



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:12 AM UTC

PDB ID : 2D3B / pdb\_00002d3b  
Title : Crystal Structure of the Maize Glutamine Synthetase complexed with AMPPNP and Methionine sulfoximine  
Authors : Unno, H.; Uchida, T.; Sugawara, H.; Kurisu, G.; Sugiyama, T.; Yamaya, T.; Sakakibara, H.; Hase, T.; Kusunoki, M.  
Deposited on : 2005-09-26  
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

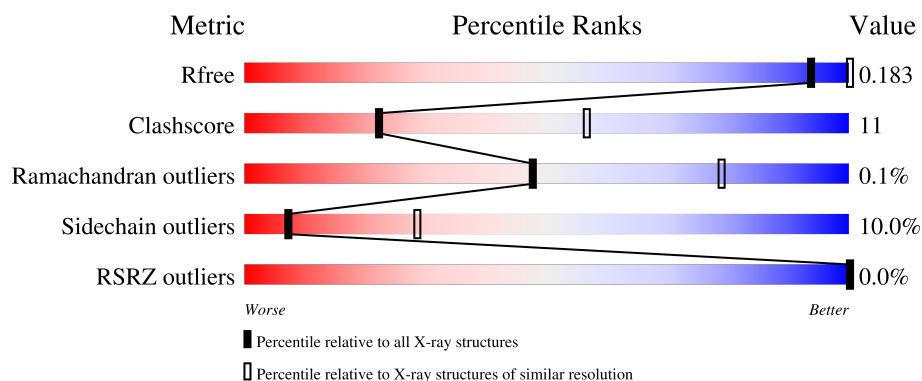
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1085 (3.54-3.46)                                      |
| Clashscore            | 190562                      | 1140 (3.54-3.46)                                      |
| Ramachandran outliers | 187476                      | 1113 (3.54-3.46)                                      |
| Sidechain outliers    | 187428                      | 1114 (3.54-3.46)                                      |
| RSRZ outliers         | 180081                      | 1084 (3.54-3.46)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 356    |  |
| 1   | B     | 356    |  |
| 1   | C     | 356    |  |
| 1   | D     | 356    |  |

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| Mol | Chain | Length | Quality of chain                                                                              |
|-----|-------|--------|-----------------------------------------------------------------------------------------------|
| 1   | E     | 356    |  74% 23% .. |
| 1   | F     | 356    |  73% 23% .. |
| 1   | G     | 356    |  73% 22% .. |
| 1   | H     | 356    |  76% 21% .. |
| 1   | I     | 356    |  76% 20% .. |
| 1   | J     | 356    |  78% 18% .. |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3   | ANP  | A     | 6001 | X         | -        | -       | -                |
| 3   | ANP  | B     | 6002 | X         | -        | -       | -                |
| 3   | ANP  | C     | 6003 | X         | -        | -       | -                |
| 3   | ANP  | D     | 6004 | X         | -        | -       | -                |
| 3   | ANP  | E     | 6005 | X         | -        | -       | -                |
| 3   | ANP  | F     | 6006 | X         | -        | -       | -                |
| 3   | ANP  | G     | 6007 | X         | -        | -       | -                |
| 3   | ANP  | H     | 6008 | X         | -        | -       | -                |
| 3   | ANP  | I     | 6009 | X         | -        | -       | -                |
| 3   | ANP  | J     | 6010 | X         | -        | -       | -                |
| 4   | MSL  | C     | 5002 | -         | -        | X       | -                |
| 4   | MSL  | C     | 5003 | -         | -        | X       | -                |
| 4   | MSL  | C     | 5005 | -         | -        | X       | -                |
| 4   | MSL  | C     | 5007 | -         | -        | X       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28277 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 glutamine synthetase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 353      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2745  | 1739 | 470 | 525 | 11 |         |         |       |
| 1   | B     | 353      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2745  | 1739 | 470 | 525 | 11 |         |         |       |
| 1   | C     | 353      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2745  | 1739 | 470 | 525 | 11 |         |         |       |
| 1   | D     | 353      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2745  | 1739 | 470 | 525 | 11 |         |         |       |
| 1   | E     | 353      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2745  | 1739 | 470 | 525 | 11 |         |         |       |
| 1   | F     | 353      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2745  | 1739 | 470 | 525 | 11 |         |         |       |
| 1   | G     | 353      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2745  | 1739 | 470 | 525 | 11 |         |         |       |
| 1   | H     | 353      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2745  | 1739 | 470 | 525 | 11 |         |         |       |
| 1   | I     | 353      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2745  | 1739 | 470 | 525 | 11 |         |         |       |
| 1   | J     | 353      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2745  | 1739 | 470 | 525 | 11 |         |         |       |

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

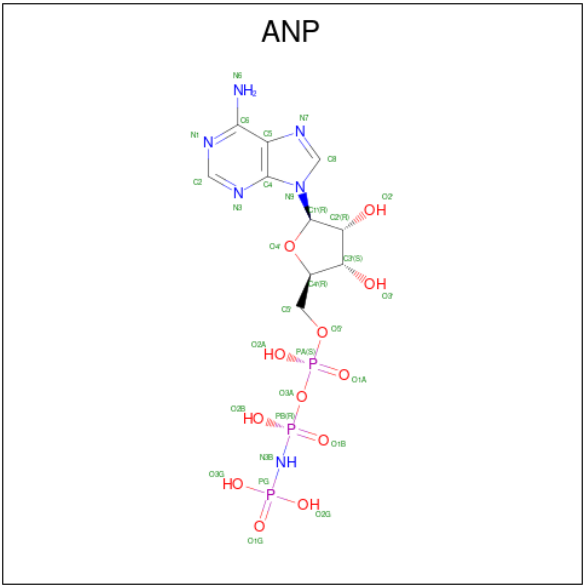
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 3        | Total | Mn | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 2   | B     | 3        | Total | Mn | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 2   | C     | 3        | Total | Mn | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 2   | D     | 3        | Total | Mn | 0       | 0       |
|     |       |          | 3     | 3  |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | E     | 3        | Total | Mn | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 2   | F     | 3        | Total | Mn | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 2   | G     | 3        | Total | Mn | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 2   | H     | 3        | Total | Mn | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 2   | I     | 3        | Total | Mn | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 2   | J     | 3        | Total | Mn | 0       | 0       |
|     |       |          | 3     | 3  |         |         |

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



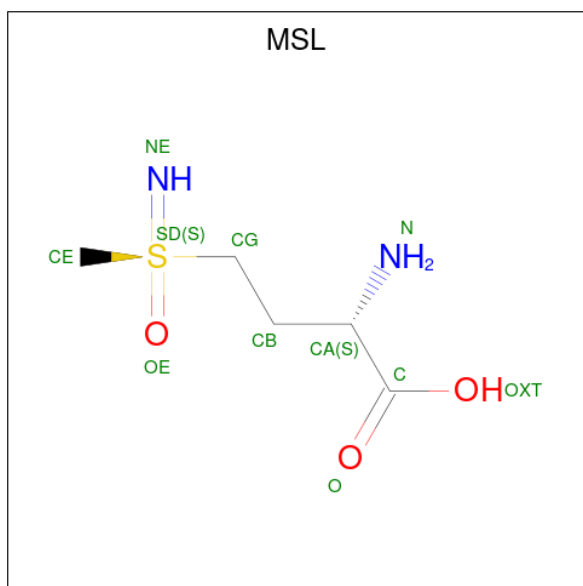
| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 6 | 12 | 3 |         |         |
| 3   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 6 | 12 | 3 |         |         |
| 3   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 6 | 12 | 3 |         |         |
| 3   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 6 | 12 | 3 |         |         |
| 3   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 6 | 12 | 3 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3   | F     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 6 | 12 | 3 |         |         |
| 3   | G     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 6 | 12 | 3 |         |         |
| 3   | H     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 6 | 12 | 3 |         |         |
| 3   | I     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 6 | 12 | 3 |         |         |
| 3   | J     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 31    | 10 | 6 | 12 | 3 |         |         |

- Molecule 4 is (2S)-2-AMINO-4-(METHYLSULFONIMIDOYL)BUTANOIC ACID (CCD ID: MSL) (formula: C<sub>5</sub>H<sub>12</sub>N<sub>2</sub>O<sub>3</sub>S).



| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 4   | C     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 11    | 5 | 2 | 3 | 1 |         |         |
| 4   | C     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 11    | 5 | 2 | 3 | 1 |         |         |
| 4   | C     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 11    | 5 | 2 | 3 | 1 |         |         |
| 4   | C     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 11    | 5 | 2 | 3 | 1 |         |         |
| 4   | C     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 11    | 5 | 2 | 3 | 1 |         |         |
| 4   | C     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 11    | 5 | 2 | 3 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 4   | C     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 11    | 5 | 2 | 3 | 1 |         |         |
| 4   | C     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 11    | 5 | 2 | 3 | 1 |         |         |
| 4   | C     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 11    | 5 | 2 | 3 | 1 |         |         |
| 4   | C     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 11    | 5 | 2 | 3 | 1 |         |         |

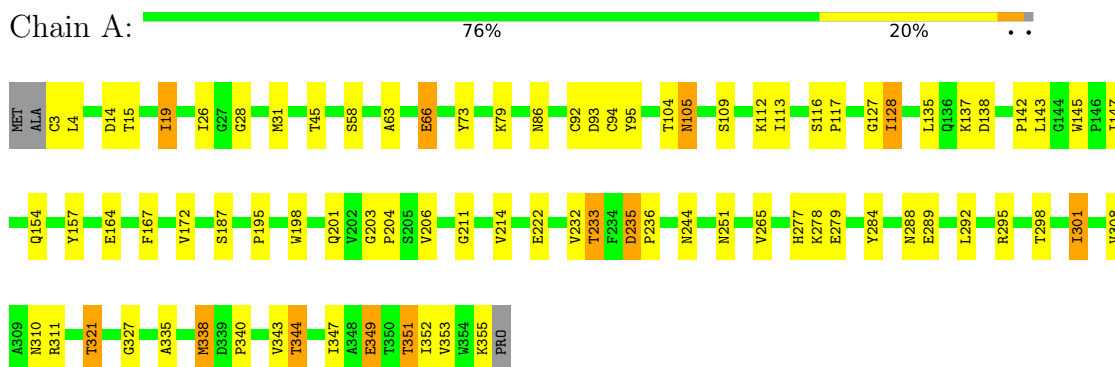
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 32       | Total | O  | 0       | 0       |
|     |       |          | 32    | 32 |         |         |
| 5   | B     | 36       | Total | O  | 0       | 0       |
|     |       |          | 36    | 36 |         |         |
| 5   | C     | 40       | Total | O  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 5   | D     | 42       | Total | O  | 0       | 0       |
|     |       |          | 42    | 42 |         |         |
| 5   | E     | 41       | Total | O  | 0       | 0       |
|     |       |          | 41    | 41 |         |         |
| 5   | F     | 39       | Total | O  | 0       | 0       |
|     |       |          | 39    | 39 |         |         |
| 5   | G     | 40       | Total | O  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 5   | H     | 32       | Total | O  | 0       | 0       |
|     |       |          | 32    | 32 |         |         |
| 5   | I     | 37       | Total | O  | 0       | 0       |
|     |       |          | 37    | 37 |         |         |
| 5   | J     | 38       | Total | O  | 0       | 0       |
|     |       |          | 38    | 38 |         |         |

