.09 | 1.29        | 1.33     |
| 3   | B     | 378 | NDP  | C5A-C4A | 2.01  | 1.46        | 1.40     |
| 3   | P     | 373 | NDP  | O4D-C4D | 2.00  | 1.49        | 1.45     |

All (388) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 3   | H     | 379 | NDP  | O4D-C1D-N1N | 34.15  | 174.82      | 108.06   |
| 3   | D     | 365 | NDP  | O4D-C1D-N1N | 34.10  | 174.73      | 108.06   |
| 3   | I     | 380 | NDP  | O4D-C1D-N1N | 33.53  | 173.61      | 108.06   |
| 3   | B     | 378 | NDP  | O4D-C1D-N1N | 33.49  | 173.52      | 108.06   |
| 3   | M     | 381 | NDP  | O4D-C1D-N1N | 32.94  | 172.46      | 108.06   |
| 3   | R     | 377 | NDP  | O4D-C1D-N1N | 32.83  | 172.24      | 108.06   |
| 3   | C     | 365 | NDP  | O4D-C1D-N1N | 31.84  | 170.30      | 108.06   |
| 3   | Q     | 375 | NDP  | O4D-C1D-N1N | 31.12  | 168.91      | 108.06   |
| 3   | L     | 369 | NDP  | O4D-C1D-N1N | 27.19  | 161.22      | 108.06   |
| 3   | P     | 373 | NDP  | O4D-C1D-N1N | 26.61  | 160.08      | 108.06   |
| 3   | O     | 372 | NDP  | O4D-C1D-N1N | 24.29  | 155.54      | 108.06   |
| 3   | A     | 376 | NDP  | O4D-C1D-C2D | -18.02 | 67.36       | 106.64   |
| 3   | A     | 376 | NDP  | O4D-C1D-N1N | 17.92  | 143.09      | 108.06   |
| 3   | O     | 372 | NDP  | O4D-C1D-C2D | -14.15 | 75.80       | 106.64   |
| 3   | A     | 376 | NDP  | C2D-C1D-N1N | -14.13 | 77.91       | 113.30   |
| 3   | L     | 369 | NDP  | O4D-C1D-C2D | -12.73 | 78.89       | 106.64   |
| 3   | A     | 376 | NDP  | C1D-N1N-C2N | -12.54 | 100.23      | 121.11   |
| 3   | O     | 372 | NDP  | C2D-C1D-N1N | -12.24 | 82.65       | 113.30   |
| 3   | O     | 372 | NDP  | C1D-N1N-C2N | -12.23 | 100.75      | 121.11   |
| 3   | Q     | 375 | NDP  | C1D-N1N-C6N | -11.42 | 96.23       | 120.83   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 3   | M     | 381 | NDP  | C1D-N1N-C6N | -11.31 | 96.46       | 120.83   |
| 3   | I     | 380 | NDP  | C1D-N1N-C6N | -11.01 | 97.11       | 120.83   |
| 3   | Q     | 375 | NDP  | O4D-C1D-C2D | -10.87 | 82.94       | 106.64   |
| 3   | P     | 373 | NDP  | O4D-C1D-C2D | -10.84 | 83.01       | 106.64   |
| 3   | C     | 365 | NDP  | O4D-C1D-C2D | -10.81 | 83.08       | 106.64   |
| 3   | L     | 369 | NDP  | C2D-C1D-N1N | -10.68 | 86.55       | 113.30   |
| 3   | B     | 378 | NDP  | C1D-N1N-C6N | -10.47 | 98.27       | 120.83   |
| 3   | Q     | 375 | NDP  | C2D-C1D-N1N | -10.44 | 87.14       | 113.30   |
| 3   | P     | 373 | NDP  | C2D-C1D-N1N | -10.32 | 87.46       | 113.30   |
| 3   | I     | 380 | NDP  | O4D-C1D-C2D | -10.14 | 84.54       | 106.64   |
| 3   | B     | 378 | NDP  | O4D-C1D-C2D | -10.01 | 84.83       | 106.64   |
| 3   | A     | 376 | NDP  | O2B-C2B-C3B | 9.58   | 146.39      | 111.68   |
| 3   | H     | 379 | NDP  | C1D-N1N-C6N | -9.55  | 100.25      | 120.83   |
| 3   | I     | 380 | NDP  | O2B-C2B-C3B | 9.46   | 145.95      | 111.68   |
| 3   | O     | 372 | NDP  | O2B-C2B-C3B | 9.34   | 145.53      | 111.68   |
| 3   | B     | 378 | NDP  | C2D-C1D-N1N | -9.31  | 89.97       | 113.30   |
| 3   | P     | 373 | NDP  | C1D-N1N-C2N | -9.30  | 105.62      | 121.11   |
| 3   | M     | 381 | NDP  | O2B-C2B-C3B | 9.26   | 145.22      | 111.68   |
| 3   | R     | 377 | NDP  | O2B-C2B-C3B | 9.21   | 145.05      | 111.68   |
| 3   | C     | 365 | NDP  | C2D-C1D-N1N | -9.19  | 90.27       | 113.30   |
| 3   | P     | 373 | NDP  | O2B-C2B-C3B | 9.19   | 144.97      | 111.68   |
| 3   | L     | 369 | NDP  | O2B-C2B-C3B | 9.14   | 144.82      | 111.68   |
| 3   | C     | 365 | NDP  | O2B-C2B-C3B | 9.14   | 144.79      | 111.68   |
| 3   | D     | 365 | NDP  | O2B-C2B-C3B | 9.07   | 144.56      | 111.68   |
| 3   | Q     | 375 | NDP  | O2B-C2B-C3B | 9.06   | 144.52      | 111.68   |
| 3   | D     | 365 | NDP  | C1D-N1N-C6N | -9.02  | 101.39      | 120.83   |
| 3   | B     | 378 | NDP  | O2B-C2B-C3B | 8.98   | 144.21      | 111.68   |
| 3   | H     | 379 | NDP  | O2B-C2B-C3B | 8.97   | 144.20      | 111.68   |
| 3   | R     | 377 | NDP  | C1B-N9A-C4A | 8.85   | 142.18      | 126.64   |
| 3   | I     | 380 | NDP  | C2D-C1D-N1N | -8.83  | 91.18       | 113.30   |
| 3   | M     | 381 | NDP  | O4D-C1D-C2D | -8.81  | 87.43       | 106.64   |
| 3   | D     | 365 | NDP  | C1B-N9A-C4A | 8.76   | 142.03      | 126.64   |
| 3   | I     | 380 | NDP  | C1B-N9A-C4A | 8.56   | 141.68      | 126.64   |
| 3   | M     | 381 | NDP  | C1B-N9A-C4A | 8.54   | 141.64      | 126.64   |
| 3   | A     | 376 | NDP  | C1D-N1N-C6N | -8.53  | 102.44      | 120.83   |
| 3   | C     | 365 | NDP  | C1B-N9A-C4A | 8.34   | 141.30      | 126.64   |
| 3   | Q     | 375 | NDP  | C1B-N9A-C4A | 8.33   | 141.27      | 126.64   |
| 3   | A     | 376 | NDP  | C1B-N9A-C4A | 8.32   | 141.25      | 126.64   |
| 3   | B     | 378 | NDP  | C1B-N9A-C4A | 8.31   | 141.24      | 126.64   |
| 3   | D     | 365 | NDP  | O4D-C1D-C2D | -8.31  | 88.53       | 106.64   |
| 3   | L     | 369 | NDP  | C1B-N9A-C4A | 8.31   | 141.24      | 126.64   |
| 3   | A     | 376 | NDP  | O2D-C2D-C3D | 8.27   | 138.57      | 111.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | R     | 377 | NDP  | O4D-C1D-C2D | -8.27 | 88.62       | 106.64   |
| 3   | P     | 373 | NDP  | C1B-N9A-C4A | 8.24  | 141.13      | 126.64   |
| 3   | M     | 381 | NDP  | C2D-C1D-N1N | -8.23 | 92.69       | 113.30   |
| 3   | H     | 379 | NDP  | O4D-C1D-C2D | -8.22 | 88.73       | 106.64   |
| 3   | R     | 377 | NDP  | PN-O3-PA    | 8.08  | 160.56      | 132.83   |
| 3   | O     | 372 | NDP  | C1B-N9A-C4A | 8.07  | 140.82      | 126.64   |
| 3   | H     | 379 | NDP  | C1B-N9A-C4A | 7.97  | 140.64      | 126.64   |
| 3   | P     | 373 | NDP  | C3B-C2B-C1B | 7.96  | 117.86      | 102.89   |
| 3   | B     | 378 | NDP  | PN-O3-PA    | 7.81  | 159.64      | 132.83   |
| 3   | O     | 372 | NDP  | PN-O3-PA    | 7.80  | 159.60      | 132.83   |
| 3   | O     | 372 | NDP  | C1D-N1N-C6N | -7.72 | 104.20      | 120.83   |
| 3   | A     | 376 | NDP  | C2D-C3D-C4D | -7.69 | 87.69       | 102.64   |
| 3   | D     | 365 | NDP  | C2D-C3D-C4D | -7.67 | 87.74       | 102.64   |
| 3   | Q     | 375 | NDP  | PN-O3-PA    | 7.65  | 159.07      | 132.83   |
| 3   | L     | 369 | NDP  | C1D-N1N-C2N | -7.65 | 108.38      | 121.11   |
| 3   | R     | 377 | NDP  | C2D-C3D-C4D | -7.60 | 87.87       | 102.64   |
| 3   | C     | 365 | NDP  | C1D-N1N-C6N | -7.59 | 104.47      | 120.83   |
| 3   | R     | 377 | NDP  | C1D-N1N-C6N | -7.56 | 104.53      | 120.83   |
| 3   | D     | 365 | NDP  | PN-O3-PA    | 7.56  | 158.77      | 132.83   |
| 3   | C     | 365 | NDP  | C3B-C2B-C1B | 7.52  | 117.03      | 102.89   |
| 3   | A     | 376 | NDP  | C3B-C2B-C1B | 7.50  | 116.99      | 102.89   |
| 3   | Q     | 375 | NDP  | C3B-C2B-C1B | 7.45  | 116.90      | 102.89   |
| 3   | H     | 379 | NDP  | C3B-C2B-C1B | 7.42  | 116.83      | 102.89   |
| 3   | C     | 365 | NDP  | PN-O3-PA    | 7.41  | 158.26      | 132.83   |
| 3   | L     | 369 | NDP  | C1D-N1N-C6N | -7.38 | 104.93      | 120.83   |
| 3   | B     | 378 | NDP  | C3B-C2B-C1B | 7.37  | 116.75      | 102.89   |
| 3   | D     | 365 | NDP  | C3B-C2B-C1B | 7.36  | 116.72      | 102.89   |
| 3   | A     | 376 | NDP  | PN-O3-PA    | 7.33  | 157.96      | 132.83   |
| 3   | P     | 373 | NDP  | C2D-C3D-C4D | -7.27 | 88.52       | 102.64   |
| 3   | O     | 372 | NDP  | C3B-C2B-C1B | 7.26  | 116.54      | 102.89   |
| 3   | L     | 369 | NDP  | C3B-C2B-C1B | 7.25  | 116.52      | 102.89   |
| 3   | M     | 381 | NDP  | C3B-C2B-C1B | 7.20  | 116.43      | 102.89   |
| 3   | L     | 369 | NDP  | C2D-C3D-C4D | -7.20 | 88.66       | 102.64   |
| 3   | P     | 373 | NDP  | PN-O3-PA    | 7.15  | 157.38      | 132.83   |
| 3   | I     | 380 | NDP  | C3B-C2B-C1B | 7.14  | 116.32      | 102.89   |
| 3   | H     | 379 | NDP  | C2D-C1D-N1N | -7.14 | 95.41       | 113.30   |
| 3   | M     | 381 | NDP  | PN-O3-PA    | 7.08  | 157.14      | 132.83   |
| 3   | R     | 377 | NDP  | C3B-C2B-C1B | 7.08  | 116.20      | 102.89   |
| 3   | I     | 380 | NDP  | PN-O3-PA    | 7.06  | 157.05      | 132.83   |
| 3   | C     | 365 | NDP  | C2D-C3D-C4D | -7.05 | 88.94       | 102.64   |
| 3   | R     | 377 | NDP  | C2D-C1D-N1N | -7.05 | 95.65       | 113.30   |
| 3   | Q     | 375 | NDP  | C2D-C3D-C4D | -7.00 | 89.04       | 102.64   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | B     | 378 | NDP  | C2D-C3D-C4D | -6.97 | 89.09       | 102.64   |
| 3   | P     | 373 | NDP  | C4D-O4D-C1D | -6.92 | 94.21       | 109.47   |
| 3   | D     | 365 | NDP  | C2D-C1D-N1N | -6.90 | 96.02       | 113.30   |
| 3   | M     | 381 | NDP  | C2D-C3D-C4D | -6.90 | 89.24       | 102.64   |
| 3   | O     | 372 | NDP  | C2D-C3D-C4D | -6.85 | 89.32       | 102.64   |
| 3   | P     | 373 | NDP  | O2D-C2D-C3D | 6.84  | 133.95      | 111.82   |
| 3   | H     | 379 | NDP  | C2D-C3D-C4D | -6.78 | 89.46       | 102.64   |
| 3   | H     | 379 | NDP  | PN-O3-PA    | 6.75  | 155.98      | 132.83   |
| 3   | L     | 369 | NDP  | PN-O3-PA    | 6.72  | 155.88      | 132.83   |
| 3   | R     | 377 | NDP  | O3B-C3B-C2B | 6.70  | 130.20      | 111.17   |
| 3   | D     | 365 | NDP  | O2D-C2D-C3D | 6.67  | 133.39      | 111.82   |
| 3   | P     | 373 | NDP  | O3B-C3B-C2B | 6.53  | 129.72      | 111.17   |
| 3   | B     | 378 | NDP  | O3B-C3B-C2B | 6.48  | 129.56      | 111.17   |
| 3   | I     | 380 | NDP  | O2D-C2D-C3D | 6.47  | 132.75      | 111.82   |
| 3   | I     | 380 | NDP  | C2D-C3D-C4D | -6.43 | 90.15       | 102.64   |
| 3   | M     | 381 | NDP  | O2D-C2D-C3D | 6.31  | 132.23      | 111.82   |
| 3   | C     | 365 | NDP  | C1D-N1N-C2N | -6.30 | 110.62      | 121.11   |
| 3   | A     | 376 | NDP  | O3B-C3B-C2B | 6.23  | 128.86      | 111.17   |
| 3   | L     | 369 | NDP  | O2D-C2D-C3D | 6.12  | 131.61      | 111.82   |
| 3   | H     | 379 | NDP  | O2D-C2D-C3D | 6.11  | 131.60      | 111.82   |
| 3   | Q     | 375 | NDP  | O2D-C2D-C3D | 6.09  | 131.53      | 111.82   |
| 3   | R     | 377 | NDP  | O2D-C2D-C3D | 6.09  | 131.51      | 111.82   |
| 3   | O     | 372 | NDP  | C5D-C4D-C3D | 6.06  | 137.88      | 115.18   |
| 3   | M     | 381 | NDP  | O3B-C3B-C2B | 6.04  | 128.31      | 111.17   |
| 3   | D     | 365 | NDP  | O3B-C3B-C2B | 5.97  | 128.13      | 111.17   |
| 3   | R     | 377 | NDP  | C4D-O4D-C1D | -5.95 | 96.35       | 109.47   |
| 3   | O     | 372 | NDP  | O2D-C2D-C3D | 5.93  | 131.01      | 111.82   |
| 3   | I     | 380 | NDP  | O3B-C3B-C2B | 5.88  | 127.88      | 111.17   |
| 3   | C     | 365 | NDP  | O3B-C3B-C2B | 5.78  | 127.58      | 111.17   |
| 3   | C     | 365 | NDP  | O2D-C2D-C3D | 5.77  | 130.47      | 111.82   |
| 3   | B     | 378 | NDP  | O2D-C2D-C3D | 5.75  | 130.43      | 111.82   |
| 3   | C     | 365 | NDP  | C5D-C4D-C3D | 5.75  | 136.73      | 115.18   |
| 3   | L     | 369 | NDP  | O3B-C3B-C2B | 5.72  | 127.41      | 111.17   |
| 3   | H     | 379 | NDP  | O3B-C3B-C2B | 5.72  | 127.40      | 111.17   |
| 3   | Q     | 375 | NDP  | O3B-C3B-C2B | 5.67  | 127.28      | 111.17   |
| 3   | O     | 372 | NDP  | O3B-C3B-C2B | 5.65  | 127.21      | 111.17   |
| 3   | I     | 380 | NDP  | C5D-C4D-C3D | 5.64  | 136.33      | 115.18   |
| 3   | D     | 365 | NDP  | C4D-O4D-C1D | -5.59 | 97.13       | 109.47   |
| 3   | A     | 376 | NDP  | C5D-C4D-C3D | 5.55  | 136.00      | 115.18   |
| 3   | B     | 378 | NDP  | C5D-C4D-C3D | 5.54  | 135.93      | 115.18   |
| 3   | R     | 377 | NDP  | C5D-C4D-C3D | 5.48  | 135.71      | 115.18   |
| 3   | P     | 373 | NDP  | C5D-C4D-C3D | 5.42  | 135.50      | 115.18   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | M     | 381 | NDP  | C5D-C4D-C3D | 5.39  | 135.36      | 115.18   |
| 3   | L     | 369 | NDP  | C5D-C4D-C3D | 5.38  | 135.34      | 115.18   |
| 3   | L     | 369 | NDP  | C4D-O4D-C1D | -5.37 | 97.63       | 109.47   |
| 3   | Q     | 375 | NDP  | C5D-C4D-C3D | 5.37  | 135.29      | 115.18   |
| 3   | H     | 379 | NDP  | C5D-C4D-C3D | 5.31  | 135.09      | 115.18   |
| 3   | D     | 365 | NDP  | C5D-C4D-C3D | 5.28  | 134.95      | 115.18   |
| 3   | P     | 373 | NDP  | C1D-N1N-C6N | -5.16 | 109.72      | 120.83   |
| 3   | D     | 365 | NDP  | O3D-C3D-C2D | 5.10  | 128.31      | 111.82   |
| 3   | M     | 381 | NDP  | O3D-C3D-C2D | 4.95  | 127.83      | 111.82   |
| 3   | R     | 377 | NDP  | O3X-P2B-O2B | -4.93 | 83.88       | 105.99   |
| 3   | I     | 380 | NDP  | O3D-C3D-C2D | 4.85  | 127.50      | 111.82   |
| 3   | O     | 372 | NDP  | C5A-C6A-N1A | -4.77 | 109.54      | 120.35   |
| 3   | B     | 378 | NDP  | O3X-P2B-O2B | -4.77 | 84.62       | 105.99   |
| 3   | C     | 365 | NDP  | O3X-P2B-O2B | -4.77 | 84.64       | 105.99   |
| 3   | Q     | 375 | NDP  | O3D-C3D-C2D | 4.70  | 127.02      | 111.82   |
| 3   | L     | 369 | NDP  | O3D-C3D-C2D | 4.69  | 126.98      | 111.82   |
| 3   | D     | 365 | NDP  | O3X-P2B-O2B | -4.69 | 85.00       | 105.99   |
| 3   | C     | 365 | NDP  | C4D-O4D-C1D | -4.67 | 99.16       | 109.47   |
| 3   | R     | 377 | NDP  | O3D-C3D-C2D | 4.65  | 126.86      | 111.82   |
| 3   | O     | 372 | NDP  | O3D-C3D-C2D | 4.65  | 126.85      | 111.82   |
| 3   | Q     | 375 | NDP  | O3X-P2B-O2B | -4.64 | 85.21       | 105.99   |
| 3   | P     | 373 | NDP  | O3D-C3D-C2D | 4.63  | 126.81      | 111.82   |
| 3   | I     | 380 | NDP  | O3X-P2B-O2B | -4.62 | 85.29       | 105.99   |
| 3   | H     | 379 | NDP  | O3D-C3D-C2D | 4.62  | 126.76      | 111.82   |
| 3   | Q     | 375 | NDP  | C1D-N1N-C2N | -4.61 | 113.44      | 121.11   |
| 3   | C     | 365 | NDP  | O3D-C3D-C2D | 4.60  | 126.69      | 111.82   |
| 3   | R     | 377 | NDP  | C2B-C3B-C4B | -4.49 | 92.23       | 101.99   |
| 3   | B     | 378 | NDP  | O3D-C3D-C2D | 4.45  | 126.22      | 111.82   |
| 3   | P     | 373 | NDP  | O3X-P2B-O2B | -4.45 | 86.05       | 105.99   |
| 3   | A     | 376 | NDP  | O3D-C3D-C2D | 4.43  | 126.15      | 111.82   |
| 3   | M     | 381 | NDP  | O3X-P2B-O2B | -4.41 | 86.23       | 105.99   |
| 3   | O     | 372 | NDP  | C3N-C2N-N1N | 4.39  | 129.36      | 123.10   |
| 3   | O     | 372 | NDP  | O3X-P2B-O2B | -4.31 | 86.70       | 105.99   |
| 3   | I     | 380 | NDP  | C1D-N1N-C2N | -4.28 | 113.99      | 121.11   |
| 3   | C     | 365 | NDP  | C3N-C2N-N1N | 4.25  | 129.17      | 123.10   |
| 3   | A     | 376 | NDP  | O3X-P2B-O2B | -4.16 | 87.34       | 105.99   |
| 3   | I     | 380 | NDP  | O2B-C2B-C1B | -4.10 | 95.36       | 110.10   |
| 3   | O     | 372 | NDP  | C5B-C4B-C3B | 4.08  | 130.45      | 115.18   |
| 3   | H     | 379 | NDP  | C2B-C3B-C4B | -4.06 | 93.17       | 101.99   |
| 3   | D     | 365 | NDP  | C5B-C4B-C3B | 4.05  | 130.37      | 115.18   |
| 3   | M     | 381 | NDP  | C2B-C3B-C4B | -4.05 | 93.20       | 101.99   |
| 3   | D     | 365 | NDP  | C2B-C3B-C4B | -4.05 | 93.20       | 101.99   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | M     | 381 | NDP  | C5B-C4B-C3B | 4.05  | 130.34      | 115.18   |
| 3   | H     | 379 | NDP  | O3X-P2B-O2B | -4.03 | 87.92       | 105.99   |
| 3   | A     | 376 | NDP  | O2B-C2B-C1B | -4.00 | 95.70       | 110.10   |
| 3   | B     | 378 | NDP  | C2B-C3B-C4B | -3.97 | 93.36       | 101.99   |