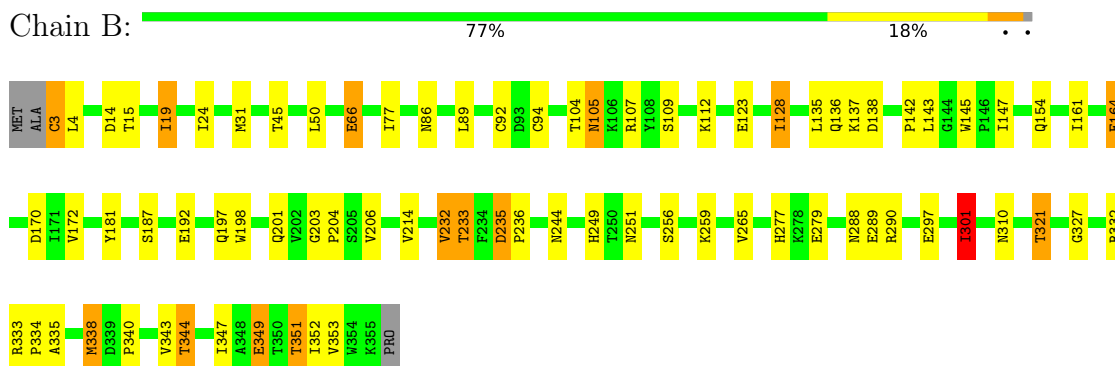
### 3 Residue-property plots [i](#)

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

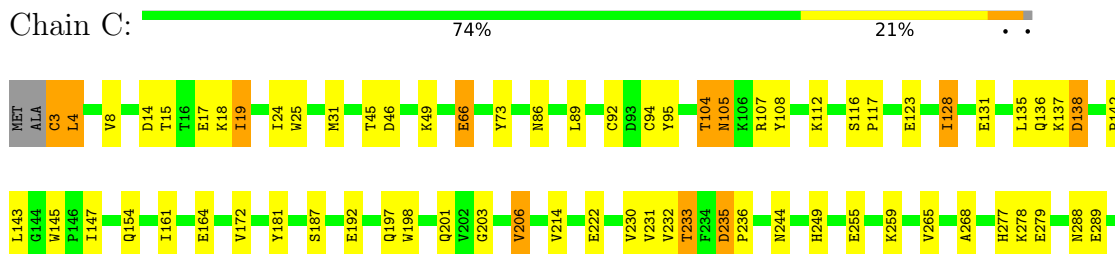
- Molecule 1: glutamine synthetase



- Molecule 1: glutamine synthetase



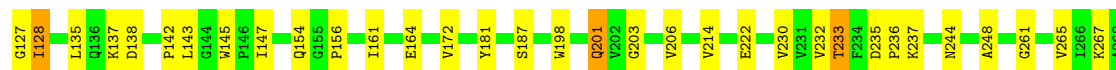
- Molecule 1: glutamine synthetase





- Molecule 1: glutamine synthetase

Chain D: 72% 23% ..



- Molecule 1: glutamine synthetase

Chain E: 74% 23% ..



- Molecule 1: glutamine synthetase

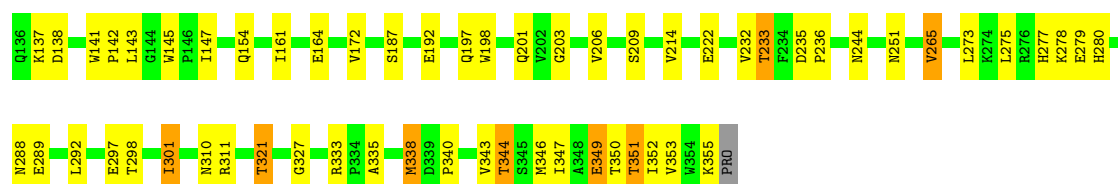
Chain F: 73% 23% ..



- Molecule 1: glutamine synthetase

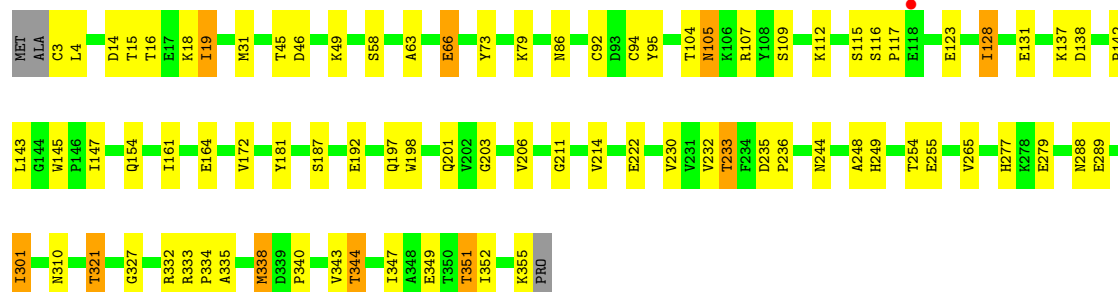
Chain G: 73% 22% ..





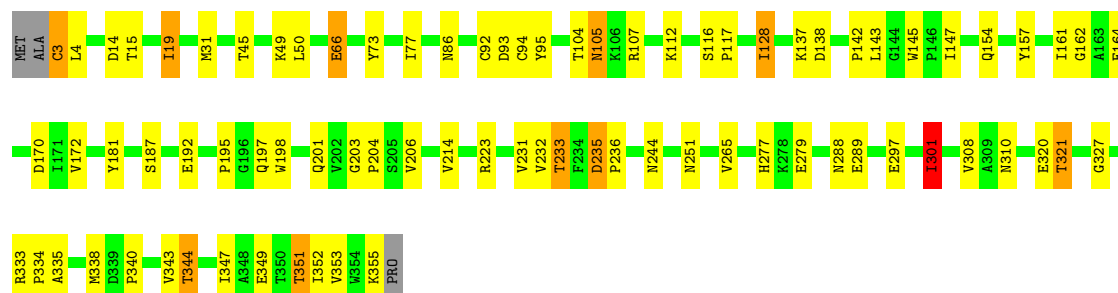
- Molecule 1: glutamine synthetase

Chain H: 76% 21% ..



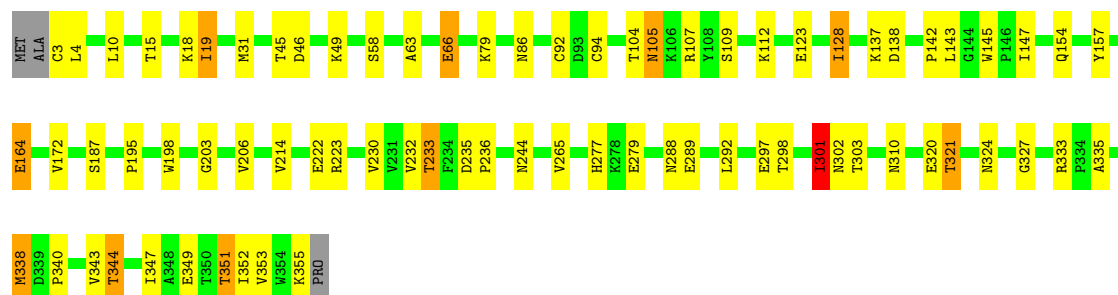
- Molecule 1: glutamine synthetase

Chain I: 76% 20% ..



- Molecule 1: glutamine synthetase

Chain J: 78% 18% ..



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 95.88Å 190.94Å 117.90Å<br>90.00° 101.23° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 33.50 – 3.50<br>33.50 – 3.50                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 83.1 (33.50-3.50)<br>83.0 (33.50-3.50)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.08                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.00 (at 3.47Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0005                                             | Depositor        |
| R, $R_{free}$                                                           | 0.166 , 0.209<br>(Not available) , 0.183                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2227 reflections (4.25%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 86.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.026                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.24 , 42.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 28277                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 75.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, MN, MSL

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.80         | 0/2819         | 1.03        | 8/3834 (0.2%)   |
| 1   | B     | 0.85         | 0/2819         | 1.02        | 8/3834 (0.2%)   |
| 1   | C     | 0.82         | 0/2819         | 1.02        | 8/3834 (0.2%)   |
| 1   | D     | 0.89         | 0/2819         | 1.02        | 5/3834 (0.1%)   |
| 1   | E     | 0.86         | 0/2819         | 1.03        | 7/3834 (0.2%)   |
| 1   | F     | 0.87         | 1/2819 (0.0%)  | 1.05        | 8/3834 (0.2%)   |
| 1   | G     | 0.87         | 0/2819         | 1.03        | 5/3834 (0.1%)   |
| 1   | H     | 0.89         | 1/2819 (0.0%)  | 1.01        | 3/3834 (0.1%)   |
| 1   | I     | 0.81         | 0/2819         | 1.01        | 8/3834 (0.2%)   |
| 1   | J     | 0.85         | 0/2819         | 1.03        | 5/3834 (0.1%)   |
| All | All   | 0.85         | 2/28190 (0.0%) | 1.02        | 65/38340 (0.2%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | H     | 16  | THR  | CA-CB | 5.15 | 1.61        | 1.53     |
| 1   | F     | 16  | THR  | CA-CB | 5.14 | 1.61        | 1.53     |

All (65) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | C     | 353 | VAL  | N-CA-C | 6.89 | 117.04      | 110.42   |
| 1   | E     | 94  | CYS  | N-CA-C | 6.68 | 119.31      | 108.41   |
| 1   | F     | 92  | CYS  | N-CA-C | 6.55 | 119.36      | 109.41   |
| 1   | A     | 92  | CYS  | N-CA-C | 6.39 | 119.12      | 109.41   |
| 1   | B     | 94  | CYS  | N-CA-C | 6.33 | 118.73      | 108.41   |
| 1   | G     | 92  | CYS  | N-CA-C | 6.33 | 119.50      | 109.81   |
| 1   | A     | 94  | CYS  | N-CA-C | 6.31 | 118.69      | 108.41   |
| 1   | I     | 92  | CYS  | N-CA-C | 6.31 | 119.29      | 109.52   |
| 1   | J     | 92  | CYS  | N-CA-C | 6.19 | 119.28      | 109.81   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | J     | 301 | ILE  | CB-CA-C | -6.19 | 103.78      | 112.14   |
| 1   | B     | 301 | ILE  | CB-CA-C | -6.17 | 103.80      | 112.14   |
| 1   | F     | 25  | TRP  | N-CA-C  | 6.15  | 117.53      | 108.86   |
| 1   | D     | 92  | CYS  | N-CA-C  | 6.09  | 118.67      | 109.41   |
| 1   | E     | 25  | TRP  | N-CA-C  | 6.09  | 117.83      | 109.18   |
| 1   | I     | 94  | CYS  | N-CA-C  | 6.07  | 118.30      | 108.41   |
| 1   | F     | 301 | ILE  | CB-CA-C | -6.06 | 103.95      | 112.14   |
| 1   | I     | 353 | VAL  | N-CA-C  | 6.03  | 116.21      | 110.42   |
| 1   | A     | 353 | VAL  | N-CA-C  | 6.00  | 116.12      | 110.30   |
| 1   | F     | 28  | GLY  | N-CA-C  | 5.96  | 119.88      | 112.73   |
| 1   | C     | 94  | CYS  | N-CA-C  | 5.93  | 118.07      | 108.41   |
| 1   | D     | 25  | TRP  | N-CA-C  | 5.90  | 117.18      | 108.86   |
| 1   | G     | 94  | CYS  | N-CA-C  | 5.87  | 118.08      | 108.52   |
| 1   | D     | 94  | CYS  | N-CA-C  | 5.81  | 117.88      | 108.41   |
| 1   | C     | 301 | ILE  | CB-CA-C | -5.78 | 103.21      | 112.16   |
| 1   | A     | 4   | LEU  | N-CA-C  | 5.74  | 118.75      | 111.69   |
| 1   | C     | 25  | TRP  | N-CA-C  | 5.69  | 116.88      | 108.86   |
| 1   | D     | 353 | VAL  | N-CA-C  | 5.65  | 115.78      | 110.30   |
| 1   | B     | 235 | ASP  | CA-C-N  | 5.65  | 125.49      | 119.28   |
| 1   | B     | 235 | ASP  | C-N-CA  | 5.65  | 125.49      | 119.28   |
| 1   | H     | 92  | CYS  | N-CA-C  | 5.62  | 117.95      | 109.41   |
| 1   | I     | 301 | ILE  | CB-CA-C | -5.60 | 103.48      | 112.16   |
| 1   | J     | 353 | VAL  | N-CA-C  | 5.57  | 115.77      | 110.42   |
| 1   | C     | 4   | LEU  | N-CA-C  | 5.55  | 118.52      | 111.69   |
| 1   | F     | 193 | VAL  | N-CA-C  | 5.54  | 116.27      | 110.62   |
| 1   | E     | 141 | TRP  | CA-C-N  | 5.54  | 125.55      | 119.90   |
| 1   | E     | 141 | TRP  | C-N-CA  | 5.54  | 125.55      | 119.90   |
| 1   | J     | 94  | CYS  | N-CA-C  | 5.54  | 117.92      | 108.90   |
| 1   | J     | 4   | LEU  | N-CA-C  | 5.52  | 118.48      | 111.69   |
| 1   | H     | 94  | CYS  | N-CA-C  | 5.51  | 117.94      | 109.07   |
| 1   | B     | 353 | VAL  | N-CA-C  | 5.47  | 115.67      | 110.42   |
| 1   | E     | 4   | LEU  | N-CA-C  | 5.46  | 118.41      | 111.69   |
| 1   | B     | 92  | CYS  | N-CA-C  | 5.46  | 118.16      | 109.81   |
| 1   | F     | 353 | VAL  | N-CA-C  | 5.37  | 115.58      | 110.42   |
| 1   | C     | 235 | ASP  | CA-C-N  | 5.36  | 125.17      | 119.28   |
| 1   | C     | 235 | ASP  | C-N-CA  | 5.36  | 125.17      | 119.28   |
| 1   | B     | 4   | LEU  | N-CA-C  | 5.33  | 118.25      | 111.69   |
| 1   | A     | 28  | GLY  | N-CA-C  | 5.30  | 119.30      | 112.83   |
| 1   | I     | 4   | LEU  | N-CA-C  | 5.30  | 118.21      | 111.69   |
| 1   | G     | 353 | VAL  | N-CA-C  | 5.29  | 115.43      | 110.30   |
| 1   | F     | 94  | CYS  | N-CA-C  | 5.28  | 117.02      | 108.41   |
| 1   | E     | 92  | CYS  | N-CA-C  | 5.27  | 117.42      | 109.41   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | F     | 4   | LEU  | N-CA-C  | 5.25  | 118.15      | 111.69   |
| 1   | E     | 353 | VAL  | N-CA-C  | 5.24  | 115.45      | 110.42   |
| 1   | I     | 235 | ASP  | CA-C-N  | 5.22  | 125.03      | 119.28   |
| 1   | I     | 235 | ASP  | C-N-CA  | 5.22  | 125.03      | 119.28   |
| 1   | H     | 4   | LEU  | N-CA-C  | 5.22  | 118.11      | 111.69   |
| 1   | A     | 235 | ASP  | CA-C-N  | 5.18  | 124.97      | 119.28   |
| 1   | A     | 235 | ASP  | C-N-CA  | 5.18  | 124.97      | 119.28   |
| 1   | D     | 4   | LEU  | N-CA-C  | 5.12  | 117.99      | 111.69   |
| 1   | A     | 167 | PHE  | N-CA-C  | 5.12  | 117.07      | 108.73   |
| 1   | I     | 320 | GLU  | N-CA-C  | 5.08  | 116.51      | 111.07   |
| 1   | B     | 232 | VAL  | CB-CA-C | -5.06 | 103.85      | 110.98   |
| 1   | G     | 141 | TRP  | CA-C-N  | 5.03  | 125.03      | 119.90   |
| 1   | G     | 141 | TRP  | C-N-CA  | 5.03  | 125.03      | 119.90   |
| 1   | C     | 92  | CYS  | N-CA-C  | 5.02  | 117.04      | 109.41   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2745  | 0        | 2653     | 51      | 0            |
| 1   | B     | 2745  | 0        | 2653     | 51      | 0            |
| 1   | C     | 2745  | 0        | 2653     | 62      | 0            |
| 1   | D     | 2745  | 0        | 2653     | 78      | 0            |
| 1   | E     | 2745  | 0        | 2653     | 59      | 0            |
| 1   | F     | 2745  | 0        | 2653     | 68      | 0            |
| 1   | G     | 2745  | 0        | 2653     | 65      | 0            |
| 1   | H     | 2745  | 0        | 2653     | 50      | 0            |
| 1   | I     | 2745  | 0        | 2653     | 52      | 0            |
| 1   | J     | 2745  | 0        | 2653     | 46      | 0            |
| 2   | A     | 3     | 0        | 0        | 0       | 0            |
| 2   | B     | 3     | 0        | 0        | 0       | 0            |
| 2   | C     | 3     | 0        | 0        | 0       | 0            |
| 2   | D     | 3     | 0        | 0        | 0       | 0            |
| 2   | E     | 3     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | F     | 3     | 0        | 0        | 0       | 0            |
| 2   | G     | 3     | 0        | 0        | 0       | 0            |
| 2   | H     | 3     | 0        | 0        | 0       | 0            |
| 2   | I     | 3     | 0        | 0        | 0       | 0            |
| 2   | J     | 3     | 0        | 0        | 0       | 0            |
| 3   | A     | 31    | 0        | 10       | 7       | 0            |
| 3   | B     | 31    | 0        | 11       | 3       | 0            |
| 3   | C     | 31    | 0        | 10       | 4       | 0            |
| 3   | D     | 31    | 0        | 11       | 6       | 0            |
| 3   | E     | 31    | 0        | 11       | 6       | 0            |
| 3   | F     | 31    | 0        | 11       | 4       | 0            |
| 3   | G     | 31    | 0        | 10       | 5       | 0            |
| 3   | H     | 31    | 0        | 10       | 3       | 0            |
| 3   | I     | 31    | 0        | 10       | 3       | 0            |
| 3   | J     | 31    | 0        | 10       | 3       | 0            |
| 4   | C     | 110   | 0        | 100      | 42      | 0            |
| 5   | A     | 32    | 0        | 0        | 7       | 0            |
| 5   | B     | 36    | 0        | 0        | 11      | 0            |
| 5   | C     | 40    | 0        | 0        | 12      | 0            |
| 5   | D     | 42    | 0        | 0        | 28      | 0            |
| 5   | E     | 41    | 0        | 0        | 14      | 0            |
| 5   | F     | 39    | 0        | 0        | 12      | 0            |
| 5   | G     | 40    | 0        | 0        | 19      | 0            |
| 5   | H     | 32    | 0        | 0        | 9       | 0            |
| 5   | I     | 37    | 0        | 0        | 7       | 0            |
| 5   | J     | 38    | 0        | 0        | 11      | 0            |
| All | All   | 28277 | 0        | 26734    | 580     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (580) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:G:12:LEU:HD23  | 5:G:6047:HOH:O  | 1.47                     | 1.11              |
| 4:C:5010:MSL:NE  | 3:H:6008:ANP:PG | 2.25                     | 1.09              |
| 1:E:354:TRP:HA   | 5:E:6026:HOH:O  | 1.56                     | 1.05              |
| 1:G:346:MET:SD   | 5:G:6041:HOH:O  | 2.14                     | 1.03              |
| 1:E:255:GLU:HG2  | 5:E:6019:HOH:O  | 1.58                     | 1.02              |
| 1:H:344:THR:HG21 | 5:H:6034:HOH:O  | 1.59                     | 0.98              |
| 1:E:154:GLN:HE22 | 1:E:244:ASN:H   | 1.08                     | 0.97              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:E:296:HIS:HD2  | 5:E:6033:HOH:O  | 1.46                     | 0.97              |
| 1:I:154:GLN:HE22 | 1:I:244:ASN:H   | 1.08                     | 0.97              |
| 1:F:128:ILE:HG21 | 5:F:6034:HOH:O  | 1.67                     | 0.95              |
| 1:F:154:GLN:HE22 | 1:F:244:ASN:H   | 1.12                     | 0.95              |
| 1:D:154:GLN:HE22 | 1:D:244:ASN:H   | 1.13                     | 0.94              |
| 1:B:154:GLN:HE22 | 1:B:244:ASN:H   | 1.15                     | 0.93              |
| 1:D:73:TYR:HB2   | 5:D:6032:HOH:O  | 1.69                     | 0.92              |
| 1:J:154:GLN:HE22 | 1:J:244:ASN:H   | 1.13                     | 0.92              |
| 1:C:154:GLN:HE22 | 1:C:244:ASN:H   | 1.07                     | 0.91              |
| 1:E:185:ASN:HB2  | 5:E:6036:HOH:O  | 1.68                     | 0.91              |
| 1:H:154:GLN:HE22 | 1:H:244:ASN:H   | 1.14                     | 0.90              |
| 1:E:274:LYS:HE3  | 5:E:6025:HOH:O  | 1.70                     | 0.90              |
| 1:A:154:GLN:HE22 | 1:A:244:ASN:H   | 1.19                     | 0.89              |
| 1:H:321:THR:HB   | 1:H:327:GLY:HA3 | 1.55                     | 0.88              |