| 3   | A     | 376 | NDP  | O4D-C4D-C5D | 3.96  | 122.41      | 109.37   |
| 3   | H     | 379 | NDP  | C4D-O4D-C1D | -3.95 | 100.76      | 109.47   |
| 3   | P     | 373 | NDP  | C2B-C3B-C4B | -3.94 | 93.44       | 101.99   |
| 3   | O     | 372 | NDP  | C5A-C6A-N6A | 3.93  | 126.33      | 120.35   |
| 3   | L     | 369 | NDP  | O3X-P2B-O2B | -3.93 | 88.38       | 105.99   |
| 3   | P     | 373 | NDP  | C5B-C4B-C3B | 3.91  | 129.82      | 115.18   |
| 3   | H     | 379 | NDP  | C5B-C4B-C3B | 3.90  | 129.79      | 115.18   |
| 3   | O     | 372 | NDP  | O2B-C2B-C1B | -3.87 | 96.17       | 110.10   |
| 3   | R     | 377 | NDP  | C5B-C4B-C3B | 3.87  | 129.67      | 115.18   |
| 3   | P     | 373 | NDP  | C3N-C7N-N7N | -3.84 | 110.84      | 117.67   |
| 3   | C     | 365 | NDP  | C5B-C4B-C3B | 3.84  | 129.56      | 115.18   |
| 3   | I     | 380 | NDP  | C5B-C4B-C3B | 3.83  | 129.55      | 115.18   |
| 3   | B     | 378 | NDP  | O2B-P2B-O1X | 3.82  | 124.13      | 109.39   |
| 3   | A     | 376 | NDP  | C4D-O4D-C1D | -3.82 | 101.05      | 109.47   |
| 3   | H     | 379 | NDP  | C3N-C7N-N7N | -3.81 | 110.90      | 117.67   |
| 3   | O     | 372 | NDP  | C4D-O4D-C1D | -3.81 | 101.07      | 109.47   |
| 3   | L     | 369 | NDP  | C5B-C4B-C3B | 3.80  | 129.40      | 115.18   |
| 3   | P     | 373 | NDP  | O2B-C2B-C1B | -3.73 | 96.67       | 110.10   |
| 3   | O     | 372 | NDP  | C2B-C3B-C4B | -3.72 | 93.92       | 101.99   |
| 3   | Q     | 375 | NDP  | C5B-C4B-C3B | 3.72  | 129.11      | 115.18   |
| 3   | A     | 376 | NDP  | C5B-C4B-C3B | 3.71  | 129.10      | 115.18   |
| 3   | B     | 378 | NDP  | C5B-C4B-C3B | 3.70  | 129.06      | 115.18   |
| 3   | A     | 376 | NDP  | O4D-C4D-C3D | -3.70 | 97.80       | 105.11   |
| 3   | L     | 369 | NDP  | C2B-C3B-C4B | -3.70 | 93.96       | 101.99   |
| 3   | I     | 380 | NDP  | C2B-C3B-C4B | -3.68 | 94.00       | 101.99   |
| 3   | M     | 381 | NDP  | C3N-C7N-N7N | -3.64 | 111.21      | 117.67   |
| 3   | I     | 380 | NDP  | C3N-C7N-N7N | -3.62 | 111.23      | 117.67   |
| 3   | M     | 381 | NDP  | O2B-C2B-C1B | -3.61 | 97.09       | 110.10   |
| 3   | C     | 365 | NDP  | C2B-C3B-C4B | -3.60 | 94.17       | 101.99   |
| 3   | B     | 378 | NDP  | C1D-N1N-C2N | -3.59 | 115.14      | 121.11   |
| 3   | M     | 381 | NDP  | O4B-C4B-C3B | -3.58 | 98.03       | 105.11   |
| 3   | C     | 365 | NDP  | O2B-C2B-C1B | -3.57 | 97.26       | 110.10   |
| 3   | A     | 376 | NDP  | C2B-C3B-C4B | -3.56 | 94.25       | 101.99   |
| 3   | L     | 369 | NDP  | C3N-C7N-N7N | -3.55 | 111.36      | 117.67   |
| 3   | Q     | 375 | NDP  | O2B-P2B-O1X | 3.53  | 123.03      | 109.39   |
| 3   | R     | 377 | NDP  | O2B-P2B-O1X | 3.53  | 123.01      | 109.39   |
| 3   | H     | 379 | NDP  | C3D-C2D-C1D | 3.50  | 108.07      | 101.43   |
| 3   | R     | 377 | NDP  | C5A-C6A-N1A | -3.47 | 112.49      | 120.35   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | C     | 365 | NDP  | O2B-P2B-O1X | 3.46  | 122.74      | 109.39   |
| 3   | D     | 365 | NDP  | O4B-C4B-C3B | -3.45 | 98.28       | 105.11   |
| 3   | R     | 377 | NDP  | O4B-C4B-C3B | -3.45 | 98.30       | 105.11   |
| 3   | P     | 373 | NDP  | O2B-P2B-O1X | 3.44  | 122.66      | 109.39   |
| 3   | I     | 380 | NDP  | O4B-C4B-C3B | -3.43 | 98.33       | 105.11   |
| 3   | Q     | 375 | NDP  | O2B-C2B-C1B | -3.43 | 97.76       | 110.10   |
| 3   | O     | 372 | NDP  | C3N-C7N-N7N | -3.41 | 111.60      | 117.67   |
| 3   | D     | 365 | NDP  | C5A-C6A-N1A | -3.35 | 112.75      | 120.35   |
| 3   | L     | 369 | NDP  | O7N-C7N-N7N | 3.35  | 130.71      | 122.88   |
| 3   | H     | 379 | NDP  | O2B-C2B-C1B | -3.35 | 98.06       | 110.10   |
| 3   | A     | 376 | NDP  | O2B-P2B-O1X | 3.34  | 122.30      | 109.39   |
| 3   | R     | 377 | NDP  | C1D-N1N-C2N | -3.34 | 115.55      | 121.11   |
| 3   | B     | 378 | NDP  | C3D-C2D-C1D | 3.33  | 107.74      | 101.43   |
| 3   | M     | 381 | NDP  | C5A-C6A-N1A | -3.32 | 112.83      | 120.35   |
| 3   | R     | 377 | NDP  | C3D-C2D-C1D | 3.32  | 107.73      | 101.43   |
| 3   | D     | 365 | NDP  | O2B-C2B-C1B | -3.30 | 98.24       | 110.10   |
| 3   | L     | 369 | NDP  | O2B-C2B-C1B | -3.29 | 98.24       | 110.10   |
| 3   | C     | 365 | NDP  | C3N-C7N-N7N | -3.29 | 111.82      | 117.67   |
| 3   | Q     | 375 | NDP  | C2B-C3B-C4B | -3.29 | 94.85       | 101.99   |
| 3   | L     | 369 | NDP  | C3N-C2N-N1N | 3.28  | 127.78      | 123.10   |
| 3   | O     | 372 | NDP  | O4B-C4B-C3B | -3.27 | 98.64       | 105.11   |
| 3   | H     | 379 | NDP  | C5A-C6A-N1A | -3.27 | 112.94      | 120.35   |
| 3   | O     | 372 | NDP  | O2B-P2B-O1X | 3.26  | 121.98      | 109.39   |
| 3   | H     | 379 | NDP  | O7N-C7N-N7N | 3.26  | 130.50      | 122.88   |
| 3   | I     | 380 | NDP  | C5A-C6A-N1A | -3.25 | 112.98      | 120.35   |
| 3   | B     | 378 | NDP  | C3N-C7N-N7N | -3.24 | 111.91      | 117.67   |
| 3   | A     | 376 | NDP  | C3N-C7N-N7N | -3.23 | 111.93      | 117.67   |
| 3   | I     | 380 | NDP  | O2B-P2B-O1X | 3.23  | 121.85      | 109.39   |
| 3   | D     | 365 | NDP  | O2B-P2B-O1X | 3.21  | 121.79      | 109.39   |
| 3   | R     | 377 | NDP  | O2B-C2B-C1B | -3.20 | 98.57       | 110.10   |
| 3   | H     | 379 | NDP  | O4B-C4B-C3B | -3.18 | 98.82       | 105.11   |
| 3   | Q     | 375 | NDP  | C5A-C6A-N1A | -3.16 | 113.20      | 120.35   |
| 3   | M     | 381 | NDP  | O2B-P2B-O1X | 3.15  | 121.53      | 109.39   |
| 3   | B     | 378 | NDP  | C5A-C6A-N1A | -3.14 | 113.24      | 120.35   |
| 3   | L     | 369 | NDP  | C5A-C6A-N1A | -3.13 | 113.26      | 120.35   |
| 3   | B     | 378 | NDP  | O2N-PN-O1N  | 3.09  | 127.51      | 112.24   |
| 3   | B     | 378 | NDP  | O2B-C2B-C1B | -3.09 | 98.99       | 110.10   |
| 3   | I     | 380 | NDP  | O7N-C7N-N7N | 3.09  | 130.10      | 122.88   |
| 3   | C     | 365 | NDP  | C5A-C6A-N1A | -3.03 | 113.49      | 120.35   |
| 3   | L     | 369 | NDP  | O4D-C4D-C5D | 3.02  | 119.30      | 109.37   |
| 3   | M     | 381 | NDP  | C5A-C6A-N6A | 3.01  | 124.93      | 120.35   |
| 3   | A     | 376 | NDP  | C3D-C2D-C1D | 3.00  | 107.13      | 101.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | A     | 376 | NDP  | C5A-C6A-N1A | -3.00 | 113.55      | 120.35   |
| 3   | P     | 373 | NDP  | C5A-C6A-N1A | -3.00 | 113.55      | 120.35   |
| 3   | B     | 378 | NDP  | O5B-PA-O1A  | 2.99  | 120.76      | 109.07   |
| 3   | M     | 381 | NDP  | C4D-O4D-C1D | -2.96 | 102.93      | 109.47   |
| 3   | M     | 381 | NDP  | O5B-C5B-C4B | 2.96  | 119.19      | 108.99   |
| 3   | B     | 378 | NDP  | C4D-O4D-C1D | -2.96 | 102.94      | 109.47   |
| 3   | M     | 381 | NDP  | O7N-C7N-N7N | 2.93  | 129.74      | 122.88   |
| 3   | D     | 365 | NDP  | O5B-C5B-C4B | 2.93  | 119.07      | 108.99   |
| 3   | R     | 377 | NDP  | O2N-PN-O1N  | 2.90  | 126.57      | 112.24   |
| 3   | B     | 378 | NDP  | C3N-C2N-N1N | 2.89  | 127.21      | 123.10   |
| 3   | H     | 379 | NDP  | O2B-P2B-O1X | 2.88  | 120.52      | 109.39   |
| 3   | P     | 373 | NDP  | O7N-C7N-N7N | 2.88  | 129.62      | 122.88   |
| 3   | Q     | 375 | NDP  | O5B-PA-O1A  | 2.87  | 120.30      | 109.07   |
| 3   | Q     | 375 | NDP  | O7N-C7N-N7N | 2.86  | 129.58      | 122.88   |
| 3   | A     | 376 | NDP  | O7N-C7N-N7N | 2.85  | 129.55      | 122.88   |
| 3   | B     | 378 | NDP  | O4B-C4B-C3B | -2.84 | 99.49       | 105.11   |
| 3   | L     | 369 | NDP  | O5B-C5B-C4B | 2.83  | 118.74      | 108.99   |
| 3   | P     | 373 | NDP  | O4D-C4D-C5D | 2.81  | 118.63      | 109.37   |
| 3   | M     | 381 | NDP  | C3D-C2D-C1D | 2.79  | 106.73      | 101.43   |
| 3   | R     | 377 | NDP  | O5B-C5B-C4B | 2.78  | 118.57      | 108.99   |
| 3   | I     | 380 | NDP  | O5B-C5B-C4B | 2.77  | 118.54      | 108.99   |
| 3   | Q     | 375 | NDP  | C3N-C7N-N7N | -2.77 | 112.75      | 117.67   |
| 3   | L     | 369 | NDP  | O2B-P2B-O1X | 2.75  | 120.00      | 109.39   |
| 3   | Q     | 375 | NDP  | C3D-C2D-C1D | 2.75  | 106.64      | 101.43   |
| 3   | Q     | 375 | NDP  | O5B-C5B-C4B | 2.74  | 118.44      | 108.99   |
| 3   | Q     | 375 | NDP  | O2N-PN-O1N  | 2.74  | 125.81      | 112.24   |
| 3   | R     | 377 | NDP  | O5B-PA-O1A  | 2.73  | 119.72      | 109.07   |
| 3   | D     | 365 | NDP  | O2N-PN-O1N  | 2.72  | 125.70      | 112.24   |
| 3   | C     | 365 | NDP  | O2N-PN-O1N  | 2.71  | 125.66      | 112.24   |
| 3   | D     | 365 | NDP  | O7N-C7N-N7N | 2.71  | 129.23      | 122.88   |
| 3   | H     | 379 | NDP  | O2N-PN-O1N  | 2.71  | 125.62      | 112.24   |
| 3   | B     | 378 | NDP  | O7N-C7N-N7N | 2.70  | 129.20      | 122.88   |
| 3   | L     | 369 | NDP  | O4B-C4B-C3B | -2.70 | 99.77       | 105.11   |
| 3   | O     | 372 | NDP  | O2N-PN-O1N  | 2.70  | 125.56      | 112.24   |
| 3   | R     | 377 | NDP  | C3N-C7N-N7N | -2.69 | 112.89      | 117.67   |
| 3   | L     | 369 | NDP  | O2N-PN-O1N  | 2.69  | 125.55      | 112.24   |
| 3   | O     | 372 | NDP  | N6A-C6A-N1A | 2.67  | 124.12      | 118.57   |
| 3   | C     | 365 | NDP  | O4B-C4B-C3B | -2.67 | 99.83       | 105.11   |
| 3   | O     | 372 | NDP  | PA-O5B-C5B  | 2.67  | 137.31      | 121.68   |
| 3   | I     | 380 | NDP  | O2N-PN-O1N  | 2.66  | 125.39      | 112.24   |
| 3   | R     | 377 | NDP  | N6A-C6A-N1A | 2.66  | 124.09      | 118.57   |
| 3   | C     | 365 | NDP  | O5B-C5B-C4B | 2.65  | 118.13      | 108.99   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | B     | 378 | NDP  | O5B-C5B-C4B | 2.65  | 118.12      | 108.99   |
| 3   | A     | 376 | NDP  | O5B-PA-O1A  | 2.64  | 119.38      | 109.07   |
| 3   | Q     | 375 | NDP  | O4B-C4B-C3B | -2.64 | 99.89       | 105.11   |
| 3   | H     | 379 | NDP  | O5B-PA-O1A  | 2.63  | 119.35      | 109.07   |
| 3   | R     | 377 | NDP  | O7N-C7N-N7N | 2.62  | 129.00      | 122.88   |
| 3   | H     | 379 | NDP  | O5B-C5B-C4B | 2.61  | 117.99      | 108.99   |
| 3   | D     | 365 | NDP  | N6A-C6A-N1A | 2.60  | 123.98      | 118.57   |
| 3   | P     | 373 | NDP  | O5B-C5B-C4B | 2.60  | 117.92      | 108.99   |
| 3   | C     | 365 | NDP  | O7N-C7N-N7N | 2.59  | 128.94      | 122.88   |
| 3   | A     | 376 | NDP  | O4B-C4B-C3B | -2.58 | 100.01      | 105.11   |
| 3   | C     | 365 | NDP  | O5D-PN-O1N  | -2.56 | 99.05       | 109.07   |
| 3   | D     | 365 | NDP  | C3D-C2D-C1D | 2.55  | 106.27      | 101.43   |
| 3   | Q     | 375 | NDP  | C3N-C2N-N1N | 2.54  | 126.72      | 123.10   |
| 3   | A     | 376 | NDP  | O2N-PN-O1N  | 2.53  | 124.75      | 112.24   |
| 3   | P     | 373 | NDP  | C3D-C2D-C1D | 2.52  | 106.22      | 101.43   |
| 3   | M     | 381 | NDP  | O2N-PN-O1N  | 2.52  | 124.72      | 112.24   |
| 3   | P     | 373 | NDP  | O2N-PN-O1N  | 2.52  | 124.71      | 112.24   |
| 3   | P     | 373 | NDP  | O5B-PA-O1A  | 2.52  | 118.92      | 109.07   |
| 3   | C     | 365 | NDP  | O5B-PA-O1A  | 2.51  | 118.88      | 109.07   |
| 3   | B     | 378 | NDP  | N6A-C6A-N1A | 2.50  | 123.77      | 118.57   |
| 3   | C     | 365 | NDP  | PA-O5B-C5B  | 2.50  | 136.33      | 121.68   |
| 3   | A     | 376 | NDP  | O5B-C5B-C4B | 2.49  | 117.55      | 108.99   |
| 3   | L     | 369 | NDP  | O5B-PA-O1A  | 2.49  | 118.78      | 109.07   |
| 3   | B     | 378 | NDP  | PA-O5B-C5B  | 2.48  | 136.25      | 121.68   |
| 3   | H     | 379 | NDP  | O3B-C3B-C4B | 2.46  | 118.16      | 111.05   |
| 3   | P     | 373 | NDP  | C5A-C6A-N6A | 2.45  | 124.07      | 120.35   |
| 3   | D     | 365 | NDP  | C3N-C7N-N7N | -2.43 | 113.35      | 117.67   |
| 3   | D     | 365 | NDP  | O5B-PA-O1A  | 2.41  | 118.49      | 109.07   |
| 3   | L     | 369 | NDP  | C3D-C2D-C1D | 2.40  | 106.00      | 101.43   |
| 3   | P     | 373 | NDP  | O3B-C3B-C4B | 2.40  | 117.99      | 111.05   |
| 3   | D     | 365 | NDP  | O3B-C3B-C4B | 2.37  | 117.89      | 111.05   |
| 3   | P     | 373 | NDP  | O4B-C4B-C3B | -2.36 | 100.45      | 105.11   |
| 3   | Q     | 375 | NDP  | O3B-C3B-C4B | 2.35  | 117.86      | 111.05   |
| 3   | Q     | 375 | NDP  | O4D-C4D-C5D | 2.35  | 117.11      | 109.37   |
| 3   | C     | 365 | NDP  | O3B-C3B-C4B | 2.34  | 117.81      | 111.05   |
| 3   | M     | 381 | NDP  | PA-O5B-C5B  | 2.33  | 135.35      | 121.68   |
| 3   | L     | 369 | NDP  | N6A-C6A-N1A | 2.33  | 123.41      | 118.57   |
| 3   | Q     | 375 | NDP  | N6A-C6A-N1A | 2.32  | 123.39      | 118.57   |
| 3   | M     | 381 | NDP  | O3B-C3B-C4B | 2.31  | 117.72      | 111.05   |
| 3   | Q     | 375 | NDP  | C4D-O4D-C1D | -2.31 | 104.38      | 109.47   |
| 3   | P     | 373 | NDP  | O2A-PA-O1A  | -2.29 | 100.93      | 112.24   |
| 3   | H     | 379 | NDP  | C5A-C6A-N6A | 2.28  | 123.82      | 120.35   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | I     | 380 | NDP  | C3N-C2N-N1N | 2.28  | 126.35      | 123.10   |
| 3   | I     | 380 | NDP  | N6A-C6A-N1A | 2.26  | 123.28      | 118.57   |
| 3   | H     | 379 | NDP  | PA-O5B-C5B  | 2.26  | 134.91      | 121.68   |
| 3   | H     | 379 | NDP  | N6A-C6A-N1A | 2.24  | 123.22      | 118.57   |
| 3   | M     | 381 | NDP  | O5B-PA-O1A  | 2.21  | 117.72      | 109.07   |
| 3   | I     | 380 | NDP  | C5A-C6A-N6A | 2.21  | 123.72      | 120.35   |
| 3   | L     | 369 | NDP  | O3B-C3B-C4B | 2.21  | 117.45      | 111.05   |
| 3   | C     | 365 | NDP  | C5A-C6A-N6A | 2.20  | 123.69      | 120.35   |
| 3   | B     | 378 | NDP  | O3B-C3B-C4B | 2.19  | 117.39      | 111.05   |
| 3   | A     | 376 | NDP  | PA-O5B-C5B  | 2.19  | 134.50      | 121.68   |
| 3   | R     | 377 | NDP  | O3B-C3B-C4B | 2.17  | 117.33      | 111.05   |
| 3   | I     | 380 | NDP  | C3D-C2D-C1D | 2.17  | 105.54      | 101.43   |
| 3   | A     | 376 | NDP  | C3N-C2N-N1N | 2.16  | 126.18      | 123.10   |
| 3   | R     | 377 | NDP  | PA-O5B-C5B  | 2.16  | 134.32      | 121.68   |
| 3   | Q     | 375 | NDP  | PA-O5B-C5B  | 2.15  | 134.29      | 121.68   |
| 3   | H     | 379 | NDP  | O2A-PA-O1A  | -2.15 | 101.61      | 112.24   |
| 3   | Q     | 375 | NDP  | O2A-PA-O1A  | -2.15 | 101.62      | 112.24   |
| 3   | I     | 380 | NDP  | C4D-O4D-C1D | -2.15 | 104.74      | 109.47   |
| 3   | L     | 369 | NDP  | O2A-PA-O1A  | -2.15 | 101.64      | 112.24   |
| 3   | D     | 365 | NDP  | O4D-C4D-C5D | 2.11  | 116.33      | 109.37   |
| 3   | A     | 376 | NDP  | N6A-C6A-N1A | 2.10  | 122.94      | 118.57   |
| 3   | P     | 373 | NDP  | C3N-C2N-N1N | 2.10  | 126.09      | 123.10   |
| 3   | A     | 376 | NDP  | O2A-PA-O1A  | -2.09 | 101.89      | 112.24   |
| 3   | M     | 381 | NDP  | O2A-PA-O1A  | -2.08 | 101.96      | 112.24   |
| 3   | L     | 369 | NDP  | PA-O5B-C5B  | 2.08  | 133.86      | 121.68   |
| 3   | C     | 365 | NDP  | C3D-C2D-C1D | 2.08  | 105.37      | 101.43   |
| 3   | A     | 376 | NDP  | C5A-C6A-N6A | 2.07  | 123.49      | 120.35   |
| 3   | B     | 378 | NDP  | O2A-PA-O1A  | -2.05 | 102.08      | 112.24   |
| 3   | M     | 381 | NDP  | C3N-C2N-N1N | 2.05  | 126.02      | 123.10   |
| 3   | I     | 380 | NDP  | PA-O5B-C5B  | 2.03  | 133.61      | 121.68   |
| 3   | C     | 365 | NDP  | N6A-C6A-N1A | 2.03  | 122.79      | 118.57   |
| 3   | D     | 365 | NDP  | O2A-PA-O1A  | -2.03 | 102.19      | 112.24   |

All (84) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 3   | B     | 378 | NDP  | C1B  |
| 3   | B     | 378 | NDP  | C3D  |
| 3   | B     | 378 | NDP  | C2B  |
| 3   | B     | 378 | NDP  | C4D  |
| 3   | B     | 378 | NDP  | C2D  |
| 3   | B     | 378 | NDP  | C1D  |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 3   | B     | 378 | NDP  | C4B  |
| 3   | O     | 372 | NDP  | C1B  |
| 3   | O     | 372 | NDP  | C3D  |
| 3   | O     | 372 | NDP  | C2B  |
| 3   | O     | 372 | NDP  | C4D  |
| 3   | O     | 372 | NDP  | C1D  |
| 3   | O     | 372 | NDP  | C2D  |
| 3   | O     | 372 | NDP  | C4B  |
| 3   | M     | 381 | NDP  | C1B  |
| 3   | M     | 381 | NDP  | C3D  |
| 3   | M     | 381 | NDP  | C2B  |
| 3   | M     | 381 | NDP  | C4D  |
| 3   | M     | 381 | NDP  | C2D  |
| 3   | M     | 381 | NDP  | C1D  |
| 3   | M     | 381 | NDP  | C4B  |
| 3   | I     | 380 | NDP  | C1B  |
| 3   | I     | 380 | NDP  | C3D  |
| 3   | I     | 380 | NDP  | C2B  |
| 3   | I     | 380 | NDP  | C4D  |
| 3   | I     | 380 | NDP  | C2D  |
| 3   | I     | 380 | NDP  | C1D  |
| 3   | I     | 380 | NDP  | C4B  |
| 3   | R     | 377 | NDP  | C1B  |
| 3   | R     | 377 | NDP  | C3D  |
| 3   | R     | 377 | NDP  | C2B  |
| 3   | R     | 377 | NDP  | C4D  |
| 3   | R     | 377 | NDP  | C2D  |
| 3   | R     | 377 | NDP  | C1D  |
| 3   | R     | 377 | NDP  | C4B  |
| 3   | A     | 376 | NDP  | C1B  |
| 3   | A     | 376 | NDP  | C3D  |
| 3   | A     | 376 | NDP  | C2B  |
| 3   | A     | 376 | NDP  | C4D  |
| 3   | A     | 376 | NDP  | C1D  |
| 3   | A     | 376 | NDP  | C2D  |
| 3   | A     | 376 | NDP  | C4B  |
| 3   | L     | 369 | NDP  | C1B  |
| 3   | L     | 369 | NDP  | C3D  |
| 3   | L     | 369 | NDP  | C2B  |
| 3   | L     | 369 | NDP  | C4D  |
| 3   | L     | 369 | NDP  | C1D  |
| 3   | L     | 369 | NDP  | C2D  |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 3   | L     | 369 | NDP  | C4B  |
| 3   | D     | 365 | NDP  | C1B  |
| 3   | D     | 365 | NDP  | C3D  |
| 3   | D     | 365 | NDP  | C2B  |
| 3   | D     | 365 | NDP  | C4D  |
| 3   | D     | 365 | NDP  | C2D  |
| 3   | D     | 365 | NDP  | C1D  |
| 3   | D     | 365 | NDP  | C4B  |
| 3   | H     | 379 | NDP  | C1B  |
| 3   | H     | 379 | NDP  | C3D  |
| 3   | H     | 379 | NDP  | C2B  |
| 3   | H     | 379 | NDP  | C4D  |
| 3   | H     | 379 | NDP  | C2D  |
| 3   | H     | 379 | NDP  | C1D  |
| 3   | H     | 379 | NDP  | C4B  |
| 3   | Q     | 375 | NDP  | C1B  |
| 3   | Q     | 375 | NDP  | C3D  |
| 3   | Q     | 375 | NDP  | C2B  |
| 3   | Q     | 375 | NDP  | C4D  |
| 3   | Q     | 375 | NDP  | C2D  |
| 3   | Q     | 375 | NDP  | C1D  |
| 3   | Q     | 375 | NDP  | C4B  |
| 3   | P     | 373 | NDP  | C1B  |
| 3   | P     | 373 | NDP  | C3D  |
| 3   | P     | 373 | NDP  | C2B  |
| 3   | P     | 373 | NDP  | C4D  |
| 3   | P     | 373 | NDP  | C1D  |
| 3   | P     | 373 | NDP  | C2D  |
| 3   | P     | 373 | NDP  | C4B  |
| 3   | C     | 365 | NDP  | C1B  |
| 3   | C     | 365 | NDP  | C3D  |
| 3   | C     | 365 | NDP  | C2B  |
| 3   | C     | 365 | NDP  | C4D  |
| 3   | C     | 365 | NDP  | C2D  |
| 3   | C     | 365 | NDP  | C1D  |
| 3   | C     | 365 | NDP  | C4B  |