| 1:D:282:ALA:HB3  | 5:D:6022:HOH:O  | 1.75                     | 0.87              |
| 1:G:154:GLN:HE22 | 1:G:244:ASN:H   | 1.19                     | 0.86              |
| 1:D:350:THR:HG22 | 5:D:6024:HOH:O  | 1.73                     | 0.86              |
| 1:D:72:LEU:HG    | 5:D:6046:HOH:O  | 1.74                     | 0.86              |
| 1:C:259:LYS:HB3  | 5:C:6028:HOH:O  | 1.76                     | 0.85              |
| 1:D:95:TYR:HE1   | 5:D:6032:HOH:O  | 1.59                     | 0.85              |
| 1:F:107:ARG:HG2  | 5:F:6016:HOH:O  | 1.76                     | 0.84              |
| 1:G:280:HIS:HA   | 5:G:6041:HOH:O  | 1.76                     | 0.84              |
| 1:C:259:LYS:HD2  | 5:C:6025:HOH:O  | 1.78                     | 0.83              |
| 1:D:321:THR:HB   | 1:D:327:GLY:HA3 | 1.59                     | 0.82              |
| 1:C:268:ALA:HB1  | 5:C:6031:HOH:O  | 1.80                     | 0.82              |
| 1:E:321:THR:HB   | 1:E:327:GLY:HA3 | 1.61                     | 0.82              |
| 1:G:275:LEU:CD2  | 5:G:6028:HOH:O  | 2.26                     | 0.82              |
| 1:A:321:THR:HB   | 1:A:327:GLY:HA3 | 1.61                     | 0.82              |
| 1:F:321:THR:HB   | 1:F:327:GLY:HA3 | 1.61                     | 0.82              |
| 1:G:321:THR:HB   | 1:G:327:GLY:HA3 | 1.59                     | 0.81              |
| 1:E:19:ILE:HD11  | 1:E:86:ASN:HB2  | 1.59                     | 0.81              |
| 1:I:321:THR:HB   | 1:I:327:GLY:HA3 | 1.61                     | 0.80              |
| 1:B:19:ILE:HD11  | 1:B:86:ASN:HB2  | 1.62                     | 0.80              |
| 1:B:321:THR:HB   | 1:B:327:GLY:HA3 | 1.63                     | 0.80              |
| 1:F:261:GLY:HA2  | 5:F:6011:HOH:O  | 1.82                     | 0.80              |
| 1:J:19:ILE:HD11  | 1:J:86:ASN:HB2  | 1.64                     | 0.79              |
| 5:B:6034:HOH:O   | 1:C:8:VAL:HG21  | 1.79                     | 0.79              |
| 1:C:321:THR:HB   | 1:C:327:GLY:HA3 | 1.61                     | 0.79              |
| 1:G:19:ILE:HD11  | 1:G:86:ASN:HB2  | 1.61                     | 0.79              |
| 1:H:49:LYS:HG2   | 5:H:6027:HOH:O  | 1.83                     | 0.79              |
| 1:D:93:ASP:HB3   | 5:D:6032:HOH:O  | 1.84                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:73:TYR:CB    | 5:D:6032:HOH:O   | 2.29                     | 0.78              |
| 1:A:19:ILE:HD11  | 1:A:86:ASN:HB2   | 1.67                     | 0.77              |
| 1:J:321:THR:HB   | 1:J:327:GLY:HA3  | 1.67                     | 0.77              |
| 1:I:19:ILE:HD11  | 1:I:86:ASN:HB2   | 1.66                     | 0.76              |
| 4:C:5007:MSL:HG3 | 1:F:332:ARG:HH22 | 1.51                     | 0.76              |
| 1:D:105:ASN:C    | 1:D:105:ASN:HD22 | 1.94                     | 0.75              |
| 1:D:19:ILE:HD11  | 1:D:86:ASN:HB2   | 1.68                     | 0.75              |
| 1:F:259:LYS:HD2  | 5:F:6008:HOH:O   | 1.88                     | 0.74              |
| 1:F:19:ILE:HD11  | 1:F:86:ASN:HB2   | 1.70                     | 0.74              |
| 1:E:296:HIS:CD2  | 5:E:6033:HOH:O   | 2.27                     | 0.74              |
| 4:C:5010:MSL:NE  | 3:H:6008:ANP:O1G | 2.16                     | 0.74              |
| 1:G:275:LEU:HD23 | 5:G:6028:HOH:O   | 1.87                     | 0.73              |
| 1:D:311:ARG:NH1  | 3:D:6004:ANP:O1G | 2.21                     | 0.73              |
| 1:H:19:ILE:HD11  | 1:H:86:ASN:HB2   | 1.71                     | 0.73              |
| 3:A:6001:ANP:PG  | 4:C:5001:MSL:NE  | 2.62                     | 0.73              |
| 1:G:128:ILE:HG12 | 1:G:214:VAL:HG21 | 1.70                     | 0.72              |
| 1:D:123:GLU:HA   | 5:D:6015:HOH:O   | 1.90                     | 0.72              |
| 1:D:54:ASN:HA    | 5:D:6046:HOH:O   | 1.89                     | 0.71              |
| 1:D:45:THR:HG22  | 5:D:6034:HOH:O   | 1.89                     | 0.71              |
| 1:J:223:ARG:NH1  | 5:J:6024:HOH:O   | 2.23                     | 0.71              |
| 1:H:355:LYS:C    | 5:H:6009:HOH:O   | 2.33                     | 0.71              |
| 1:C:128:ILE:HG12 | 1:C:214:VAL:HG21 | 1.73                     | 0.70              |
| 1:B:344:THR:HG21 | 5:B:6009:HOH:O   | 1.90                     | 0.70              |
| 1:F:18:LYS:HE2   | 5:I:6021:HOH:O   | 1.92                     | 0.70              |
| 1:A:128:ILE:HG12 | 1:A:214:VAL:HG21 | 1.73                     | 0.70              |
| 1:A:311:ARG:NH1  | 3:A:6001:ANP:O1G | 2.24                     | 0.70              |
| 4:C:5005:MSL:HE3 | 1:E:297:GLU:OE2  | 1.91                     | 0.70              |
| 1:I:105:ASN:C    | 1:I:105:ASN:HD22 | 1.97                     | 0.70              |
| 1:J:320:GLU:HB3  | 5:J:6019:HOH:O   | 1.92                     | 0.70              |
| 1:C:19:ILE:HD11  | 1:C:86:ASN:HB2   | 1.74                     | 0.69              |
| 4:C:5009:MSL:HG3 | 1:J:297:GLU:OE2  | 1.92                     | 0.69              |
| 1:E:128:ILE:HG12 | 1:E:214:VAL:HG21 | 1.74                     | 0.69              |
| 1:D:66:GLU:HA    | 1:E:310:ASN:OD1  | 1.92                     | 0.69              |
| 1:C:105:ASN:C    | 1:C:105:ASN:HD22 | 2.00                     | 0.68              |
| 1:A:3:CYS:HB3    | 5:E:6009:HOH:O   | 1.93                     | 0.68              |
| 1:D:95:TYR:CE1   | 5:D:6032:HOH:O   | 2.38                     | 0.68              |
| 1:J:128:ILE:HG12 | 1:J:214:VAL:HG21 | 1.76                     | 0.68              |
| 1:I:128:ILE:HG12 | 1:I:214:VAL:HG21 | 1.74                     | 0.68              |
| 1:F:66:GLU:HA    | 1:I:310:ASN:OD1  | 1.93                     | 0.68              |
| 1:D:237:LYS:HE2  | 5:D:6009:HOH:O   | 1.93                     | 0.67              |
| 1:E:105:ASN:C    | 1:E:105:ASN:HD22 | 2.03                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:118:GLU:HG3  | 5:G:6021:HOH:O   | 1.94                     | 0.67              |
| 1:J:105:ASN:C    | 1:J:105:ASN:HD22 | 2.02                     | 0.67              |
| 1:D:128:ILE:HG12 | 1:D:214:VAL:HG21 | 1.78                     | 0.66              |
| 1:G:123:GLU:HG3  | 5:G:6016:HOH:O   | 1.95                     | 0.66              |
| 1:B:332:ARG:HH22 | 4:C:5002:MSL:HG3 | 1.61                     | 0.66              |
| 1:D:203:GLY:HA2  | 3:D:6004:ANP:O3' | 1.95                     | 0.66              |
| 1:C:297:GLU:OE2  | 4:C:5003:MSL:HE3 | 1.96                     | 0.66              |
| 1:D:277:HIS:HE1  | 1:D:301:ILE:O    | 1.79                     | 0.65              |
| 1:F:128:ILE:HG12 | 1:F:214:VAL:HG21 | 1.78                     | 0.65              |
| 1:G:105:ASN:C    | 1:G:105:ASN:HD22 | 2.05                     | 0.65              |
| 1:G:107:ARG:HG2  | 5:G:6019:HOH:O   | 1.95                     | 0.65              |
| 4:C:5004:MSL:NE  | 3:D:6004:ANP:PG  | 2.69                     | 0.65              |
| 1:B:105:ASN:C    | 1:B:105:ASN:HD22 | 2.02                     | 0.65              |
| 1:J:355:LYS:HB2  | 5:J:6033:HOH:O   | 1.97                     | 0.65              |
| 1:G:112:LYS:HD3  | 5:G:6031:HOH:O   | 1.97                     | 0.65              |
| 1:A:347:ILE:O    | 1:A:351:THR:HB   | 1.97                     | 0.65              |
| 1:J:338:MET:HG3  | 1:J:343:VAL:HG21 | 1.77                     | 0.65              |
| 1:F:347:ILE:O    | 1:F:351:THR:HB   | 1.97                     | 0.64              |
| 1:B:154:GLN:HB2  | 5:B:6026:HOH:O   | 1.96                     | 0.64              |
| 1:E:115:SER:HB3  | 5:E:6016:HOH:O   | 1.95                     | 0.64              |
| 1:C:278:LYS:HD3  | 5:C:6029:HOH:O   | 1.96                     | 0.64              |
| 1:F:154:GLN:HB2  | 5:F:6013:HOH:O   | 1.96                     | 0.64              |
| 1:F:351:THR:HG22 | 1:F:352:ILE:HG13 | 1.80                     | 0.64              |
| 4:C:5008:MSL:HG3 | 1:I:297:GLU:OE2  | 1.96                     | 0.64              |
| 4:C:5006:MSL:HG3 | 1:G:297:GLU:OE2  | 1.98                     | 0.64              |
| 1:D:338:MET:HG3  | 1:D:343:VAL:HG21 | 1.80                     | 0.64              |
| 1:H:347:ILE:O    | 1:H:351:THR:HB   | 1.98                     | 0.64              |
| 1:G:275:LEU:HD21 | 5:G:6028:HOH:O   | 1.89                     | 0.64              |
| 4:C:5007:MSL:HB2 | 1:F:249:HIS:CE1  | 2.33                     | 0.63              |
| 1:C:4:LEU:HB3    | 5:C:6019:HOH:O   | 1.98                     | 0.63              |
| 1:F:340:PRO:O    | 1:F:344:THR:HB   | 1.99                     | 0.63              |
| 1:F:94:CYS:N     | 5:F:6010:HOH:O   | 2.31                     | 0.63              |
| 1:E:351:THR:HG22 | 1:E:352:ILE:HG13 | 1.81                     | 0.63              |
| 1:H:277:HIS:HE1  | 1:H:301:ILE:O    | 1.82                     | 0.62              |
| 1:E:347:ILE:O    | 1:E:351:THR:HB   | 1.99                     | 0.62              |
| 1:F:310:ASN:OD1  | 1:G:66:GLU:HA    | 1.99                     | 0.62              |
| 1:H:128:ILE:HG12 | 1:H:214:VAL:HG21 | 1.81                     | 0.62              |
| 1:F:105:ASN:HD22 | 1:F:105:ASN:C    | 2.08                     | 0.62              |
| 1:B:249:HIS:CE1  | 4:C:5002:MSL:HB2 | 2.35                     | 0.62              |
| 1:H:203:GLY:HA2  | 3:H:6008:ANP:O3' | 2.00                     | 0.62              |
| 1:E:338:MET:HG3  | 1:E:343:VAL:HG21 | 1.82                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:J:277:HIS:HE1  | 1:J:301:ILE:O     | 1.82                     | 0.62              |
| 1:D:3:CYS:HB3    | 5:D:6017:HOH:O    | 2.00                     | 0.61              |
| 1:F:251:ASN:ND2  | 3:F:6006:ANP:H5'2 | 2.15                     | 0.61              |