All (194) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 3   | B     | 378 | NDP  | C5B-O5B-PA-O1A |
| 3   | B     | 378 | NDP  | C5B-O5B-PA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | B     | 378 | NDP  | C5B-O5B-PA-O3   |
| 3   | B     | 378 | NDP  | C4B-C5B-O5B-PA  |
| 3   | B     | 378 | NDP  | C3B-C2B-O2B-P2B |
| 3   | B     | 378 | NDP  | C5D-O5D-PN-O2N  |
| 3   | O     | 372 | NDP  | C5B-O5B-PA-O1A  |
| 3   | O     | 372 | NDP  | C5B-O5B-PA-O2A  |
| 3   | O     | 372 | NDP  | C5B-O5B-PA-O3   |
| 3   | O     | 372 | NDP  | C4B-C5B-O5B-PA  |
| 3   | O     | 372 | NDP  | C5D-O5D-PN-O2N  |
| 3   | M     | 381 | NDP  | C5B-O5B-PA-O1A  |
| 3   | M     | 381 | NDP  | C5B-O5B-PA-O2A  |
| 3   | M     | 381 | NDP  | C5B-O5B-PA-O3   |
| 3   | M     | 381 | NDP  | C4B-C5B-O5B-PA  |
| 3   | M     | 381 | NDP  | C5D-O5D-PN-O2N  |
| 3   | M     | 381 | NDP  | O4D-C1D-N1N-C6N |
| 3   | I     | 380 | NDP  | C5B-O5B-PA-O1A  |
| 3   | I     | 380 | NDP  | C5B-O5B-PA-O2A  |
| 3   | I     | 380 | NDP  | C5B-O5B-PA-O3   |
| 3   | I     | 380 | NDP  | C4B-C5B-O5B-PA  |
| 3   | I     | 380 | NDP  | C3B-C2B-O2B-P2B |
| 3   | I     | 380 | NDP  | C5D-O5D-PN-O2N  |
| 3   | I     | 380 | NDP  | O4D-C1D-N1N-C6N |
| 3   | R     | 377 | NDP  | C5B-O5B-PA-O1A  |
| 3   | R     | 377 | NDP  | C5B-O5B-PA-O2A  |
| 3   | R     | 377 | NDP  | C5B-O5B-PA-O3   |
| 3   | R     | 377 | NDP  | C4B-C5B-O5B-PA  |
| 3   | R     | 377 | NDP  | C5D-O5D-PN-O2N  |
| 3   | A     | 376 | NDP  | C5B-O5B-PA-O1A  |
| 3   | A     | 376 | NDP  | C5B-O5B-PA-O2A  |
| 3   | A     | 376 | NDP  | C5B-O5B-PA-O3   |
| 3   | A     | 376 | NDP  | C4B-C5B-O5B-PA  |
| 3   | A     | 376 | NDP  | C5D-O5D-PN-O2N  |
| 3   | A     | 376 | NDP  | O4D-C1D-N1N-C2N |
| 3   | L     | 369 | NDP  | C5B-O5B-PA-O1A  |
| 3   | L     | 369 | NDP  | C5B-O5B-PA-O2A  |
| 3   | L     | 369 | NDP  | C5B-O5B-PA-O3   |
| 3   | L     | 369 | NDP  | C4B-C5B-O5B-PA  |
| 3   | D     | 365 | NDP  | C5B-O5B-PA-O1A  |
| 3   | D     | 365 | NDP  | C5B-O5B-PA-O2A  |
| 3   | D     | 365 | NDP  | C5B-O5B-PA-O3   |
| 3   | D     | 365 | NDP  | C4B-C5B-O5B-PA  |
| 3   | D     | 365 | NDP  | C5D-O5D-PN-O2N  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | H     | 379 | NDP  | C5B-O5B-PA-O1A  |
| 3   | H     | 379 | NDP  | C5B-O5B-PA-O2A  |
| 3   | H     | 379 | NDP  | C5B-O5B-PA-O3   |
| 3   | H     | 379 | NDP  | C4B-C5B-O5B-PA  |
| 3   | H     | 379 | NDP  | C5D-O5D-PN-O2N  |
| 3   | Q     | 375 | NDP  | C5B-O5B-PA-O1A  |
| 3   | Q     | 375 | NDP  | C5B-O5B-PA-O2A  |
| 3   | Q     | 375 | NDP  | C5B-O5B-PA-O3   |
| 3   | Q     | 375 | NDP  | C4B-C5B-O5B-PA  |
| 3   | Q     | 375 | NDP  | C5D-O5D-PN-O2N  |
| 3   | P     | 373 | NDP  | C5B-O5B-PA-O1A  |
| 3   | P     | 373 | NDP  | C5B-O5B-PA-O2A  |
| 3   | P     | 373 | NDP  | C5B-O5B-PA-O3   |
| 3   | P     | 373 | NDP  | C4B-C5B-O5B-PA  |
| 3   | P     | 373 | NDP  | C5D-O5D-PN-O2N  |
| 3   | C     | 365 | NDP  | C5B-O5B-PA-O1A  |
| 3   | C     | 365 | NDP  | C5B-O5B-PA-O2A  |
| 3   | C     | 365 | NDP  | C5B-O5B-PA-O3   |
| 3   | C     | 365 | NDP  | C4B-C5B-O5B-PA  |
| 3   | C     | 365 | NDP  | C5D-O5D-PN-O2N  |
| 3   | C     | 365 | NDP  | C3D-C4D-C5D-O5D |
| 3   | B     | 378 | NDP  | O4D-C1D-N1N-C6N |
| 3   | O     | 372 | NDP  | O4D-C1D-N1N-C2N |
| 3   | L     | 369 | NDP  | O4D-C1D-N1N-C2N |
| 3   | P     | 373 | NDP  | O4D-C1D-N1N-C2N |
| 3   | C     | 365 | NDP  | O4D-C1D-N1N-C2N |
| 3   | B     | 378 | NDP  | C3D-C4D-C5D-O5D |
| 3   | O     | 372 | NDP  | C3D-C4D-C5D-O5D |
| 3   | M     | 381 | NDP  | C3D-C4D-C5D-O5D |
| 3   | I     | 380 | NDP  | C3D-C4D-C5D-O5D |
| 3   | R     | 377 | NDP  | C3D-C4D-C5D-O5D |
| 3   | A     | 376 | NDP  | C3D-C4D-C5D-O5D |
| 3   | L     | 369 | NDP  | C3D-C4D-C5D-O5D |
| 3   | D     | 365 | NDP  | C3D-C4D-C5D-O5D |
| 3   | H     | 379 | NDP  | C3D-C4D-C5D-O5D |
| 3   | Q     | 375 | NDP  | C3D-C4D-C5D-O5D |
| 3   | P     | 373 | NDP  | O4B-C4B-C5B-O5B |
| 3   | P     | 373 | NDP  | C3D-C4D-C5D-O5D |
| 3   | C     | 365 | NDP  | O4B-C4B-C5B-O5B |
| 3   | O     | 372 | NDP  | C3B-C2B-O2B-P2B |
| 3   | M     | 381 | NDP  | C3B-C2B-O2B-P2B |
| 3   | R     | 377 | NDP  | C3B-C2B-O2B-P2B |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | A     | 376 | NDP  | C3B-C2B-O2B-P2B |
| 3   | L     | 369 | NDP  | C3B-C2B-O2B-P2B |
| 3   | D     | 365 | NDP  | C3B-C2B-O2B-P2B |
| 3   | H     | 379 | NDP  | C3B-C2B-O2B-P2B |
| 3   | Q     | 375 | NDP  | C3B-C2B-O2B-P2B |
| 3   | P     | 373 | NDP  | C3B-C2B-O2B-P2B |
| 3   | C     | 365 | NDP  | C3B-C2B-O2B-P2B |
| 3   | B     | 378 | NDP  | O4D-C4D-C5D-O5D |
| 3   | R     | 377 | NDP  | O4D-C4D-C5D-O5D |
| 3   | A     | 376 | NDP  | O4B-C4B-C5B-O5B |
| 3   | A     | 376 | NDP  | O4D-C4D-C5D-O5D |
| 3   | P     | 373 | NDP  | O4D-C4D-C5D-O5D |
| 3   | Q     | 375 | NDP  | O4D-C1D-N1N-C6N |
| 3   | D     | 365 | NDP  | O4D-C4D-C5D-O5D |
| 3   | Q     | 375 | NDP  | O4D-C4D-C5D-O5D |
| 3   | O     | 372 | NDP  | O4D-C4D-C5D-O5D |
| 3   | L     | 369 | NDP  | O4D-C4D-C5D-O5D |
| 3   | M     | 381 | NDP  | O4D-C4D-C5D-O5D |
| 3   | I     | 380 | NDP  | O4D-C4D-C5D-O5D |
| 3   | L     | 369 | NDP  | O4B-C4B-C5B-O5B |
| 3   | H     | 379 | NDP  | O4D-C4D-C5D-O5D |
| 3   | Q     | 375 | NDP  | O4B-C4B-C5B-O5B |
| 3   | C     | 365 | NDP  | O4D-C4D-C5D-O5D |
| 3   | B     | 378 | NDP  | PA-O3-PN-O1N    |
| 3   | M     | 381 | NDP  | PA-O3-PN-O1N    |
| 3   | A     | 376 | NDP  | PA-O3-PN-O1N    |
| 3   | B     | 378 | NDP  | O4B-C4B-C5B-O5B |
| 3   | H     | 379 | NDP  | O4B-C4B-C5B-O5B |
| 3   | O     | 372 | NDP  | PN-O3-PA-O5B    |
| 3   | M     | 381 | NDP  | PN-O3-PA-O5B    |
| 3   | I     | 380 | NDP  | PN-O3-PA-O5B    |
| 3   | R     | 377 | NDP  | PN-O3-PA-O5B    |
| 3   | L     | 369 | NDP  | PN-O3-PA-O5B    |
| 3   | D     | 365 | NDP  | PN-O3-PA-O5B    |
| 3   | H     | 379 | NDP  | PN-O3-PA-O5B    |
| 3   | Q     | 375 | NDP  | PN-O3-PA-O5B    |
| 3   | P     | 373 | NDP  | PN-O3-PA-O5B    |
| 3   | C     | 365 | NDP  | PN-O3-PA-O5B    |
| 3   | D     | 365 | NDP  | O4B-C4B-C5B-O5B |
| 3   | O     | 372 | NDP  | C2D-C1D-N1N-C2N |
| 3   | B     | 378 | NDP  | C5D-O5D-PN-O3   |
| 3   | O     | 372 | NDP  | C5D-O5D-PN-O3   |

*Continued on next page...*

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | M     | 381 | NDP  | C5D-O5D-PN-O3   |
| 3   | I     | 380 | NDP  | C5D-O5D-PN-O3   |
| 3   | R     | 377 | NDP  | C5D-O5D-PN-O3   |
| 3   | A     | 376 | NDP  | C5D-O5D-PN-O3   |
| 3   | D     | 365 | NDP  | C5D-O5D-PN-O3   |
| 3   | H     | 379 | NDP  | C2B-O2B-P2B-O3X |
| 3   | H     | 379 | NDP  | C5D-O5D-PN-O3   |
| 3   | Q     | 375 | NDP  | C5D-O5D-PN-O3   |
| 3   | P     | 373 | NDP  | C5D-O5D-PN-O3   |
| 3   | C     | 365 | NDP  | C5D-O5D-PN-O3   |
| 3   | I     | 380 | NDP  | PA-O3-PN-O1N    |
| 3   | I     | 380 | NDP  | PA-O3-PN-O2N    |
| 3   | L     | 369 | NDP  | PA-O3-PN-O2N    |
| 3   | D     | 365 | NDP  | PA-O3-PN-O1N    |
| 3   | D     | 365 | NDP  | PA-O3-PN-O2N    |
| 3   | H     | 379 | NDP  | PA-O3-PN-O1N    |
| 3   | H     | 379 | NDP  | PA-O3-PN-O2N    |
| 3   | P     | 373 | NDP  | PA-O3-PN-O1N    |
| 3   | P     | 373 | NDP  | PA-O3-PN-O2N    |
| 3   | C     | 365 | NDP  | PA-O3-PN-O2N    |
| 3   | B     | 378 | NDP  | O4D-C1D-N1N-C2N |
| 3   | I     | 380 | NDP  | O4D-C1D-N1N-C2N |
| 3   | A     | 376 | NDP  | O4D-C1D-N1N-C6N |
| 3   | C     | 365 | NDP  | C2D-C1D-N1N-C2N |
| 3   | B     | 378 | NDP  | C5D-O5D-PN-O1N  |
| 3   | R     | 377 | NDP  | C5D-O5D-PN-O1N  |
| 3   | O     | 372 | NDP  | O4B-C4B-C5B-O5B |
| 3   | R     | 377 | NDP  | O4D-C1D-N1N-C2N |
| 3   | D     | 365 | NDP  | O4D-C1D-N1N-C2N |
| 3   | H     | 379 | NDP  | O4D-C1D-N1N-C6N |
| 3   | O     | 372 | NDP  | O4D-C1D-N1N-C6N |
| 3   | Q     | 375 | NDP  | O4D-C1D-N1N-C2N |
| 3   | B     | 378 | NDP  | PA-O3-PN-O2N    |
| 3   | O     | 372 | NDP  | PA-O3-PN-O2N    |
| 3   | M     | 381 | NDP  | PA-O3-PN-O2N    |
| 3   | R     | 377 | NDP  | PA-O3-PN-O2N    |
| 3   | A     | 376 | NDP  | PA-O3-PN-O2N    |
| 3   | Q     | 375 | NDP  | PA-O3-PN-O2N    |
| 3   | M     | 381 | NDP  | O4B-C4B-C5B-O5B |
| 3   | R     | 377 | NDP  | O4B-C4B-C5B-O5B |
| 3   | B     | 378 | NDP  | C2D-C1D-N1N-C2N |
| 3   | I     | 380 | NDP  | C2D-C1D-N1N-C2N |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | R     | 377 | NDP  | C2D-C1D-N1N-C2N |
| 3   | A     | 376 | NDP  | C2D-C1D-N1N-C2N |
| 3   | L     | 369 | NDP  | C2D-C1D-N1N-C2N |
| 3   | Q     | 375 | NDP  | C2D-C1D-N1N-C2N |
| 3   | P     | 373 | NDP  | C2D-C1D-N1N-C2N |
| 3   | M     | 381 | NDP  | C2D-C1D-N1N-C2N |
| 3   | R     | 377 | NDP  | PA-O3-PN-O1N    |
| 3   | C     | 365 | NDP  | PA-O3-PN-O1N    |
| 3   | I     | 380 | NDP  | O4B-C4B-C5B-O5B |
| 3   | B     | 378 | NDP  | PN-O3-PA-O5B    |
| 3   | A     | 376 | NDP  | PN-O3-PA-O5B    |
| 3   | O     | 372 | NDP  | C2B-O2B-P2B-O2X |
| 3   | O     | 372 | NDP  | C2B-O2B-P2B-O3X |
| 3   | I     | 380 | NDP  | C2B-O2B-P2B-O3X |
| 3   | L     | 369 | NDP  | C2B-O2B-P2B-O2X |
| 3   | L     | 369 | NDP  | C2B-O2B-P2B-O3X |
| 3   | L     | 369 | NDP  | C5D-O5D-PN-O3   |
| 3   | H     | 379 | NDP  | C2B-O2B-P2B-O2X |
| 3   | O     | 372 | NDP  | PA-O3-PN-O1N    |
| 3   | H     | 379 | NDP  | C2D-C1D-N1N-C2N |
| 3   | A     | 376 | NDP  | C5D-O5D-PN-O1N  |
| 3   | H     | 379 | NDP  | C5D-O5D-PN-O1N  |
| 3   | Q     | 375 | NDP  | C5D-O5D-PN-O1N  |
| 3   | P     | 373 | NDP  | C5D-O5D-PN-O1N  |

There are no ring outliers.

29 monomers are involved in 181 short contacts:

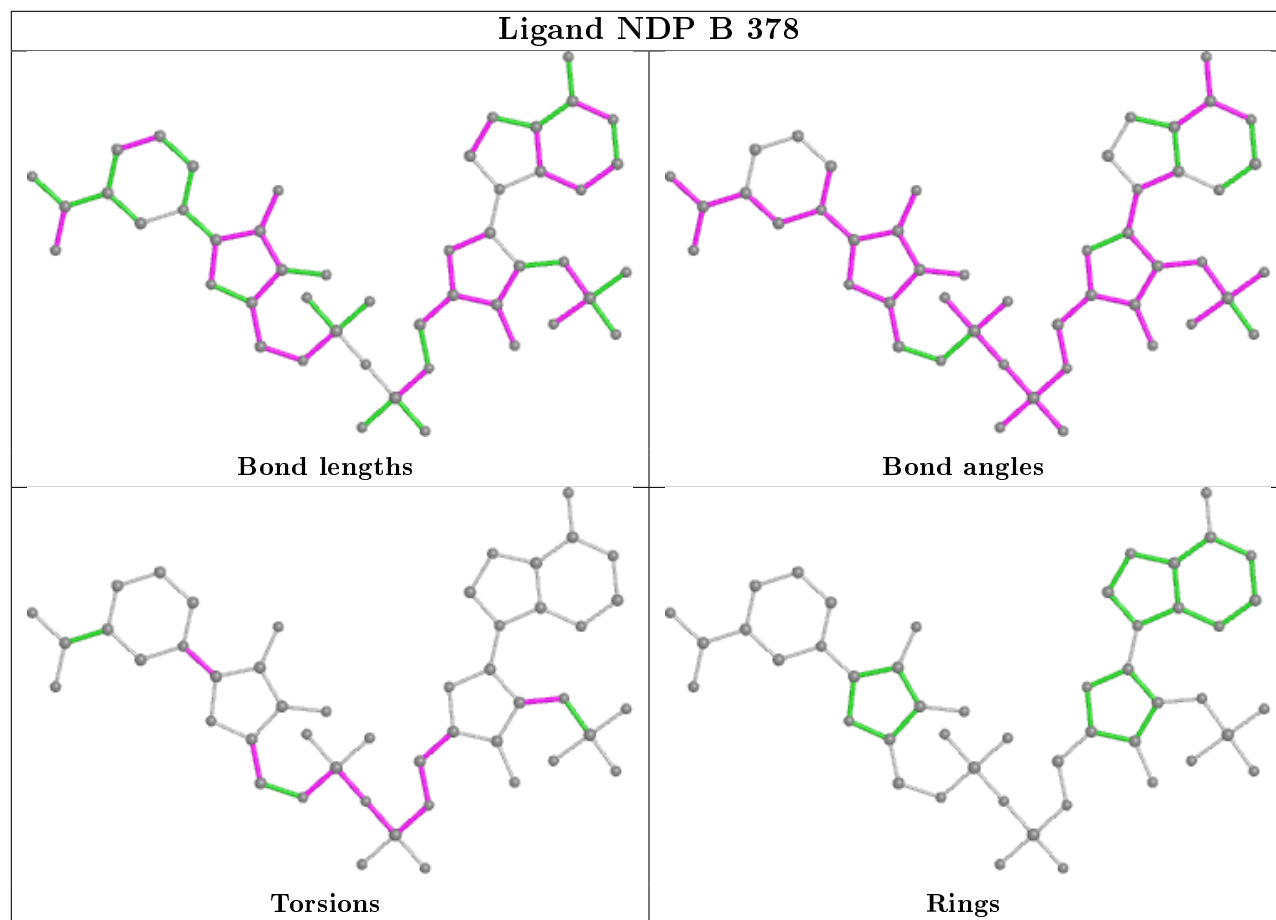
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | B     | 378 | NDP  | 13      | 0            |
| 3   | O     | 372 | NDP  | 15      | 0            |
| 3   | M     | 381 | NDP  | 10      | 0            |
| 2   | R     | 363 | SO4  | 1       | 0            |
| 3   | I     | 380 | NDP  | 10      | 0            |
| 2   | H     | 364 | SO4  | 2       | 0            |
| 2   | O     | 371 | SO4  | 2       | 0            |
| 2   | H     | 378 | SO4  | 1       | 0            |
| 2   | P     | 364 | SO4  | 4       | 0            |
| 3   | R     | 377 | NDP  | 5       | 0            |
| 3   | A     | 376 | NDP  | 19      | 0            |
| 2   | Q     | 373 | SO4  | 1       | 0            |
| 2   | B     | 364 | SO4  | 2       | 0            |

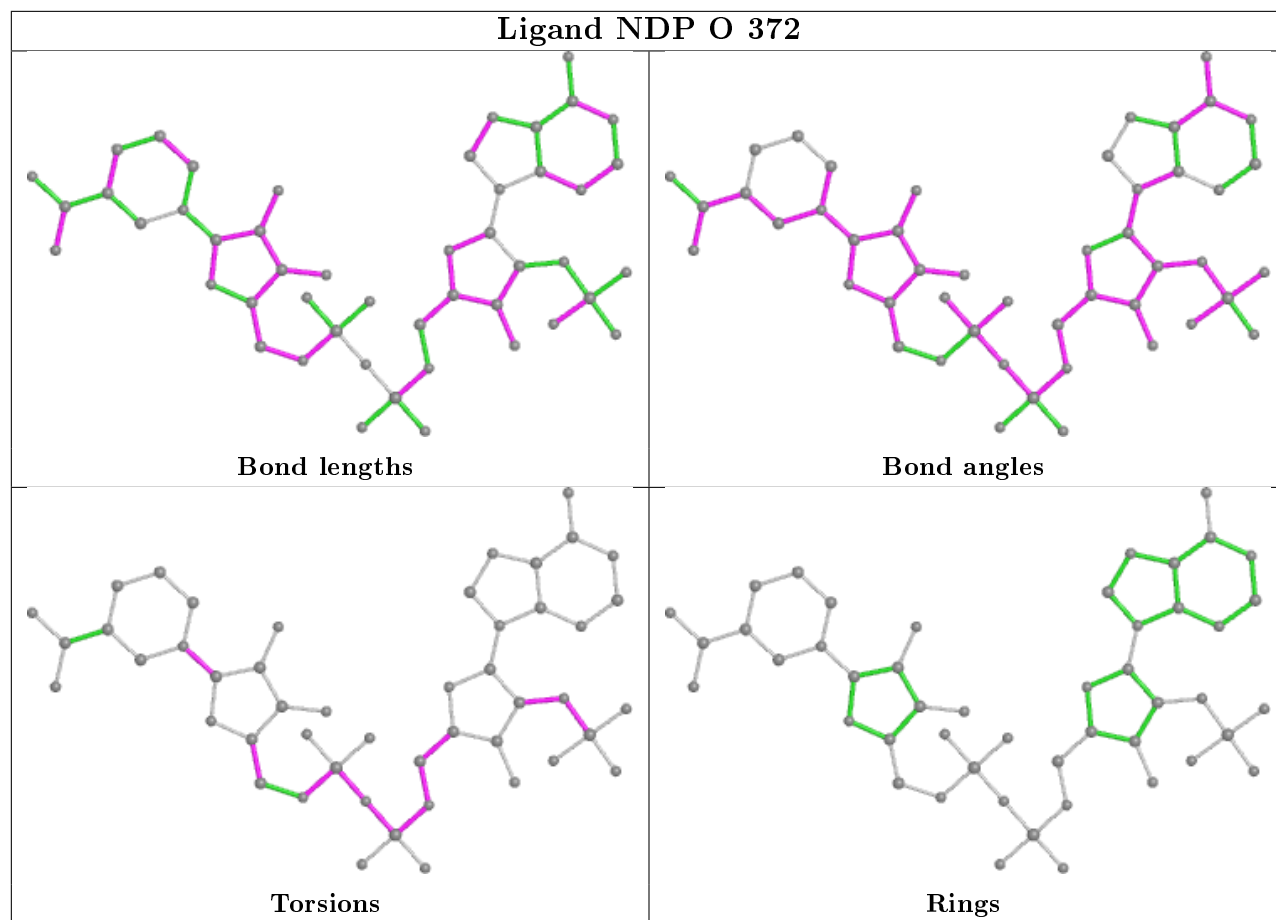
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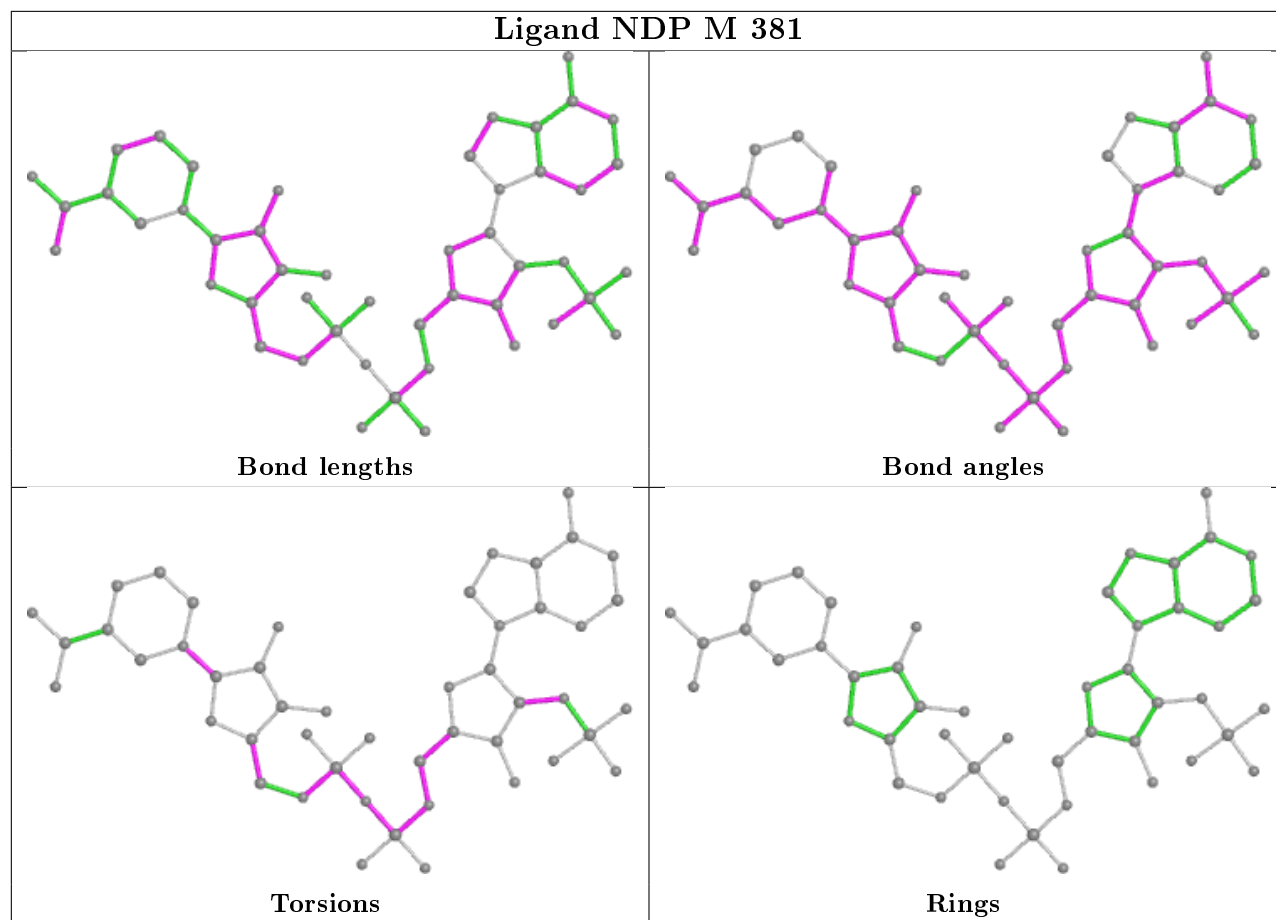
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | R     | 376 | SO4  | 2       | 0            |
| 2   | D     | 364 | SO4  | 2       | 0            |
| 2   | L     | 367 | SO4  | 1       | 0            |
| 2   | O     | 364 | SO4  | 2       | 0            |
| 2   | P     | 363 | SO4  | 1       | 0            |
| 3   | L     | 369 | NDP  | 14      | 0            |
| 3   | D     | 365 | NDP  | 6       | 0            |
| 2   | I     | 366 | SO4  | 5       | 0            |
| 2   | P     | 372 | SO4  | 1       | 0            |
| 2   | H     | 363 | SO4  | 1       | 0            |
| 3   | H     | 379 | NDP  | 14      | 0            |
| 2   | M     | 370 | SO4  | 3       | 0            |
| 2   | I     | 379 | SO4  | 1       | 0            |
| 3   | Q     | 375 | NDP  | 16      | 0            |
| 3   | P     | 373 | NDP  | 11      | 0            |
| 3   | C     | 365 | NDP  | 16      | 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.