| 4:C:5006:MSL:NE  | 3:G:6007:ANP:PG   | 2.74                     | 0.61              |
| 1:B:351:THR:HG22 | 1:B:352:ILE:HG13  | 1.83                     | 0.61              |
| 1:G:347:ILE:O    | 1:G:351:THR:HB    | 2.00                     | 0.61              |
| 1:B:277:HIS:HE1  | 1:B:301:ILE:O     | 1.83                     | 0.61              |
| 1:D:347:ILE:O    | 1:D:351:THR:HB    | 2.01                     | 0.61              |
| 5:H:6016:HOH:O   | 1:I:3:CYS:HB3     | 2.00                     | 0.61              |
| 1:C:154:GLN:HE22 | 1:C:244:ASN:N     | 1.90                     | 0.61              |
| 1:E:277:HIS:HE1  | 1:E:301:ILE:O     | 1.84                     | 0.61              |
| 1:A:105:ASN:HD22 | 1:A:105:ASN:C     | 2.07                     | 0.60              |
| 1:A:172:VAL:HG21 | 1:A:198:TRP:CD2   | 2.36                     | 0.60              |
| 1:A:340:PRO:O    | 1:A:344:THR:HB    | 2.01                     | 0.60              |
| 1:D:267:LYS:HD3  | 5:D:6020:HOH:O    | 2.01                     | 0.60              |
| 1:B:338:MET:HG3  | 1:B:343:VAL:HG21  | 1.84                     | 0.60              |
| 1:G:277:HIS:HE1  | 1:G:301:ILE:O     | 1.84                     | 0.60              |
| 1:H:105:ASN:C    | 1:H:105:ASN:HD22  | 2.08                     | 0.60              |
| 1:D:172:VAL:HG21 | 1:D:198:TRP:CD2   | 2.37                     | 0.60              |
| 1:B:128:ILE:HG12 | 1:B:214:VAL:HG21  | 1.82                     | 0.60              |
| 1:C:310:ASN:OD1  | 1:E:66:GLU:HA     | 2.01                     | 0.60              |
| 1:E:128:ILE:HD13 | 1:E:338:MET:HE1   | 1.82                     | 0.60              |
| 1:F:128:ILE:HD13 | 1:F:338:MET:HE1   | 1.83                     | 0.60              |
| 1:F:3:CYS:HB3    | 5:J:6048:HOH:O    | 2.01                     | 0.60              |
| 4:C:5005:MSL:OE  | 3:E:6005:ANP:O3G  | 2.20                     | 0.60              |
| 1:G:73:TYR:CD2   | 1:G:95:TYR:CE1    | 2.89                     | 0.60              |
| 1:G:273:LEU:HA   | 5:G:6036:HOH:O    | 2.02                     | 0.60              |
| 1:A:278:LYS:HB2  | 5:A:6011:HOH:O    | 2.02                     | 0.59              |
| 1:D:17:GLU:HG2   | 5:D:6030:HOH:O    | 2.02                     | 0.59              |
| 1:H:310:ASN:OD1  | 1:J:66:GLU:HA     | 2.02                     | 0.59              |
| 4:C:5004:MSL:HG3 | 1:D:297:GLU:OE2   | 2.02                     | 0.59              |
| 4:C:5004:MSL:HE1 | 3:D:6004:ANP:O3G  | 2.02                     | 0.59              |
| 1:F:203:GLY:HA2  | 3:F:6006:ANP:O3'  | 2.02                     | 0.59              |
| 4:C:5009:MSL:NE  | 3:J:6010:ANP:PG   | 2.76                     | 0.59              |
| 1:B:170:ASP:HA   | 5:B:6034:HOH:O    | 2.02                     | 0.59              |
| 1:D:123:GLU:HG2  | 5:D:6015:HOH:O    | 2.01                     | 0.59              |
| 1:A:277:HIS:HE1  | 1:A:301:ILE:O     | 1.85                     | 0.59              |
| 1:B:204:PRO:HD2  | 5:B:6028:HOH:O    | 2.02                     | 0.58              |
| 1:J:203:GLY:HA2  | 3:J:6010:ANP:O3'  | 2.03                     | 0.58              |
| 1:C:105:ASN:C    | 1:C:105:ASN:ND2   | 2.60                     | 0.58              |
| 1:C:347:ILE:O    | 1:C:351:THR:HB    | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:277:HIS:HE1  | 1:F:301:ILE:O    | 1.87                     | 0.58              |
| 1:I:105:ASN:C    | 1:I:105:ASN:ND2  | 2.58                     | 0.58              |
| 1:E:105:ASN:C    | 1:E:105:ASN:ND2  | 2.61                     | 0.58              |
| 1:C:277:HIS:HE1  | 1:C:301:ILE:O    | 1.86                     | 0.58              |
| 1:H:338:MET:HG3  | 1:H:343:VAL:HG21 | 1.85                     | 0.58              |
| 1:B:340:PRO:O    | 1:B:344:THR:HB   | 2.04                     | 0.58              |
| 1:E:187:SER:HB3  | 1:E:203:GLY:HA3  | 1.84                     | 0.58              |
| 1:E:187:SER:HB3  | 1:E:203:GLY:CA   | 2.34                     | 0.58              |
| 1:H:340:PRO:O    | 1:H:344:THR:HB   | 2.03                     | 0.58              |
| 1:B:105:ASN:C    | 1:B:105:ASN:ND2  | 2.61                     | 0.58              |
| 1:D:128:ILE:HD13 | 1:D:338:MET:HE1  | 1.86                     | 0.57              |
| 1:F:274:LYS:HE2  | 5:F:6041:HOH:O   | 2.04                     | 0.57              |
| 1:I:154:GLN:HE22 | 1:I:244:ASN:N    | 1.91                     | 0.57              |
| 1:C:351:THR:HG22 | 1:C:352:ILE:HG13 | 1.85                     | 0.57              |
| 1:I:66:GLU:HA    | 1:J:310:ASN:OD1  | 2.03                     | 0.57              |
| 1:B:347:ILE:O    | 1:B:351:THR:HB   | 2.04                     | 0.57              |
| 1:D:105:ASN:C    | 1:D:105:ASN:ND2  | 2.56                     | 0.57              |
| 1:D:269:ALA:HA   | 5:D:6006:HOH:O   | 2.04                     | 0.57              |
| 1:J:347:ILE:O    | 1:J:351:THR:HB   | 2.05                     | 0.57              |
| 1:F:172:VAL:HG21 | 1:F:198:TRP:CD2  | 2.39                     | 0.57              |
| 1:J:351:THR:HG22 | 1:J:352:ILE:HG13 | 1.85                     | 0.57              |
| 1:A:204:PRO:HD3  | 3:A:6001:ANP:O2' | 2.05                     | 0.57              |
| 1:A:351:THR:HG22 | 1:A:352:ILE:HG13 | 1.87                     | 0.57              |
| 1:I:351:THR:HG22 | 1:I:352:ILE:HG13 | 1.87                     | 0.57              |
| 1:I:355:LYS:HB3  | 5:I:6022:HOH:O   | 2.04                     | 0.57              |
| 1:J:172:VAL:HG21 | 1:J:198:TRP:CD2  | 2.39                     | 0.57              |
| 1:C:73:TYR:CD2   | 1:C:95:TYR:CE1   | 2.93                     | 0.57              |
| 1:G:340:PRO:O    | 1:G:344:THR:HB   | 2.04                     | 0.57              |
| 1:B:128:ILE:HD13 | 1:B:338:MET:HE1  | 1.87                     | 0.57              |
| 1:B:172:VAL:HG21 | 1:B:198:TRP:CD2  | 2.39                     | 0.57              |
| 1:I:347:ILE:O    | 1:I:351:THR:HB   | 2.05                     | 0.57              |
| 1:C:172:VAL:HG21 | 1:C:198:TRP:CD2  | 2.40                     | 0.56              |
| 1:F:187:SER:HB3  | 1:F:203:GLY:HA3  | 1.86                     | 0.56              |
| 1:F:187:SER:HB3  | 1:F:203:GLY:CA   | 2.35                     | 0.56              |
| 1:J:172:VAL:HG13 | 5:J:6011:HOH:O   | 2.04                     | 0.56              |
| 1:B:19:ILE:HD11  | 1:B:86:ASN:CB    | 2.34                     | 0.56              |
| 4:C:5005:MSL:HB2 | 1:E:249:HIS:CE1  | 2.40                     | 0.56              |
| 1:E:154:GLN:HE22 | 1:E:244:ASN:N    | 1.91                     | 0.56              |
| 1:J:19:ILE:HD11  | 1:J:86:ASN:CB    | 2.34                     | 0.56              |
| 1:B:310:ASN:OD1  | 1:C:66:GLU:HA    | 2.05                     | 0.56              |
| 1:C:187:SER:HB3  | 1:C:203:GLY:CA   | 2.36                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:187:SER:HB3  | 1:I:203:GLY:CA    | 2.35                     | 0.56              |
| 1:J:340:PRO:O    | 1:J:344:THR:HB    | 2.05                     | 0.56              |
| 1:G:31:MET:HE3   | 1:G:31:MET:O      | 2.05                     | 0.56              |
| 1:G:338:MET:HG3  | 1:G:343:VAL:HG21  | 1.88                     | 0.56              |
| 1:I:355:LYS:HB2  | 5:I:6029:HOH:O    | 2.06                     | 0.56              |
| 1:E:311:ARG:NH1  | 3:E:6005:ANP:O3G  | 2.38                     | 0.56              |
| 1:G:172:VAL:HG21 | 1:G:198:TRP:CD2   | 2.41                     | 0.56              |
| 1:G:311:ARG:NH1  | 3:G:6007:ANP:O1G  | 2.39                     | 0.56              |
| 1:I:128:ILE:HD13 | 1:I:338:MET:HE1   | 1.88                     | 0.56              |
| 1:J:105:ASN:C    | 1:J:105:ASN:ND2   | 2.62                     | 0.56              |
| 1:C:128:ILE:HD13 | 1:C:338:MET:HE1   | 1.87                     | 0.56              |
| 1:D:351:THR:HG22 | 1:D:352:ILE:HG13  | 1.87                     | 0.56              |
| 1:G:310:ASN:OD1  | 1:H:66:GLU:HA     | 2.06                     | 0.56              |
| 1:C:131:GLU:OE1  | 4:C:5003:MSL:HB3  | 2.06                     | 0.55              |
| 1:H:351:THR:HG22 | 1:H:352:ILE:HG13  | 1.88                     | 0.55              |
| 1:G:128:ILE:HD13 | 1:G:338:MET:HE1   | 1.88                     | 0.55              |
| 1:G:278:LYS:HB2  | 5:G:6014:HOH:O    | 2.05                     | 0.55              |
| 1:D:187:SER:HB3  | 1:D:203:GLY:CA    | 2.37                     | 0.55              |
| 1:E:19:ILE:HD11  | 1:E:86:ASN:CB     | 2.35                     | 0.55              |
| 1:I:338:MET:HG3  | 1:I:343:VAL:HG21  | 1.88                     | 0.55              |
| 1:A:3:CYS:HA     | 5:A:6012:HOH:O    | 2.04                     | 0.55              |
| 1:H:172:VAL:HG21 | 1:H:198:TRP:CD2   | 2.41                     | 0.55              |
| 1:C:187:SER:HB3  | 1:C:203:GLY:HA3   | 1.88                     | 0.55              |
| 1:F:154:GLN:NE2  | 1:F:244:ASN:H     | 1.95                     | 0.55              |
| 1:G:251:ASN:ND2  | 3:G:6007:ANP:H5'2 | 2.22                     | 0.55              |
| 1:J:10:LEU:HD23  | 5:J:6031:HOH:O    | 2.06                     | 0.55              |
| 1:I:277:HIS:HE1  | 1:I:301:ILE:O     | 1.90                     | 0.55              |
| 1:A:63:ALA:HA    | 5:A:6031:HOH:O    | 2.06                     | 0.55              |
| 1:A:310:ASN:OD1  | 1:B:66:GLU:HA     | 2.07                     | 0.55              |
| 1:C:338:MET:HG3  | 1:C:343:VAL:HG21  | 1.88                     | 0.55              |
| 1:D:187:SER:HB3  | 1:D:203:GLY:HA3   | 1.89                     | 0.55              |
| 1:D:237:LYS:NZ   | 5:D:6013:HOH:O    | 2.39                     | 0.55              |
| 1:E:172:VAL:HG21 | 1:E:198:TRP:CD2   | 2.42                     | 0.55              |