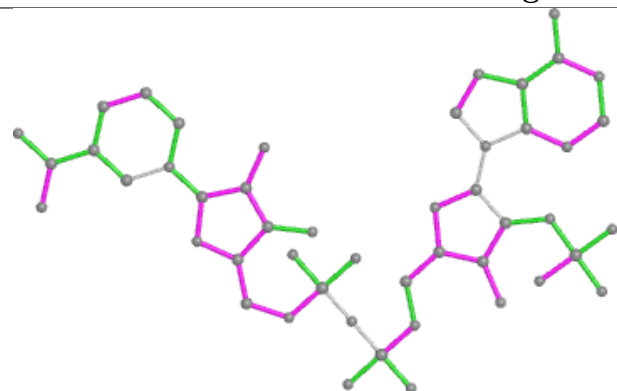




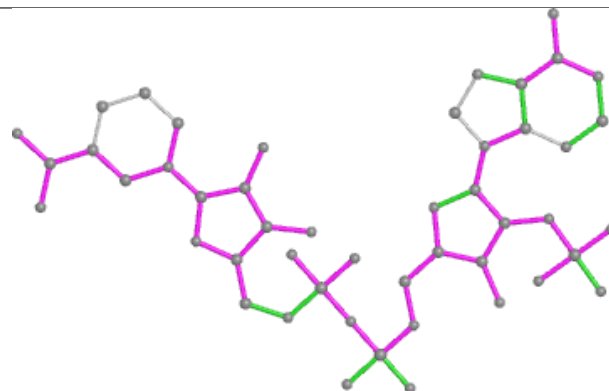




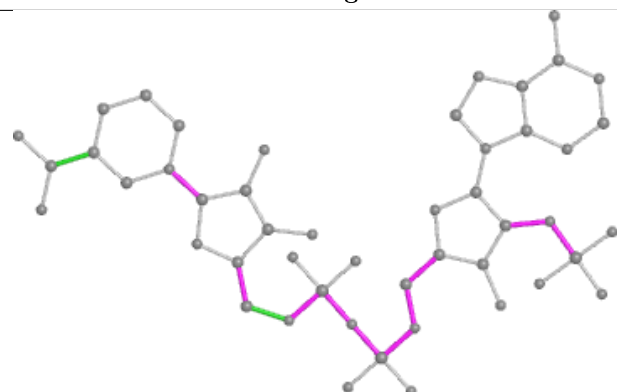
## Ligand NDP I 380



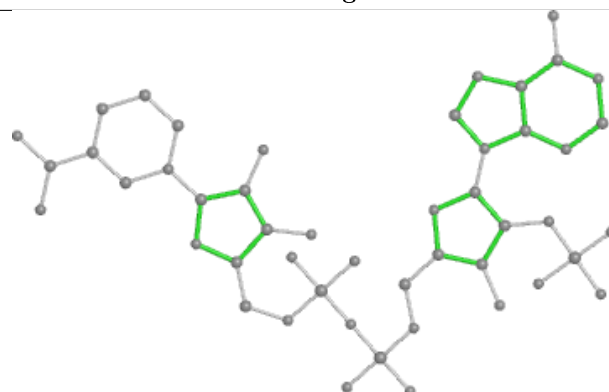
Bond lengths



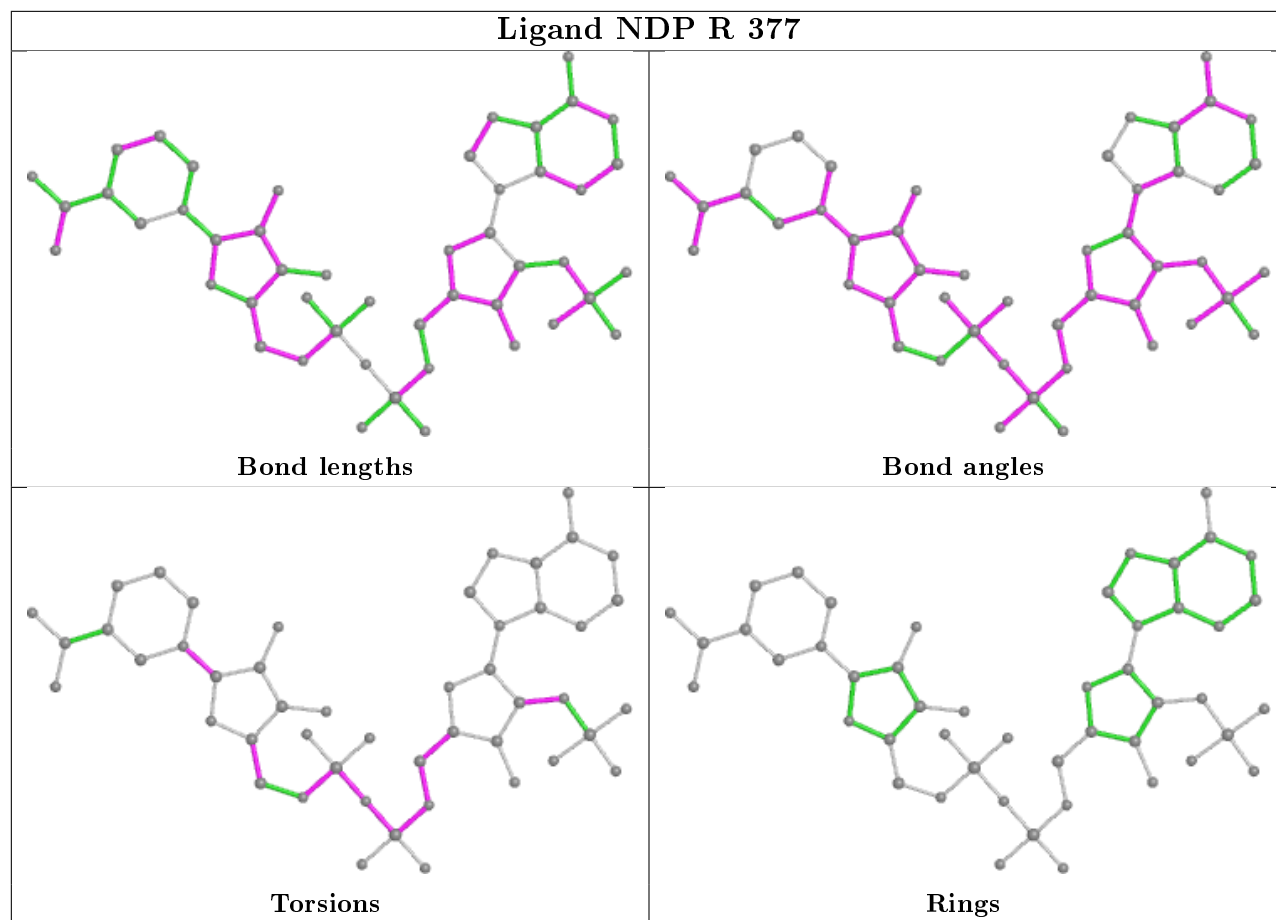
Bond angles

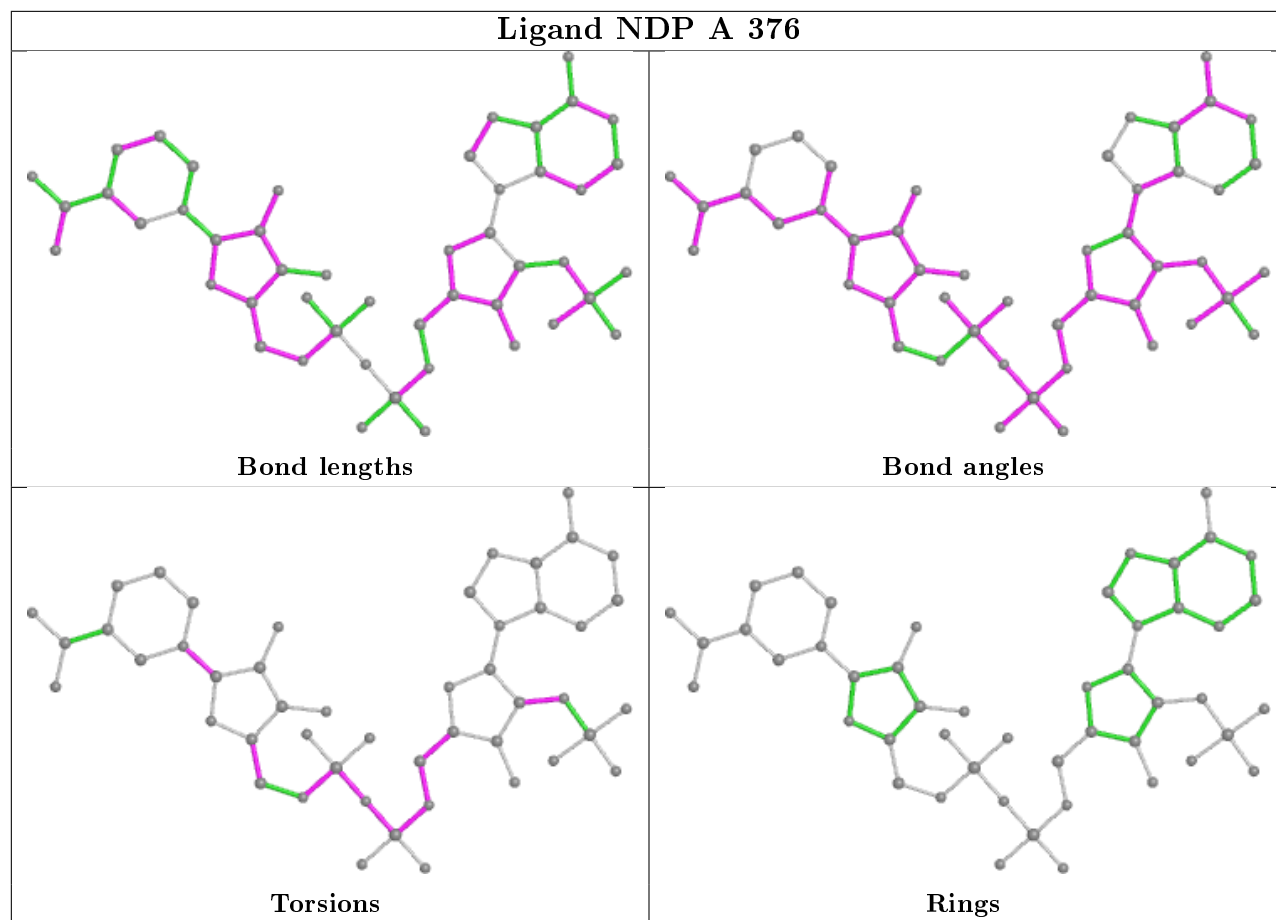


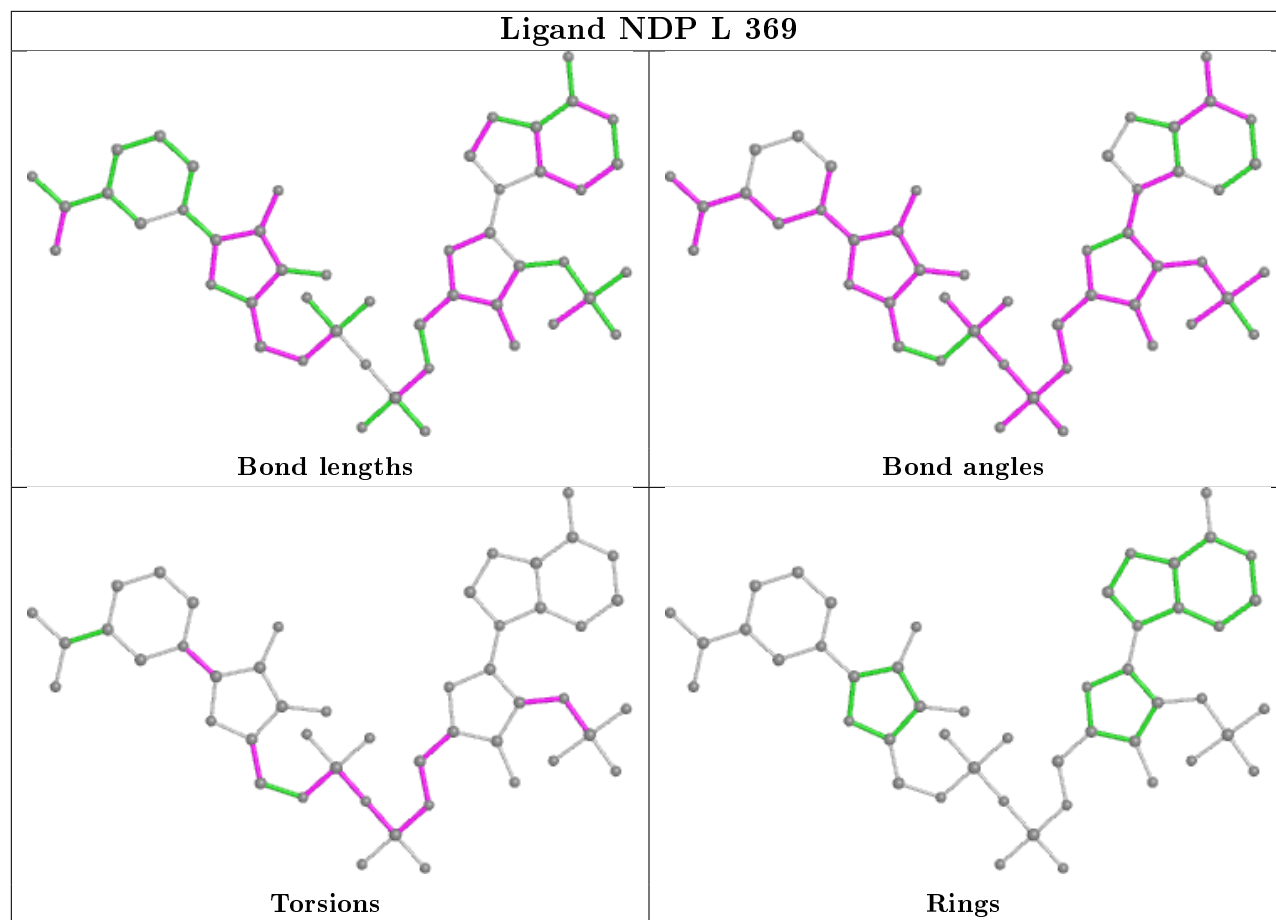
Torsions

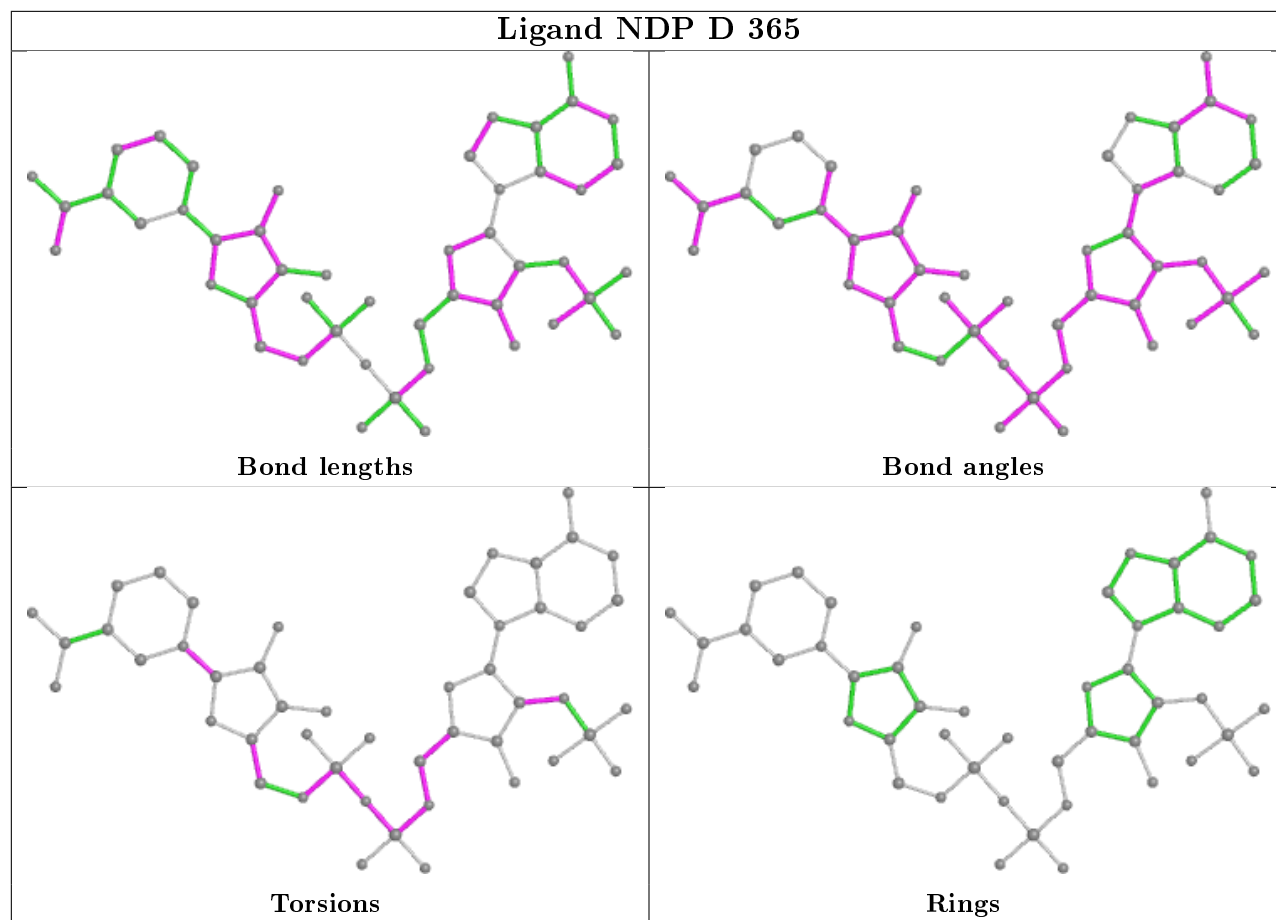


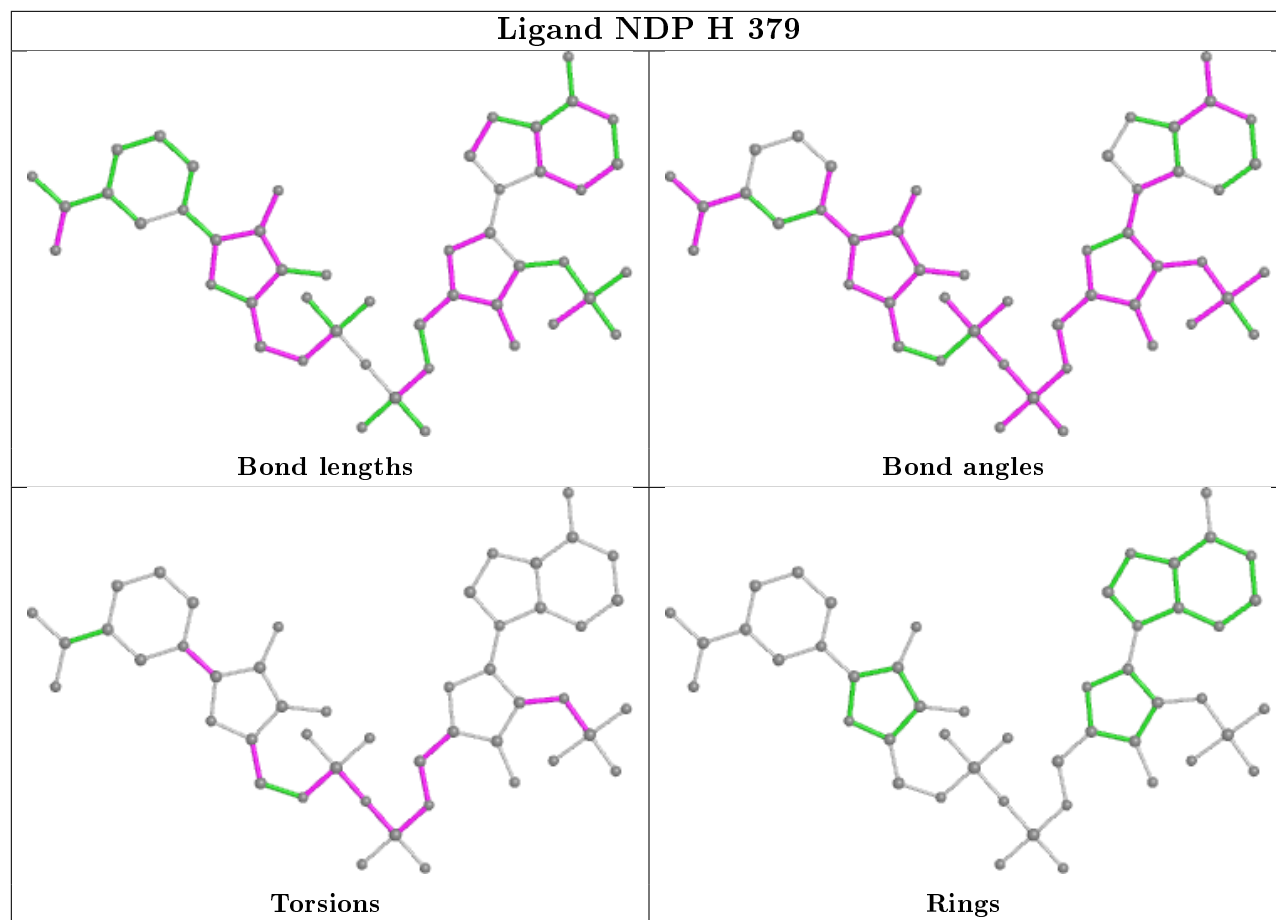
Rings

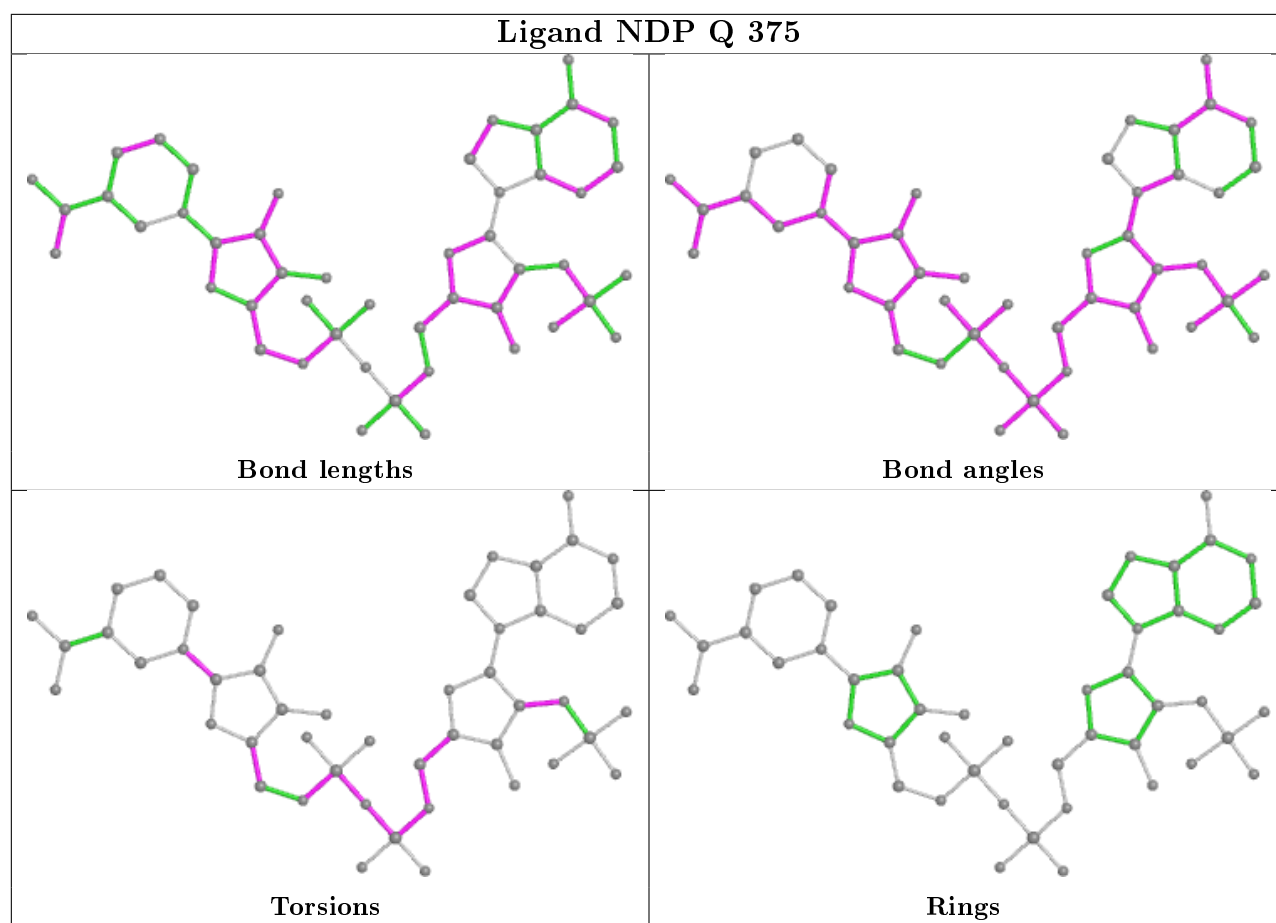


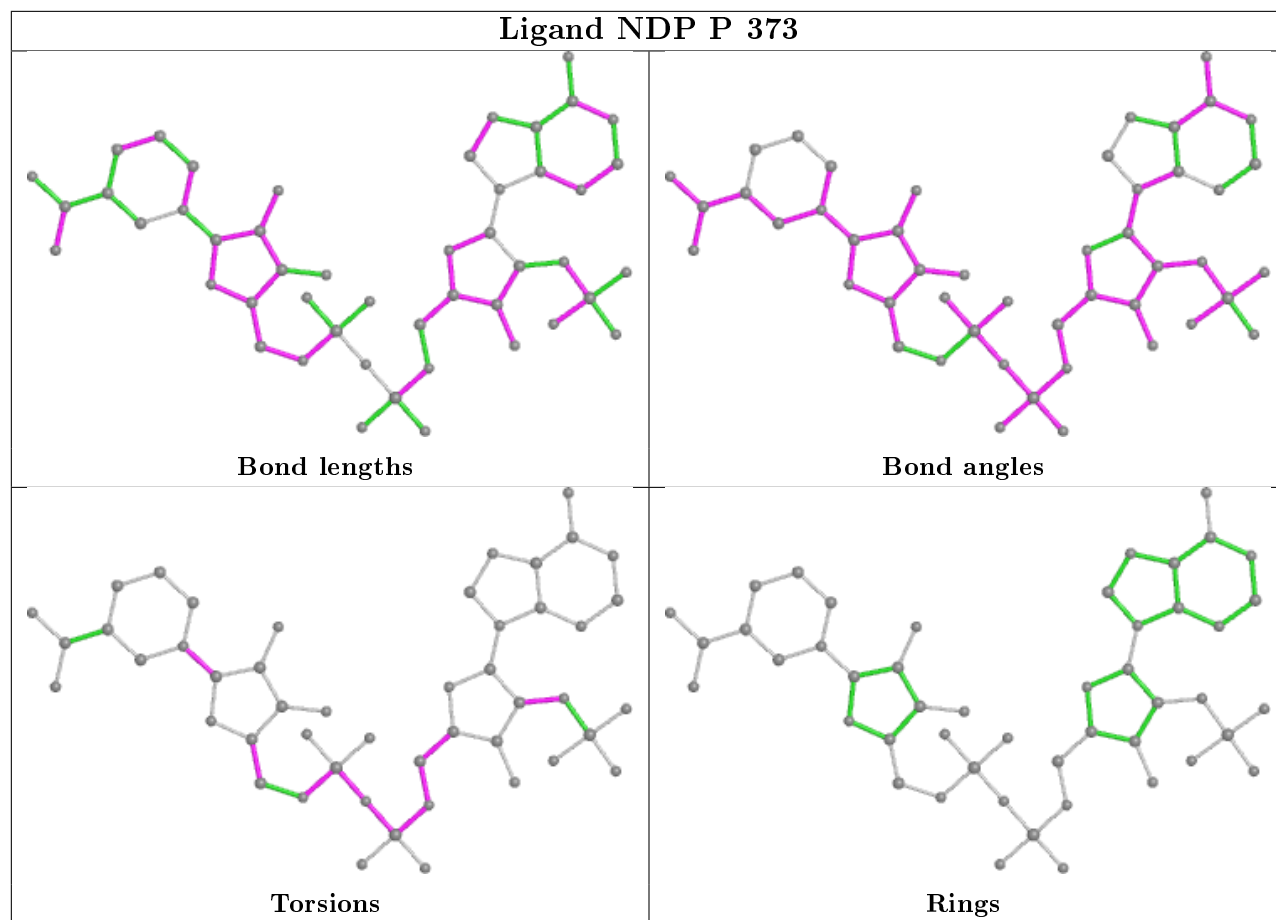




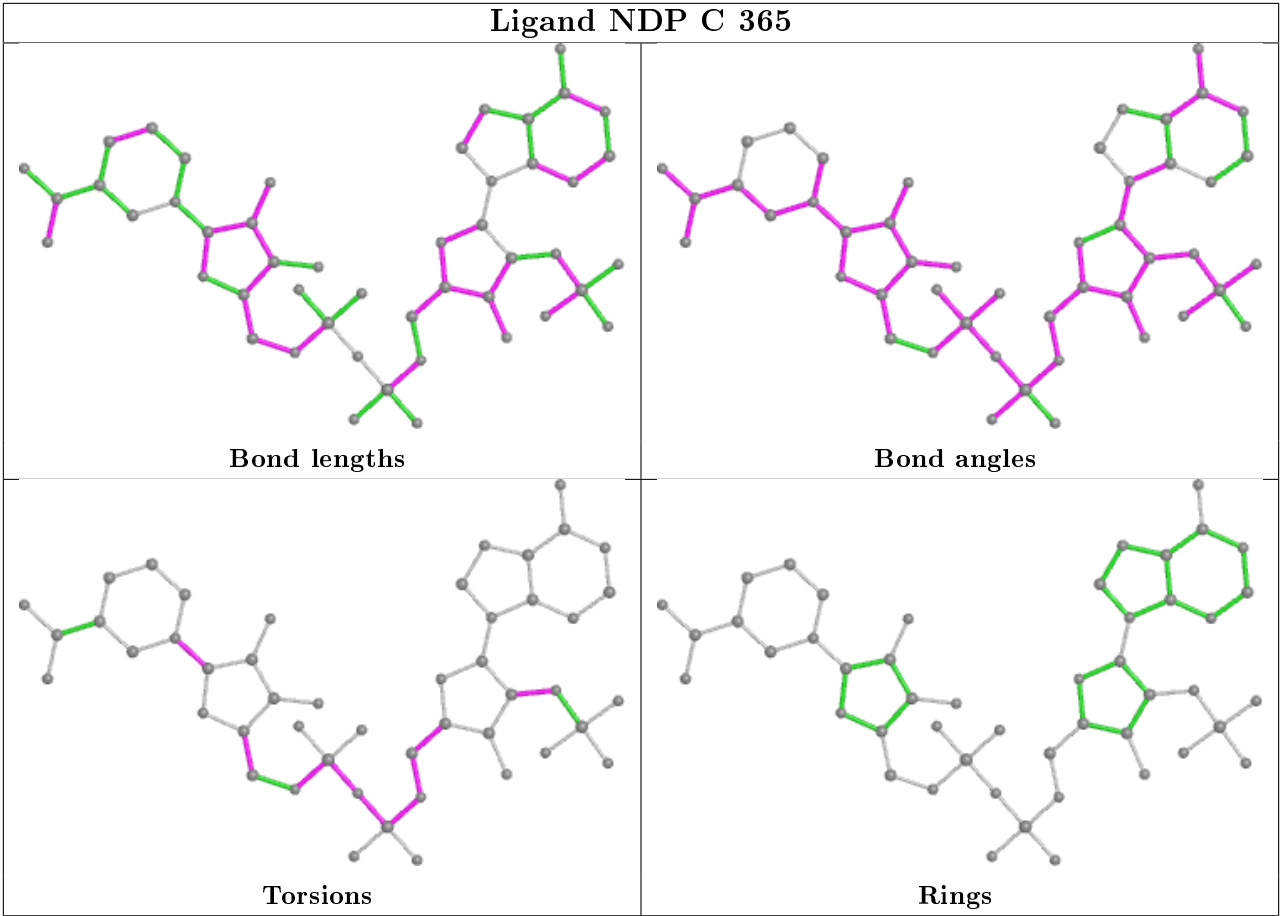












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | B     | 2                |
| 1   | A     | 1                |
| 1   | L     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | B     | 210:ALA   | C      | 211:ALA   | N      | 1.68         |
| 1     | A     | 206:THR   | C      | 207:SER   | N      | 1.18         |
| 1     | L     | 205:PRO   | C      | 206:THR   | N      | 1.16         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | B     | 333:GLN   | C      | 334:GLY   | N      | 1.12         |

## 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     | 337/365 (92%)   | 0.12   | 2 (0%) 89 88  | 7, 24, 42, 53         | 1 (0%)  |
| 1   | B     | 337/365 (92%)   | 0.02   | 1 (0%) 94 93  | 7, 18, 35, 54         | 1 (0%)  |
| 1   | C     | 337/365 (92%)   | -0.05  | 1 (0%) 94 93  | 6, 16, 31, 43         | 1 (0%)  |
| 1   | D     | 336/365 (92%)   | 0.25   | 12 (3%) 42 42 | 7, 27, 56, 65         | 1 (0%)  |
| 1   | H     | 336/365 (92%)   | 0.29   | 9 (2%) 54 52  | 9, 28, 55, 67         | 1 (0%)  |
| 1   | I     | 337/365 (92%)   | -0.00  | 1 (0%) 94 93  | 7, 22, 37, 50         | 1 (0%)  |
| 1   | L     | 336/365 (92%)   | 0.32   | 14 (4%) 36 35 | 11, 30, 57, 73        | 1 (0%)  |
| 1   | M     | 337/365 (92%)   | 0.01   | 0 100 100     | 10, 21, 38, 44        | 1 (0%)  |
| 1   | O     | 337/365 (92%)   | -0.04  | 2 (0%) 89 88  | 6, 17, 32, 47         | 1 (0%)  |
| 1   | P     | 337/365 (92%)   | 0.19   | 4 (1%) 79 77  | 9, 25, 42, 54         | 1 (0%)  |
| 1   | Q     | 337/365 (92%)   | -0.04  | 1 (0%) 94 93  | 7, 18, 34, 44         | 1 (0%)  |
| 1   | R     | 337/365 (92%)   | 0.30   | 13 (3%) 39 38 | 6, 26, 55, 68         | 1 (0%)  |
| All | All   | 4041/4380 (92%) | 0.11   | 60 (1%) 73 72 | 6, 22, 50, 73         | 12 (0%) |

All (60) RSRZ outliers are listed below:

| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | L     | 332   | TRP  | 5.1  |
| 1   | H     | 332   | TRP  | 4.0  |
| 1   | L     | 61    | ASP  | 3.6  |
| 1   | D     | 80    | VAL  | 3.5  |
| 1   | L     | 60(A) | GLY  | 3.3  |
| 1   | H     | 61    | ASP  | 3.3  |
| 1   | R     | 77    | ARG  | 3.2  |
| 1   | D     | 77    | ARG  | 3.1  |
| 1   | D     | 332   | TRP  | 3.0  |
| 1   | P     | 139   | HIS  | 3.0  |
| 1   | L     | 103   | ASP  | 3.0  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | R     | 68    | GLY  | 3.0  |
| 1   | R     | 333   | GLN  | 2.9  |
| 1   | L     | 85    | GLY  | 2.9  |
| 1   | R     | 83    | PRO  | 2.9  |
| 1   | L     | 116   | VAL  | 2.8  |
| 1   | H     | 86    | ASP  | 2.8  |
| 1   | R     | 332   | TRP  | 2.8  |
| 1   | L     | 86    | ASP  | 2.7  |
| 1   | H     | 60(A) | GLY  | 2.6  |
| 1   | H     | 78    | ASN  | 2.6  |
| 1   | D     | 98    | VAL  | 2.5  |
| 1   | R     | 1     | LEU  | 2.5  |
| 1   | L     | 110   | GLN  | 2.5  |
| 1   | H     | 143   | ILE  | 2.5  |
| 1   | L     | 0     | LYS  | 2.4  |
| 1   | L     | 333   | GLN  | 2.4  |
| 1   | L     | 72    | LYS  | 2.4  |
| 1   | L     | 89    | ILE  | 2.4  |
| 1   | R     | 86    | ASP  | 2.3  |
| 1   | B     | 56    | ASP  | 2.3  |
| 1   | R     | 72    | LYS  | 2.3  |
| 1   | A     | 61    | ASP  | 2.3  |
| 1   | R     | 88    | GLY  | 2.2  |
| 1   | D     | 78    | ASN  | 2.2  |
| 1   | O     | 62    | SER  | 2.2  |
| 1   | H     | 211   | ALA  | 2.2  |
| 1   | D     | 329   | ALA  | 2.2  |
| 1   | L     | 78    | ASN  | 2.2  |
| 1   | A     | 215   | ALA  | 2.2  |
| 1   | R     | 209   | GLY  | 2.2  |
| 1   | I     | 191   | ARG  | 2.2  |
| 1   | P     | 333   | GLN  | 2.2  |
| 1   | D     | 83    | PRO  | 2.2  |
| 1   | D     | 0     | LYS  | 2.2  |
| 1   | D     | 2     | LYS  | 2.2  |
| 1   | R     | 111   | ALA  | 2.1  |
| 1   | P     | 140   | ALA  | 2.1  |
| 1   | H     | 1     | LEU  | 2.1  |
| 1   | R     | 78    | ASN  | 2.1  |
| 1   | R     | 329   | ALA  | 2.1  |
| 1   | P     | 212   | LYS  | 2.1  |
| 1   | D     | 85    | GLY  | 2.1  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | Q     | 61     | ASP  | 2.1  |
| 1   | D     | 91     | LEU  | 2.1  |
| 1   | H     | 209    | GLY  | 2.0  |
| 1   | C     | 62     | SER  | 2.0  |
| 1   | L     | 211    | ALA  | 2.0  |
| 1   | D     | 191    | ARG  | 2.0  |
| 1   | O     | 122(A) | LYS  | 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 carbohydrates 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | SO4  | O     | 371 | 5/5   | 0.49 | 0.88 | 148,148,148,148            | 5     |
| 2   | SO4  | I     | 366 | 5/5   | 0.76 | 0.38 | 69,69,70,70                | 5     |
| 2   | SO4  | M     | 370 | 5/5   | 0.78 | 0.48 | 70,71,71,71                | 5     |
| 2   | SO4  | H     | 364 | 5/5   | 0.82 | 0.26 | 55,57,57,58                | 5     |
| 2   | SO4  | Q     | 373 | 5/5   | 0.84 | 0.43 | 74,74,74,75                | 5     |
| 2   | SO4  | B     | 377 | 5/5   | 0.85 | 0.36 | 77,77,77,77                | 5     |
| 2   | SO4  | C     | 364 | 5/5   | 0.87 | 0.17 | 57,57,59,59                | 0     |
| 2   | SO4  | A     | 363 | 5/5   | 0.87 | 0.28 | 56,56,57,58                | 5     |
| 3   | NDP  | H     | 379 | 48/48 | 0.89 | 0.23 | 31,38,54,57                | 0     |
| 3   | NDP  | L     | 369 | 48/48 | 0.89 | 0.22 | 31,40,58,60                | 0     |
| 2   | SO4  | D     | 364 | 5/5   | 0.89 | 0.22 | 54,54,55,55                | 5     |
| 3   | NDP  | R     | 377 | 48/48 | 0.90 | 0.23 | 30,43,53,54                | 0     |
| 2   | SO4  | L     | 368 | 5/5   | 0.91 | 0.21 | 49,50,51,53                | 0     |
| 2   | SO4  | M     | 380 | 5/5   | 0.92 | 0.41 | 65,65,66,66                | 5     |
| 3   | NDP  | O     | 372 | 48/48 | 0.92 | 0.20 | 16,25,39,43                | 0     |
| 3   | NDP  | D     | 365 | 48/48 | 0.92 | 0.22 | 30,40,55,57                | 0     |

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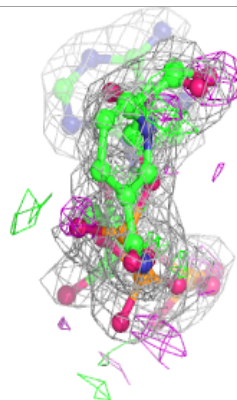
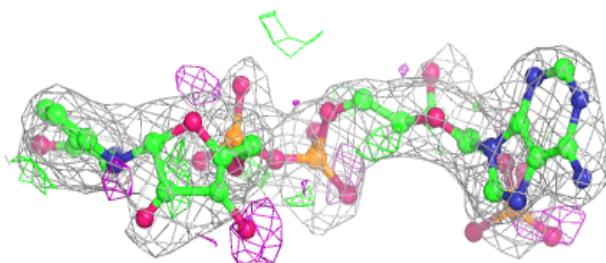
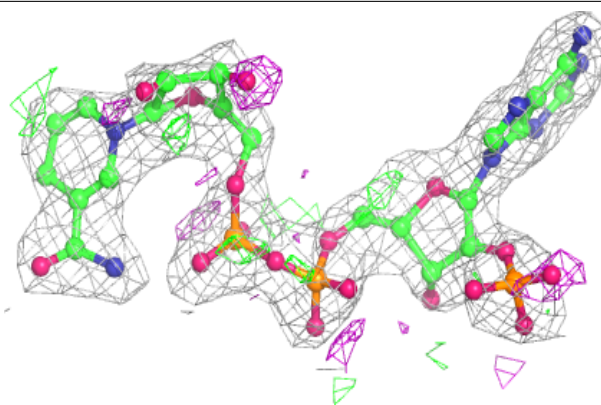
*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | SO4  | I     | 379 | 5/5   | 0.92 | 0.23 | 64,64,65,65                 | 0     |
| 2   | SO4  | R     | 364 | 5/5   | 0.92 | 0.23 | 50,50,51,51                 | 5     |
| 3   | NDP  | B     | 378 | 48/48 | 0.93 | 0.19 | 17,23,45,46                 | 0     |
| 2   | SO4  | O     | 364 | 5/5   | 0.93 | 0.22 | 56,56,56,57                 | 5     |
| 2   | SO4  | R     | 376 | 5/5   | 0.93 | 0.17 | 62,63,63,63                 | 0     |
| 3   | NDP  | M     | 381 | 48/48 | 0.93 | 0.18 | 21,26,41,43                 | 0     |
| 3   | NDP  | Q     | 375 | 48/48 | 0.93 | 0.19 | 25,30,49,51                 | 0     |
| 3   | NDP  | C     | 365 | 48/48 | 0.93 | 0.20 | 17,24,40,43                 | 0     |
| 3   | NDP  | A     | 376 | 48/48 | 0.93 | 0.17 | 19,25,47,48                 | 0     |
| 2   | SO4  | M     | 369 | 5/5   | 0.93 | 0.23 | 60,60,61,62                 | 0     |
| 2   | SO4  | B     | 364 | 5/5   | 0.94 | 0.23 | 40,42,43,45                 | 0     |
| 2   | SO4  | D     | 363 | 5/5   | 0.94 | 0.22 | 60,60,61,62                 | 0     |
| 2   | SO4  | Q     | 363 | 5/5   | 0.94 | 0.19 | 51,51,52,53                 | 0     |
| 2   | SO4  | B     | 363 | 5/5   | 0.94 | 0.23 | 52,53,54,54                 | 0     |
| 3   | NDP  | P     | 373 | 48/48 | 0.94 | 0.17 | 11,26,45,47                 | 0     |
| 3   | NDP  | I     | 380 | 48/48 | 0.94 | 0.19 | 19,26,42,46                 | 0     |
| 2   | SO4  | O     | 363 | 5/5   | 0.94 | 0.25 | 50,51,51,52                 | 5     |
| 2   | SO4  | H     | 378 | 5/5   | 0.94 | 0.17 | 55,56,56,56                 | 0     |
| 2   | SO4  | A     | 364 | 5/5   | 0.95 | 0.21 | 48,49,51,51                 | 0     |
| 2   | SO4  | C     | 363 | 5/5   | 0.95 | 0.19 | 62,62,63,63                 | 0     |
| 2   | SO4  | Q     | 374 | 5/5   | 0.95 | 0.24 | 51,52,52,52                 | 5     |
| 2   | SO4  | L     | 367 | 5/5   | 0.95 | 0.22 | 63,63,64,65                 | 0     |
| 2   | SO4  | R     | 363 | 5/5   | 0.95 | 0.22 | 35,36,37,37                 | 5     |
| 2   | SO4  | Q     | 364 | 5/5   | 0.95 | 0.17 | 40,41,42,42                 | 0     |
| 2   | SO4  | P     | 363 | 5/5   | 0.95 | 0.20 | 60,60,61,62                 | 0     |
| 2   | SO4  | P     | 364 | 5/5   | 0.96 | 0.18 | 44,44,45,45                 | 0     |
| 2   | SO4  | I     | 365 | 5/5   | 0.96 | 0.19 | 64,65,65,66                 | 0     |
| 2   | SO4  | H     | 363 | 5/5   | 0.96 | 0.20 | 60,61,61,62                 | 0     |
| 2   | SO4  | P     | 372 | 5/5   | 0.97 | 0.13 | 61,61,62,62                 | 0     |
| 2   | SO4  | A     | 375 | 5/5   | 0.97 | 0.16 | 55,55,55,56                 | 0     |

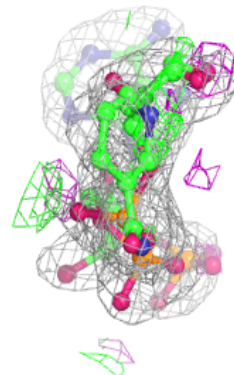
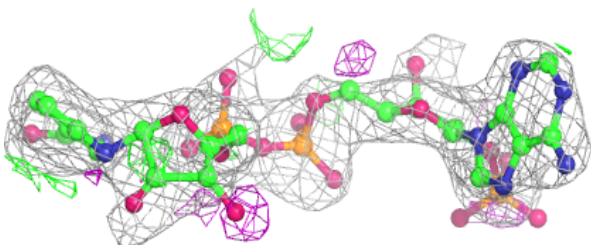
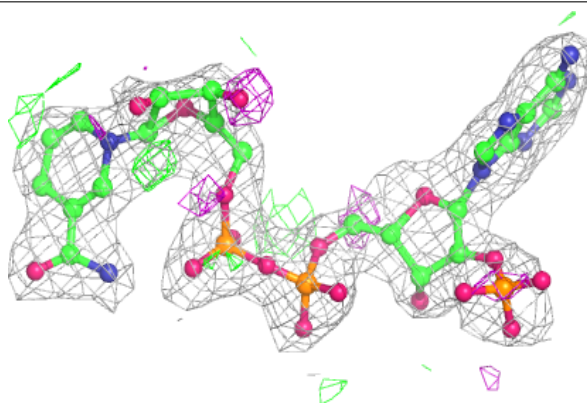
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NDP H 379:**