| 1:C:312:GLY:N    | 5:C:6030:HOH:O    | 2.39                     | 0.54              |
| 1:I:340:PRO:O    | 1:I:344:THR:HB    | 2.07                     | 0.54              |
| 1:C:3:CYS:HB3    | 5:C:6015:HOH:O    | 2.08                     | 0.54              |
| 1:H:105:ASN:C    | 1:H:105:ASN:ND2   | 2.65                     | 0.54              |
| 1:I:170:ASP:HB2  | 5:I:6046:HOH:O    | 2.06                     | 0.54              |
| 1:G:137:LYS:O    | 1:G:138:ASP:HB2   | 2.07                     | 0.54              |
| 1:A:73:TYR:CD2   | 1:A:95:TYR:CE1    | 2.95                     | 0.54              |
| 1:D:340:PRO:O    | 1:D:344:THR:HB    | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:19:ILE:HD11  | 1:I:86:ASN:CB    | 2.35                     | 0.54              |
| 1:A:26:ILE:N     | 5:A:6007:HOH:O   | 2.35                     | 0.54              |
| 1:A:137:LYS:O    | 1:A:138:ASP:HB2  | 2.07                     | 0.54              |
| 1:G:105:ASN:C    | 1:G:105:ASN:ND2  | 2.65                     | 0.54              |
| 1:B:161:ILE:HD12 | 1:C:222:GLU:HB3  | 1.89                     | 0.54              |
| 1:G:115:SER:HB3  | 5:G:6027:HOH:O   | 2.07                     | 0.54              |
| 1:H:137:LYS:O    | 1:H:138:ASP:HB2  | 2.08                     | 0.54              |
| 1:E:316:ARG:NH1  | 3:E:6005:ANP:O1B | 2.27                     | 0.53              |
| 1:C:340:PRO:O    | 1:C:344:THR:HB   | 2.09                     | 0.53              |
| 1:A:105:ASN:C    | 1:A:105:ASN:ND2  | 2.65                     | 0.53              |
| 4:C:5008:MSL:NE  | 3:I:6009:ANP:PG  | 2.82                     | 0.53              |
| 1:F:105:ASN:C    | 1:F:105:ASN:ND2  | 2.66                     | 0.53              |
| 1:A:66:GLU:HA    | 1:D:310:ASN:OD1  | 2.08                     | 0.53              |
| 1:J:187:SER:HB3  | 1:J:203:GLY:HA3  | 1.90                     | 0.53              |
| 1:G:187:SER:HB3  | 1:G:203:GLY:CA   | 2.38                     | 0.53              |
| 1:F:26:ILE:HG21  | 5:F:6042:HOH:O   | 2.07                     | 0.53              |
| 1:D:19:ILE:HD11  | 1:D:86:ASN:CB    | 2.36                     | 0.53              |
| 1:E:105:ASN:HD22 | 1:E:107:ARG:H    | 1.55                     | 0.53              |
| 1:I:49:LYS:HE2   | 5:I:6036:HOH:O   | 2.08                     | 0.52              |
| 1:I:137:LYS:O    | 1:I:138:ASP:HB2  | 2.09                     | 0.52              |
| 1:J:187:SER:HB3  | 1:J:203:GLY:CA   | 2.40                     | 0.52              |
| 1:C:31:MET:HE3   | 1:C:31:MET:O     | 2.08                     | 0.52              |
| 1:C:137:LYS:O    | 1:C:138:ASP:HB2  | 2.10                     | 0.52              |
| 1:I:172:VAL:HG21 | 1:I:198:TRP:CD2  | 2.45                     | 0.52              |
| 4:C:5003:MSL:OE  | 3:C:6003:ANP:O1G | 2.27                     | 0.52              |
| 1:G:209:SER:HA   | 5:G:6013:HOH:O   | 2.09                     | 0.52              |
| 1:G:351:THR:HG22 | 1:G:352:ILE:HG13 | 1.92                     | 0.52              |
| 1:H:321:THR:CB   | 1:H:327:GLY:HA3  | 2.35                     | 0.52              |
| 1:G:19:ILE:HD11  | 1:G:86:ASN:CB    | 2.36                     | 0.52              |
| 1:H:142:PRO:HB2  | 1:H:145:TRP:CD1  | 2.45                     | 0.52              |
| 1:A:19:ILE:HD11  | 1:A:86:ASN:CB    | 2.39                     | 0.52              |
| 1:F:19:ILE:HD11  | 1:F:86:ASN:CB    | 2.37                     | 0.52              |
| 1:G:105:ASN:HD22 | 1:G:107:ARG:H    | 1.57                     | 0.52              |
| 1:A:338:MET:HG3  | 1:A:343:VAL:HG21 | 1.92                     | 0.51              |
| 1:E:203:GLY:HA2  | 3:E:6005:ANP:O3' | 2.11                     | 0.51              |
| 1:B:31:MET:HE3   | 1:B:31:MET:O     | 2.10                     | 0.51              |
| 1:D:105:ASN:HD22 | 1:D:107:ARG:H    | 1.58                     | 0.51              |
| 1:E:236:PRO:HB3  | 1:E:335:ALA:HB1  | 1.91                     | 0.51              |
| 1:E:318:GLY:HA3  | 5:E:6020:HOH:O   | 2.09                     | 0.51              |
| 1:F:311:ARG:NH1  | 3:F:6006:ANP:O1G | 2.42                     | 0.51              |
| 1:I:142:PRO:HB2  | 1:I:145:TRP:CD1  | 2.45                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:105:ASN:ND2  | 1:E:107:ARG:H     | 2.08                     | 0.51              |
| 1:F:338:MET:HG3  | 1:F:343:VAL:HG21  | 1.92                     | 0.51              |
| 1:F:50:LEU:HD11  | 1:F:77:ILE:HD11   | 1.92                     | 0.51              |
| 1:H:142:PRO:HB2  | 1:H:145:TRP:CG    | 2.46                     | 0.51              |
| 1:E:206:VAL:CG1  | 5:E:6022:HOH:O    | 2.58                     | 0.51              |
| 1:I:187:SER:HB3  | 1:I:203:GLY:HA3   | 1.93                     | 0.51              |
| 1:H:192:GLU:HB3  | 1:H:197:GLN:HE21  | 1.75                     | 0.51              |
| 1:A:295:ARG:HG3  | 5:A:6009:HOH:O    | 2.10                     | 0.51              |
| 1:F:31:MET:O     | 1:F:31:MET:HE3    | 2.10                     | 0.51              |
| 1:J:105:ASN:HD22 | 1:J:107:ARG:H     | 1.58                     | 0.51              |
| 1:B:233:THR:HB   | 1:B:235:ASP:H     | 1.77                     | 0.50              |
| 1:A:128:ILE:HD13 | 1:A:338:MET:HE1   | 1.93                     | 0.50              |
| 1:D:73:TYR:CD2   | 5:D:6032:HOH:O    | 2.55                     | 0.50              |
| 1:I:73:TYR:CD2   | 1:I:95:TYR:CE1    | 2.99                     | 0.50              |
| 1:I:142:PRO:HB2  | 1:I:145:TRP:CG    | 2.46                     | 0.50              |
| 1:A:142:PRO:HB2  | 1:A:145:TRP:CD1   | 2.47                     | 0.50              |
| 1:J:137:LYS:O    | 1:J:138:ASP:HB2   | 2.11                     | 0.50              |
| 1:I:157:TYR:CD1  | 1:I:195:PRO:HD3   | 2.47                     | 0.50              |
| 1:A:187:SER:HB3  | 1:A:203:GLY:HA3   | 1.93                     | 0.50              |
| 1:G:50:LEU:HD11  | 1:G:77:ILE:HD11   | 1.94                     | 0.49              |
| 1:G:236:PRO:HB3  | 1:G:335:ALA:HB1   | 1.94                     | 0.49              |
| 1:C:192:GLU:HB3  | 1:C:197:GLN:HE21  | 1.76                     | 0.49              |
| 1:C:203:GLY:HA2  | 3:C:6003:ANP:O3'  | 2.13                     | 0.49              |
| 1:D:236:PRO:HB3  | 1:D:335:ALA:HB1   | 1.94                     | 0.49              |
| 1:H:187:SER:HB3  | 1:H:203:GLY:CA    | 2.42                     | 0.49              |
| 1:A:187:SER:HB3  | 1:A:203:GLY:CA    | 2.43                     | 0.49              |
| 1:C:105:ASN:HD22 | 1:C:107:ARG:H     | 1.60                     | 0.49              |
| 1:E:154:GLN:NE2  | 1:E:244:ASN:H     | 1.92                     | 0.49              |
| 1:F:274:LYS:CE   | 5:F:6041:HOH:O    | 2.61                     | 0.49              |
| 1:E:121:ALA:HA   | 5:E:6027:HOH:O    | 2.11                     | 0.49              |
| 1:E:137:LYS:O    | 1:E:138:ASP:HB2   | 2.12                     | 0.49              |
| 1:I:251:ASN:ND2  | 3:I:6009:ANP:H5'2 | 2.27                     | 0.49              |
| 1:G:115:SER:CB   | 5:G:6027:HOH:O    | 2.61                     | 0.49              |
| 1:E:31:MET:HE3   | 1:E:31:MET:O      | 2.13                     | 0.49              |
| 1:H:161:ILE:HD12 | 1:J:222:GLU:HB3   | 1.95                     | 0.49              |
| 1:B:135:LEU:HD23 | 1:B:142:PRO:HA    | 1.95                     | 0.49              |
| 1:D:222:GLU:HB3  | 1:E:161:ILE:HD12  | 1.94                     | 0.49              |
| 1:A:58:SER:HA    | 1:A:63:ALA:O      | 2.12                     | 0.48              |
| 1:C:236:PRO:HB3  | 1:C:335:ALA:HB1   | 1.95                     | 0.48              |
| 1:H:31:MET:HE3   | 1:H:31:MET:O      | 2.13                     | 0.48              |
| 1:B:259:LYS:HD2  | 5:B:6016:HOH:O    | 2.12                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:142:PRO:HB2  | 1:E:145:TRP:CD1   | 2.48                     | 0.48              |
| 1:G:233:THR:HB   | 1:G:235:ASP:H     | 1.78                     | 0.48              |
| 1:B:137:LYS:O    | 1:B:138:ASP:HB2   | 2.14                     | 0.48              |
| 1:D:109:SER:HB2  | 5:D:6005:HOH:O    | 2.12                     | 0.48              |
| 4:C:5008:MSL:HE2 | 1:I:192:GLU:OE2   | 2.14                     | 0.48              |
| 1:D:58:SER:HA    | 1:D:63:ALA:O      | 2.14                     | 0.48              |
| 1:I:105:ASN:HD22 | 1:I:107:ARG:H     | 1.61                     | 0.48              |
| 1:B:297:GLU:OE2  | 4:C:5002:MSL:HG2  | 2.14                     | 0.48              |
| 1:E:142:PRO:HB2  | 1:E:145:TRP:CG    | 2.48                     | 0.48              |
| 1:F:73:TYR:CD2   | 1:F:95:TYR:CE1    | 3.02                     | 0.48              |
| 1:J:303:THR:HG21 | 5:J:6045:HOH:O    | 2.13                     | 0.48              |
| 1:D:113:ILE:HD13 | 1:D:349:GLU:HG3   | 1.95                     | 0.48              |
| 1:E:73:TYR:CD2   | 1:E:95:TYR:CE1    | 3.01                     | 0.48              |
| 1:J:31:MET:HE3   | 1:J:31:MET:O      | 2.14                     | 0.48              |
| 1:G:187:SER:HB3  | 1:G:203:GLY:HA3   | 1.94                     | 0.48              |
| 1:G:273:LEU:HD23 | 5:G:6036:HOH:O    | 2.14                     | 0.48              |
| 1:I:31:MET:HE3   | 1:I:31:MET:O      | 2.14                     | 0.48              |
| 1:A:203:GLY:HA2  | 3:A:6001:ANP:O3'  | 2.14                     | 0.48              |
| 1:F:142:PRO:HB2  | 1:F:145:TRP:CG    | 2.49                     | 0.48              |
| 1:A:251:ASN:ND2  | 3:A:6001:ANP:H5'2 | 2.29                     | 0.48              |
| 1:H:236:PRO:HB3  | 1:H:335:ALA:HB1   | 1.96                     | 0.48              |
| 1:A:142:PRO:HB2  | 1:A:145:TRP:CG    | 2.49                     | 0.47              |
| 3:A:6001:ANP:O1G | 4:C:5001:MSL:NE   | 2.48                     | 0.47              |
| 1:C:233:THR:HB   | 1:C:235:ASP:H     | 1.79                     | 0.47              |
| 1:H:332:ARG:HD3  | 5:H:6035:HOH:O    | 2.14                     | 0.47              |
| 1:B:187:SER:HB3  | 1:B:203:GLY:CA    | 2.44                     | 0.47              |
| 1:F:137:LYS:O    | 1:F:138:ASP:HB2   | 2.14                     | 0.47              |
| 1:J:157:TYR:CD1  | 1:J:195:PRO:HD3   | 2.49                     | 0.47              |
| 1:B:142:PRO:HB2  | 1:B:145:TRP:CD1   | 2.50                     | 0.47              |
| 1:B:251:ASN:ND2  | 3:B:6002:ANP:H5'2 | 2.29                     | 0.47              |
| 1:C:255:GLU:HG2  | 5:C:6042:HOH:O    | 2.13                     | 0.47              |
| 4:C:5006:MSL:HE1 | 3:G:6007:ANP:O3G  | 2.13                     | 0.47              |
| 1:E:340:PRO:O    | 1:E:344:THR:HB    | 2.14                     | 0.47              |
| 4:C:5007:MSL:OE  | 3:F:6006:ANP:O1G  | 2.33                     | 0.47              |
| 1:H:333:ARG:N    | 1:H:334:PRO:CD    | 2.77                     | 0.47              |
| 1:J:105:ASN:ND2  | 1:J:107:ARG:H     | 2.13                     | 0.47              |
| 1:A:31:MET:HE3   | 1:A:31:MET:O      | 2.15                     | 0.47              |
| 1:A:292:LEU:HD23 | 1:A:298:THR:HB    | 1.96                     | 0.47              |
| 1:J:128:ILE:HD13 | 1:J:338:MET:HE1   | 1.96                     | 0.47              |
| 1:D:142:PRO:HB2  | 1:D:145:TRP:CD1   | 2.50                     | 0.47              |
| 1:E:233:THR:HB   | 1:E:235:ASP:H     | 1.80                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:18:LYS:O     | 1:F:19:ILE:HD12  | 2.15                     | 0.47              |
| 1:G:105:ASN:ND2  | 1:G:107:ARG:H    | 2.13                     | 0.47              |
| 1:G:142:PRO:HB2  | 1:G:145:TRP:CD1  | 2.50                     | 0.47              |
| 1:J:236:PRO:HB3  | 1:J:335:ALA:HB1  | 1.97                     | 0.47              |
| 1:G:265:VAL:HG12 | 5:G:6011:HOH:O   | 2.15                     | 0.47              |
| 1:I:181:TYR:C    | 1:I:181:TYR:CD2  | 2.93                     | 0.47              |
| 1:J:320:GLU:HB2  | 5:J:6039:HOH:O   | 2.15                     | 0.47              |
| 1:A:236:PRO:HB3  | 1:A:335:ALA:HB1  | 1.95                     | 0.47              |
| 1:D:261:GLY:HA2  | 5:D:6010:HOH:O   | 2.14                     | 0.47              |
| 1:G:135:LEU:HD23 | 1:G:142:PRO:HA   | 1.97                     | 0.47              |
| 1:H:19:ILE:HD11  | 1:H:86:ASN:CB    | 2.43                     | 0.47              |
| 1:H:73:TYR:CD2   | 1:H:95:TYR:CE1   | 3.03                     | 0.47              |
| 1:C:206:VAL:HG22 | 5:C:6022:HOH:O   | 2.15                     | 0.46              |
| 1:C:104:THR:HA   | 5:C:6006:HOH:O   | 2.14                     | 0.46              |
| 1:B:192:GLU:HB3  | 1:B:197:GLN:HE21 | 1.80                     | 0.46              |
| 1:C:105:ASN:HD21 | 1:C:108:TYR:H    | 1.63                     | 0.46              |
| 1:C:161:ILE:HD12 | 1:E:222:GLU:HB3  | 1.97                     | 0.46              |
| 4:C:5007:MSL:HG3 | 1:F:332:ARG:NH2  | 2.27                     | 0.46              |
| 1:F:222:GLU:HB3  | 1:I:161:ILE:HD12 | 1.98                     | 0.46              |
| 1:I:233:THR:HB   | 1:I:235:ASP:H    | 1.81                     | 0.46              |
| 1:J:233:THR:HB   | 1:J:235:ASP:H    | 1.81                     | 0.46              |
| 1:C:17:GLU:HA    | 5:C:6035:HOH:O   | 2.15                     | 0.46              |
| 1:B:187:SER:HB2  | 5:B:6028:HOH:O   | 2.15                     | 0.46              |
| 1:C:249:HIS:CE1  | 4:C:5003:MSL:HB2 | 2.50                     | 0.46              |
| 1:H:49:LYS:NZ    | 5:H:6039:HOH:O   | 2.47                     | 0.46              |
| 1:E:206:VAL:HG13 | 5:E:6022:HOH:O   | 2.14                     | 0.46              |
| 1:D:201:GLN:HG2  | 3:D:6004:ANP:O2A | 2.16                     | 0.46              |
| 1:H:187:SER:HB3  | 1:H:203:GLY:HA3  | 1.98                     | 0.46              |
| 1:E:192:GLU:HB3  | 1:E:197:GLN:HE21 | 1.81                     | 0.46              |
| 1:C:19:ILE:HD11  | 1:C:86:ASN:CB    | 2.44                     | 0.46              |
| 4:C:5007:MSL:HE2 | 1:F:192:GLU:OE1  | 2.15                     | 0.46              |
| 1:D:142:PRO:HB2  | 1:D:145:TRP:CG   | 2.51                     | 0.46              |
| 1:D:31:MET:HE3   | 1:D:31:MET:O     | 2.16                     | 0.45              |
| 1:F:142:PRO:HB2  | 1:F:145:TRP:CD1  | 2.51                     | 0.45              |
| 1:I:236:PRO:HB3  | 1:I:335:ALA:HB1  | 1.98                     | 0.45              |
| 1:F:301:ILE:H    | 1:F:301:ILE:HG13 | 1.52                     | 0.45              |
| 1:G:203:GLY:HA2  | 3:G:6007:ANP:O3' | 2.16                     | 0.45              |
| 1:I:105:ASN:ND2  | 1:I:107:ARG:H    | 2.14                     | 0.45              |
| 1:I:192:GLU:HB3  | 1:I:197:GLN:HE21 | 1.82                     | 0.45              |
| 1:D:116:SER:HA   | 1:D:117:PRO:HD3  | 1.82                     | 0.45              |
| 1:F:236:PRO:HB3  | 1:F:335:ALA:HB1  | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:105:ASN:HD22 | 1:B:107:ARG:H    | 1.65                     | 0.45              |
| 3:B:6002:ANP:PG  | 4:C:5002:MSL:NE  | 2.89                     | 0.45              |
| 1:D:105:ASN:ND2  | 1:D:107:ARG:H    | 2.14                     | 0.45              |
| 1:F:161:ILE:HD12 | 1:G:222:GLU:HB3  | 1.98                     | 0.45              |
| 1:H:248:ALA:O    | 1:H:249:HIS:C    | 2.60                     | 0.45              |
| 1:C:105:ASN:ND2  | 1:C:108:TYR:H    | 2.15                     | 0.45              |
| 1:C:181:TYR:C    | 1:C:181:TYR:CD2  | 2.95                     | 0.45              |
| 1:E:10:LEU:HA    | 5:E:6013:HOH:O   | 2.17                     | 0.45              |
| 1:F:46:ASP:HB3   | 1:F:49:LYS:HD3   | 1.99                     | 0.45              |
| 1:F:73:TYR:HB2   | 1:F:93:ASP:HB3   | 1.97                     | 0.45              |
| 1:G:49:LYS:HE2   | 5:G:6025:HOH:O   | 2.16                     | 0.45              |
| 1:A:295:ARG:HD2  | 5:A:6013:HOH:O   | 2.17                     | 0.45              |
| 1:E:46:ASP:HB3   | 1:E:49:LYS:HD3   | 1.97                     | 0.45              |
| 1:C:277:HIS:CD2  | 1:C:333:ARG:HH11 | 2.35                     | 0.44              |
| 4:C:5005:MSL:NE  | 3:E:6005:ANP:PG  | 2.90                     | 0.44              |
| 1:D:105:ASN:ND2  | 1:D:108:TYR:H    | 2.15                     | 0.44              |
| 1:G:301:ILE:H    | 1:G:301:ILE:HG13 | 1.48                     | 0.44              |
| 1:I:355:LYS:HG2  | 5:I:6044:HOH:O   | 2.16                     | 0.44              |
| 1:C:24:ILE:HD11  | 1:C:89:LEU:HD22  | 2.00                     | 0.44              |
| 1:D:46:ASP:HB3   | 1:D:49:LYS:HD3   | 1.98                     | 0.44              |
| 1:F:355:LYS:HB3  | 5:F:6014:HOH:O   | 2.16                     | 0.44              |
| 1:E:18:LYS:O     | 1:E:19:ILE:HD12  | 2.17                     | 0.44              |
| 1:F:93:ASP:HB3   | 1:F:95:TYR:HE1   | 1.83                     | 0.44              |
| 1:A:203:GLY:O    | 1:A:204:PRO:C    | 2.60                     | 0.44              |
| 4:C:5009:MSL:OE  | 3:J:6010:ANP:O1G | 2.35                     | 0.44              |
| 1:A:284:TYR:CD2  | 1:A:343:VAL:HG22 | 2.53                     | 0.44              |
| 1:C:136:GLN:HB3  | 5:C:6009:HOH:O   | 2.17                     | 0.44              |
| 4:C:5003:MSL:NE  | 3:C:6003:ANP:PG  | 2.90                     | 0.44              |
| 4:C:5005:MSL:OE  | 1:E:311:ARG:HD3  | 2.18                     | 0.44              |
| 1:D:73:TYR:CD2   | 1:D:95:TYR:CE1   | 3.06                     | 0.44              |
| 1:G:73:TYR:HB2   | 1:G:93:ASP:HB3   | 1.98                     | 0.44              |
| 1:H:233:THR:HB   | 1:H:235:ASP:H    | 1.83                     | 0.44              |
| 1:H:355:LYS:HB3  | 5:H:6009:HOH:O   | 2.16                     | 0.44              |
| 1:I:203:GLY:O    | 1:I:204:PRO:C    | 2.60                     | 0.44              |
| 1:D:72:LEU:CG    | 5:D:6046:HOH:O   | 2.48                     | 0.44              |
| 1:J:292:LEU:HD23 | 1:J:298:THR:HB   | 2.00                     | 0.44              |
| 1:F:135:LEU:HD23 | 1:F:142:PRO:HA   | 2.00                     | 0.44              |
| 1:I:73:TYR:HB2   | 1:I:93:ASP:HB3   | 2.00                     | 0.44              |
| 1:J:324:ASN:CB   | 5:J:6034:HOH:O   | 2.64                     | 0.44              |
| 1:A:157:TYR:CD1  | 1:A:195:PRO:HD3  | 2.53                     | 0.44              |
| 1:B:187:SER:HB3  | 1:B:203:GLY:HA3  | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:5005:MSL:HG3 | 1:E:332:ARG:HH22 | 1.83                     | 0.43              |
| 1:D:105:ASN:HD21 | 1:D:108:TYR:H    | 1.66                     | 0.43              |
| 1:A:172:VAL:HG21 | 1:A:198:TRP:CE3  | 2.54                     | 0.43              |
| 1:B:154:GLN:NE2  | 1:B:244:ASN:H    | 1.98                     | 0.43              |
| 1:C:116:SER:HA   | 1:C:117:PRO:HD3  | 1.85                     | 0.43              |
| 1:E:310:ASN:HD22 | 1:E:313:ALA:HB2  | 1.83                     | 0.43              |
| 1:F:233:THR:HB   | 1:F:235:ASP:H    | 1.83                     | 0.43              |
| 1:G:142:PRO:HB2  | 1:G:145:TRP:CG   | 2.53                     | 0.43              |
| 1:H:254:THR:O    | 1:H:255:GLU:C    | 2.61                     | 0.43              |
| 1:A:73:TYR:HB2   | 1:A:93:ASP:HB3   | 2.00                     | 0.43              |