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

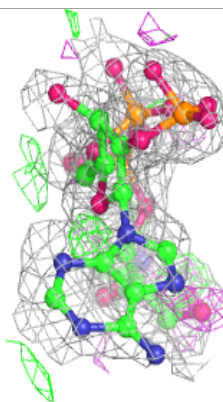
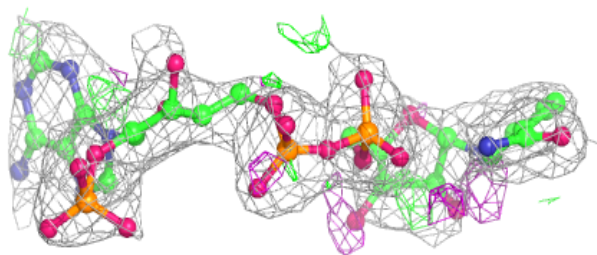
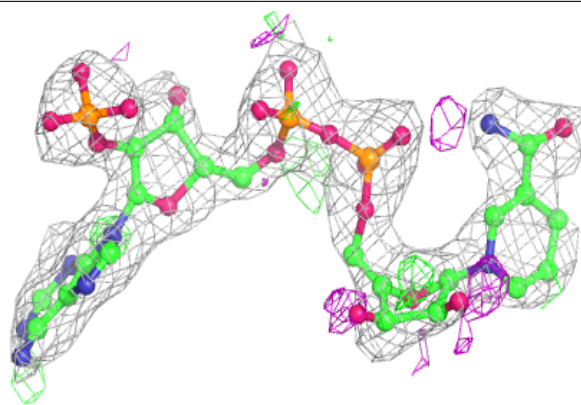
**Electron density around NDP L 369:**

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

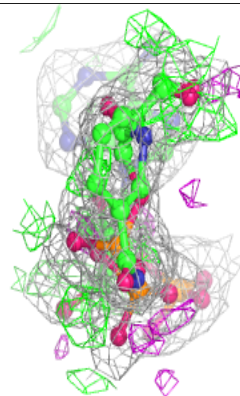
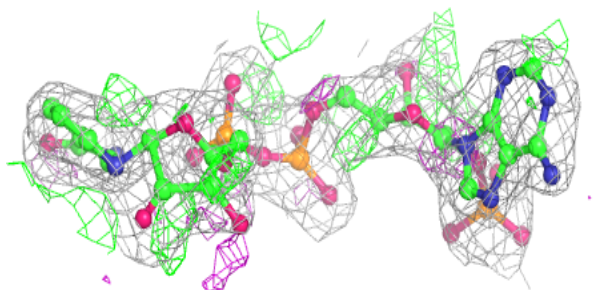
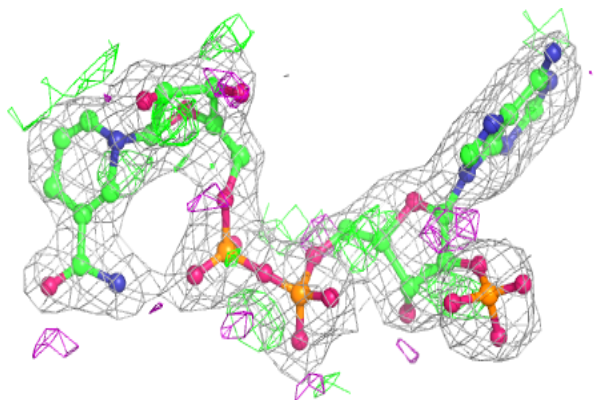


**Electron density around NDP R 377:**

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

**Electron density around NDP O 372:**

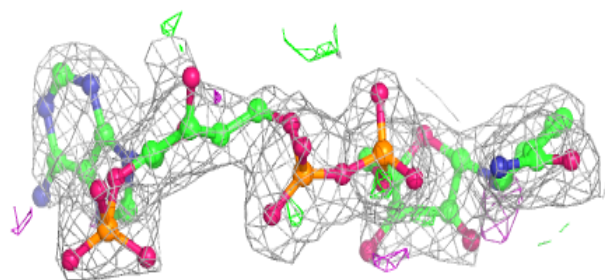
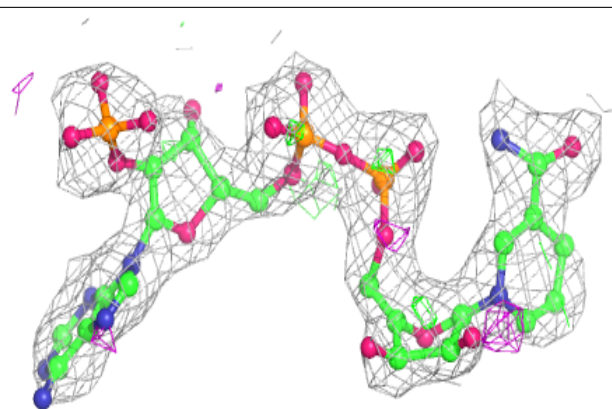
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



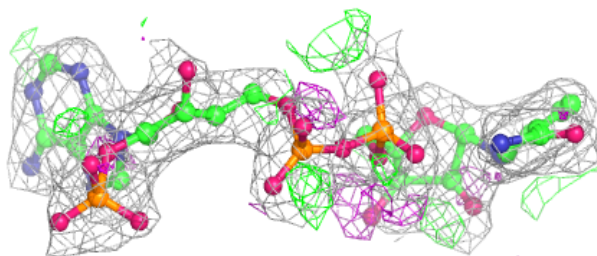
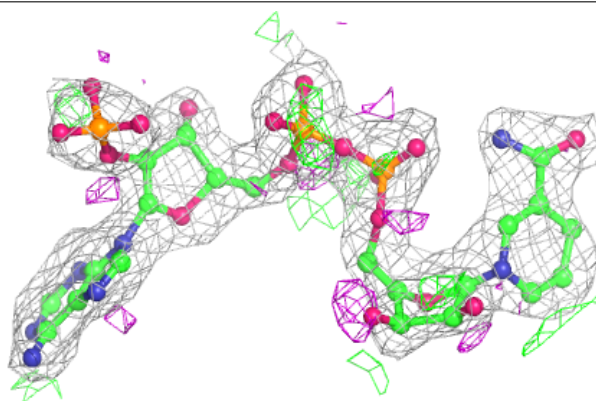


**Electron density around NDP D 365:**

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

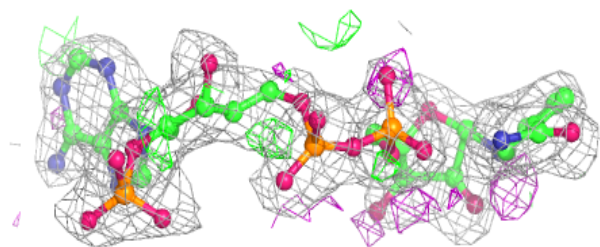
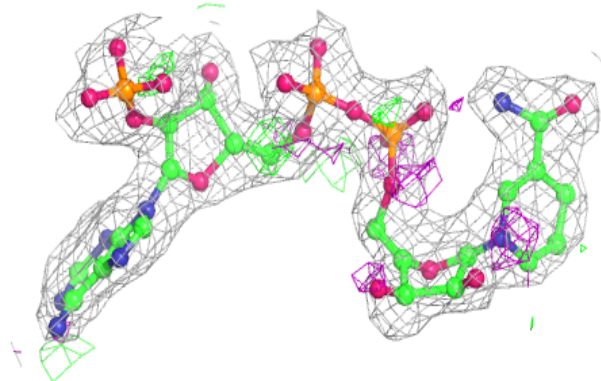
**Electron density around NDP B 378:**

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

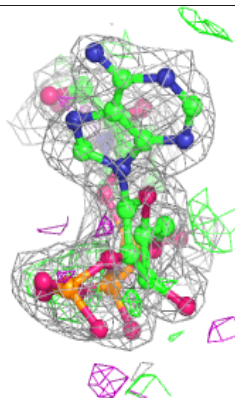
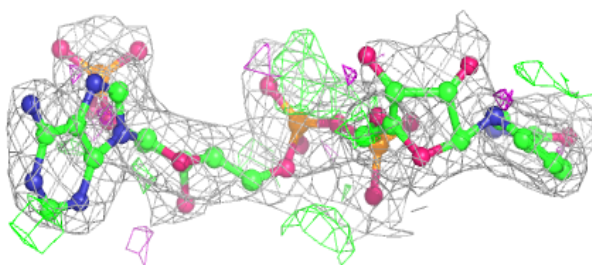
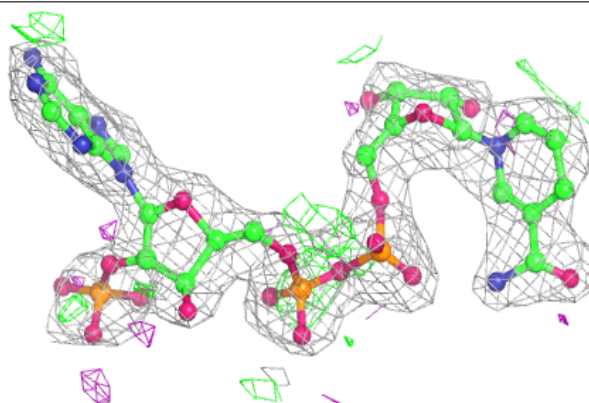


**Electron density around NDP M 381:**

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

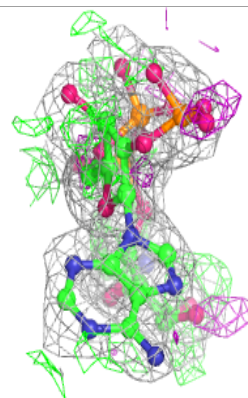
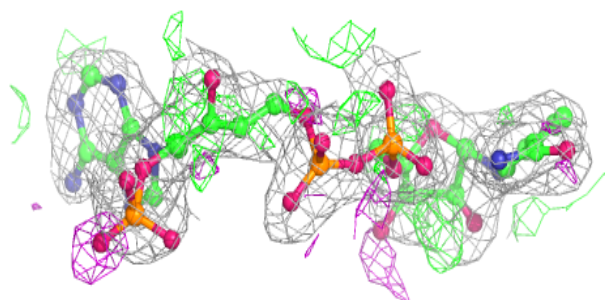
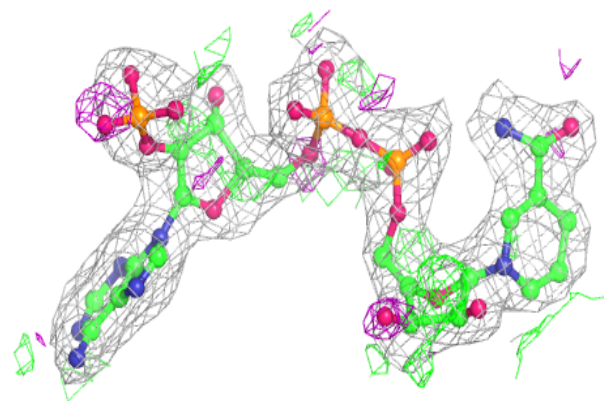
**Electron density around NDP Q 375:**

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

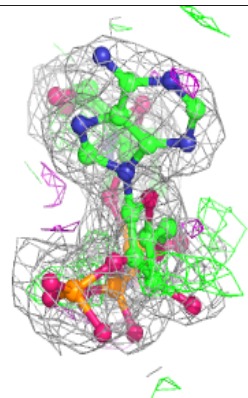
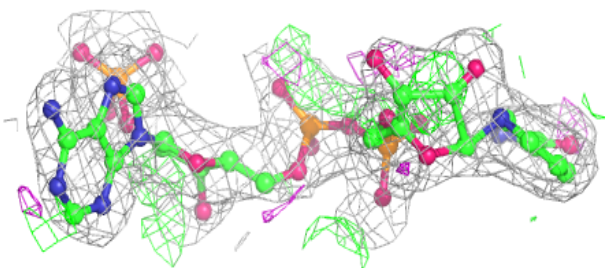
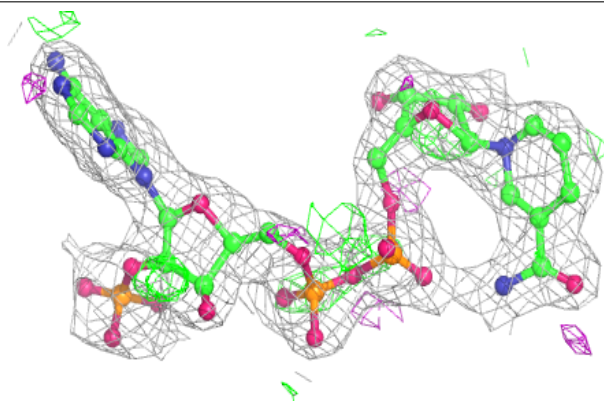


**Electron density around NDP C 365:**

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

**Electron density around NDP A 376:**

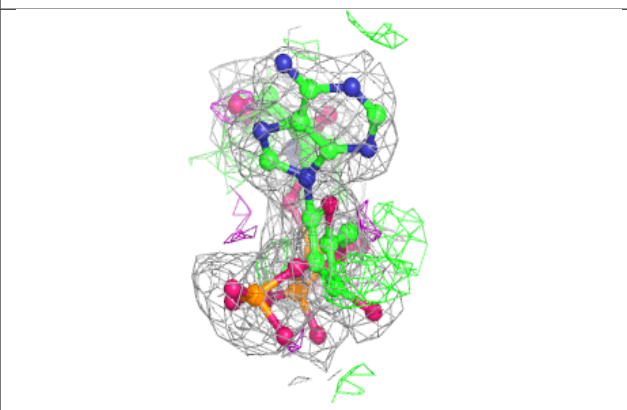
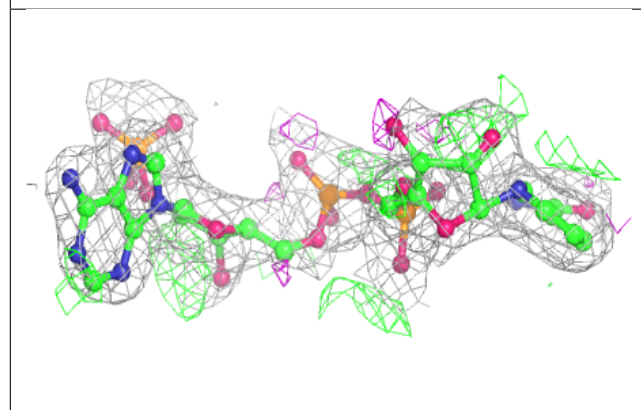
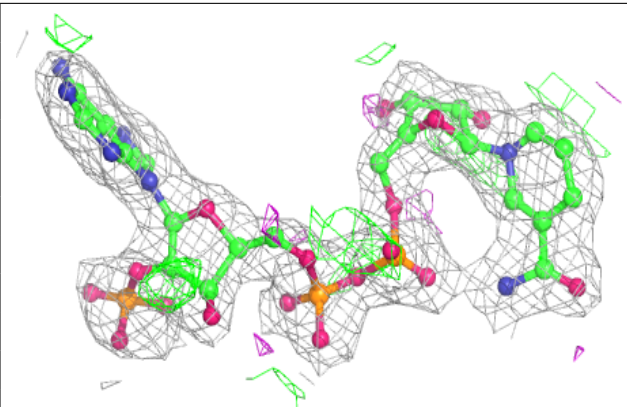
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



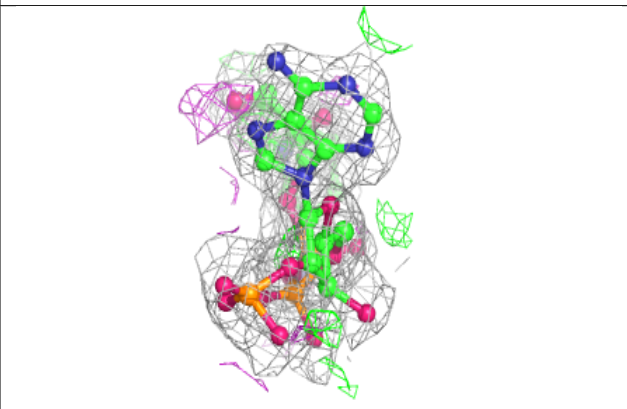
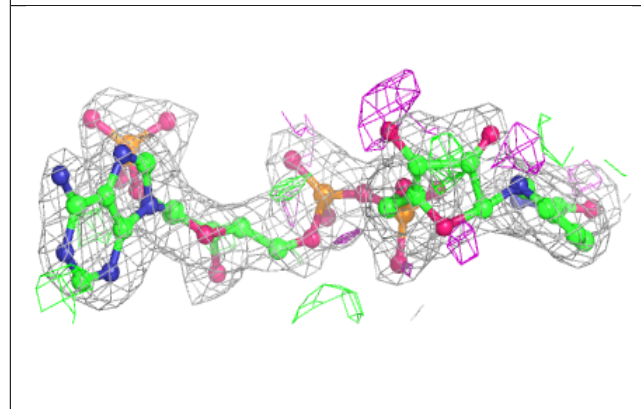
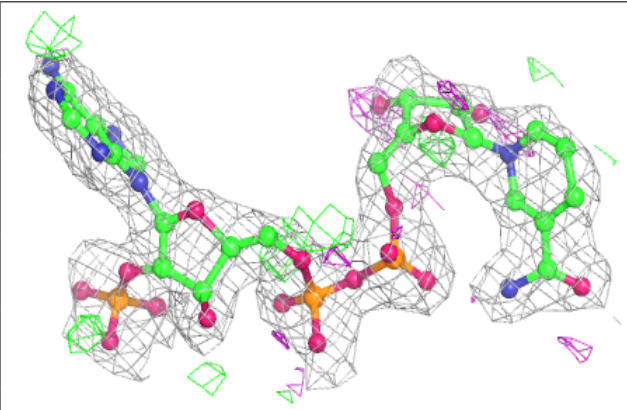


**Electron density around NDP P 373:**

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

**Electron density around NDP I 380:**

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



## 6.5 Other polymers

There are no such residues in this entry.