| 1:A:284:TYR:CE2  | 1:A:343:VAL:HG22 | 2.54                     | 0.43              |
| 1:D:233:THR:HB   | 1:D:235:ASP:H    | 1.84                     | 0.43              |
| 1:H:115:SER:O    | 1:H:116:SER:C    | 2.61                     | 0.43              |
| 1:J:58:SER:HA    | 1:J:63:ALA:O     | 2.19                     | 0.43              |
| 1:D:310:ASN:HD22 | 1:D:313:ALA:HB2  | 1.82                     | 0.43              |
| 1:E:272:LYS:HA   | 5:E:6035:HOH:O   | 2.19                     | 0.43              |
| 5:F:6037:HOH:O   | 1:G:97:PRO:HG2   | 2.19                     | 0.43              |
| 1:I:116:SER:HA   | 1:I:117:PRO:HD3  | 1.86                     | 0.43              |
| 1:B:3:CYS:N      | 5:B:6032:HOH:O   | 2.52                     | 0.43              |
| 1:B:301:ILE:H    | 1:B:301:ILE:HG13 | 1.53                     | 0.43              |
| 1:F:113:ILE:HD13 | 1:F:349:GLU:HG3  | 1.99                     | 0.43              |
| 1:C:316:ARG:NH1  | 3:C:6003:ANP:O1B | 2.43                     | 0.43              |
| 4:C:5007:MSL:CB  | 1:F:249:HIS:CE1  | 3.01                     | 0.43              |
| 1:D:93:ASP:CB    | 5:D:6032:HOH:O   | 2.55                     | 0.43              |
| 1:D:127:GLY:HA3  | 3:D:6004:ANP:O4' | 2.19                     | 0.43              |
| 1:G:113:ILE:HD13 | 1:G:349:GLU:HG3  | 2.01                     | 0.43              |
| 1:G:192:GLU:HB3  | 1:G:197:GLN:HE21 | 1.84                     | 0.43              |
| 1:H:46:ASP:HB3   | 1:H:49:LYS:HD3   | 2.01                     | 0.43              |
| 1:B:154:GLN:HE22 | 1:B:244:ASN:N    | 1.98                     | 0.42              |
| 1:A:211:GLY:HA2  | 1:A:340:PRO:HB2  | 2.01                     | 0.42              |
| 1:G:116:SER:HA   | 1:G:117:PRO:HD3  | 1.80                     | 0.42              |
| 1:H:18:LYS:O     | 1:H:19:ILE:HD12  | 2.20                     | 0.42              |
| 1:D:235:ASP:OD2  | 1:D:290:ARG:NH2  | 2.52                     | 0.42              |
| 1:E:93:ASP:HB3   | 1:E:95:TYR:HE1   | 1.84                     | 0.42              |
| 1:F:226:GLU:HG3  | 1:I:162:GLY:C    | 2.45                     | 0.42              |
| 1:H:116:SER:HA   | 1:H:117:PRO:HD3  | 1.76                     | 0.42              |
| 1:I:50:LEU:HD11  | 1:I:77:ILE:HD11  | 2.00                     | 0.42              |
| 1:B:333:ARG:N    | 1:B:334:PRO:CD   | 2.82                     | 0.42              |
| 1:C:333:ARG:N    | 1:C:334:PRO:CD   | 2.82                     | 0.42              |
| 1:F:157:TYR:CD1  | 1:F:195:PRO:HD3  | 2.54                     | 0.42              |
| 1:F:180:LEU:HG   | 1:F:186:ILE:CG2  | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:277:HIS:CD2  | 1:F:333:ARG:HH11 | 2.38                     | 0.42              |
| 1:J:66:GLU:H     | 1:J:66:GLU:CD    | 2.26                     | 0.42              |
| 1:E:58:SER:HA    | 1:E:63:ALA:O     | 2.19                     | 0.42              |
| 1:B:249:HIS:HE1  | 4:C:5002:MSL:HB2 | 1.82                     | 0.42              |
| 3:B:6002:ANP:O1G | 4:C:5002:MSL:OE  | 2.38                     | 0.42              |
| 1:C:135:LEU:HD23 | 1:C:142:PRO:HA   | 2.02                     | 0.42              |
| 1:F:116:SER:HA   | 1:F:117:PRO:HD3  | 1.82                     | 0.42              |
| 1:G:105:ASN:ND2  | 1:G:108:TYR:H    | 2.17                     | 0.42              |
| 1:H:58:SER:HA    | 1:H:63:ALA:O     | 2.20                     | 0.42              |
| 1:H:131:GLU:HG2  | 1:H:192:GLU:HG3  | 2.02                     | 0.42              |
| 1:B:235:ASP:OD2  | 1:B:290:ARG:NH2  | 2.53                     | 0.42              |
| 1:D:45:THR:CG2   | 5:D:6034:HOH:O   | 2.56                     | 0.42              |
| 1:D:102:ILE:HD11 | 5:D:6039:HOH:O   | 2.19                     | 0.42              |
| 1:D:156:PRO:HB3  | 5:D:6008:HOH:O   | 2.19                     | 0.42              |
| 1:I:333:ARG:N    | 1:I:334:PRO:CD   | 2.83                     | 0.42              |
| 1:J:324:ASN:CA   | 5:J:6034:HOH:O   | 2.68                     | 0.42              |
| 1:B:349:GLU:HB3  | 5:B:6027:HOH:O   | 2.18                     | 0.42              |
| 1:D:172:VAL:HG21 | 1:D:198:TRP:CE3  | 2.54                     | 0.42              |
| 1:F:248:ALA:CB   | 1:F:338:MET:HE3  | 2.50                     | 0.42              |
| 1:G:350:THR:HG21 | 5:G:6036:HOH:O   | 2.20                     | 0.42              |
| 1:B:142:PRO:HB2  | 1:B:145:TRP:CG   | 2.54                     | 0.42              |
| 1:H:105:ASN:HD22 | 1:H:107:ARG:H    | 1.67                     | 0.42              |
| 1:H:355:LYS:CB   | 5:H:6009:HOH:O   | 2.68                     | 0.42              |
| 1:C:105:ASN:ND2  | 1:C:107:ARG:H    | 2.17                     | 0.41              |
| 1:D:292:LEU:HD23 | 1:D:298:THR:HB   | 2.02                     | 0.41              |
| 1:J:18:LYS:O     | 1:J:19:ILE:HD12  | 2.20                     | 0.41              |
| 1:J:142:PRO:HB2  | 1:J:145:TRP:CD1  | 2.55                     | 0.41              |
| 1:A:116:SER:HA   | 1:A:117:PRO:HD3  | 1.87                     | 0.41              |
| 1:A:135:LEU:HD23 | 1:A:142:PRO:HA   | 2.02                     | 0.41              |
| 5:B:6034:HOH:O   | 1:C:8:VAL:CG2    | 2.54                     | 0.41              |
| 1:G:161:ILE:HD12 | 1:H:222:GLU:HB3  | 2.02                     | 0.41              |
| 1:I:308:VAL:HG22 | 5:I:6041:HOH:O   | 2.20                     | 0.41              |
| 1:B:164:GLU:HG3  | 1:C:231:VAL:HG22 | 2.01                     | 0.41              |
| 1:D:123:GLU:CG   | 5:D:6015:HOH:O   | 2.64                     | 0.41              |
| 1:D:137:LYS:O    | 1:D:138:ASP:HB2  | 2.20                     | 0.41              |
| 1:I:203:GLY:HA2  | 3:I:6009:ANP:O3' | 2.19                     | 0.41              |
| 1:B:136:GLN:HB3  | 5:B:6018:HOH:O   | 2.20                     | 0.41              |
| 1:I:231:VAL:HG22 | 1:J:164:GLU:HG3  | 2.02                     | 0.41              |
| 1:C:332:ARG:HH22 | 4:C:5003:MSL:HG3 | 1.85                     | 0.41              |
| 1:D:248:ALA:CB   | 1:D:338:MET:HE3  | 2.51                     | 0.41              |
| 1:D:248:ALA:HB3  | 1:D:338:MET:HE3  | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:5005:MSL:NE  | 3:E:6005:ANP:O1G | 2.54                     | 0.41              |
| 1:C:46:ASP:HB3   | 1:C:49:LYS:HD3   | 2.03                     | 0.41              |
| 1:C:142:PRO:HB2  | 1:C:145:TRP:CD1  | 2.56                     | 0.41              |
| 1:D:181:TYR:CD2  | 1:D:181:TYR:C    | 2.99                     | 0.41              |
| 1:E:191:GLY:HA2  | 1:E:198:TRP:CE3  | 2.56                     | 0.41              |
| 1:A:222:GLU:HB3  | 1:D:161:ILE:HD12 | 2.01                     | 0.41              |
| 1:B:24:ILE:HD11  | 1:B:89:LEU:HD22  | 2.02                     | 0.41              |
| 1:B:236:PRO:HB3  | 1:B:335:ALA:HB1  | 2.03                     | 0.41              |
| 1:C:18:LYS:O     | 1:C:19:ILE:HD12  | 2.20                     | 0.41              |
| 1:C:142:PRO:HB2  | 1:C:145:TRP:CG   | 2.56                     | 0.41              |
| 1:D:66:GLU:H     | 1:D:66:GLU:CD    | 2.29                     | 0.41              |
| 1:D:75:GLN:NE2   | 5:D:6032:HOH:O   | 2.50                     | 0.41              |
| 1:F:128:ILE:O    | 1:F:128:ILE:HG13 | 2.21                     | 0.41              |
| 1:G:46:ASP:HB3   | 1:G:49:LYS:HD3   | 2.03                     | 0.41              |
| 1:G:277:HIS:CD2  | 1:G:333:ARG:HH11 | 2.38                     | 0.41              |
| 1:J:302:ASN:HA   | 5:J:6028:HOH:O   | 2.21                     | 0.41              |
| 1:B:181:TYR:CD2  | 1:B:181:TYR:C    | 2.99                     | 0.41              |
| 1:F:284:TYR:CD2  | 1:F:343:VAL:HG22 | 2.56                     | 0.41              |
| 1:H:128:ILE:HD13 | 1:H:338:MET:HE1  | 2.03                     | 0.41              |
| 1:I:223:ARG:HH11 | 1:I:223:ARG:HD2  | 1.71                     | 0.41              |
| 4:C:5007:MSL:HB2 | 1:F:249:HIS:HE1  | 1.84                     | 0.40              |
| 1:H:181:TYR:CD2  | 1:H:181:TYR:C    | 2.98                     | 0.40              |
| 1:A:233:THR:HB   | 1:A:235:ASP:H    | 1.86                     | 0.40              |
| 1:D:135:LEU:HD23 | 1:D:142:PRO:HA   | 2.03                     | 0.40              |
| 1:J:46:ASP:HB3   | 1:J:49:LYS:HD3   | 2.02                     | 0.40              |
| 1:J:277:HIS:CD2  | 1:J:333:ARG:HH11 | 2.39                     | 0.40              |
| 1:B:50:LEU:HD11  | 1:B:77:ILE:HD11  | 2.03                     | 0.40              |
| 1:E:292:LEU:HD23 | 1:E:298:THR:HB   | 2.02                     | 0.40              |
| 1:F:192:GLU:HB3  | 1:F:197:GLN:HE21 | 1.87                     | 0.40              |
| 1:G:58:SER:HA    | 1:G:63:ALA:O     | 2.21                     | 0.40              |
| 1:G:292:LEU:HD23 | 1:G:298:THR:HB   | 2.03                     | 0.40              |
| 1:H:211:GLY:HA2  | 1:H:340:PRO:HB2  | 2.02                     | 0.40              |
| 1:A:127:GLY:HA3  | 3:A:6001:ANP:O4' | 2.21                     | 0.40              |
| 1:A:308:VAL:N    | 5:A:6028:HOH:O   | 2.48                     | 0.40              |
| 1:A:113:ILE:HD13 | 1:A:349:GLU:HG3  | 2.02                     | 0.40              |
| 1:D:154:GLN:HE22 | 1:D:244:ASN:N    | 1.96                     | 0.40              |
| 1:F:105:ASN:HD22 | 1:F:107:ARG:H    | 1.68                     | 0.40              |
| 1:F:323:GLN:HG2  | 5:F:6035:HOH:O   | 2.22                     | 0.40              |
| 1:H:105:ASN:ND2  | 1:H:107:ARG:H    | 2.20                     | 0.40              |
| 5:H:6015:HOH:O   | 1:I:3:CYS:HA     | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 351/356 (99%)   | 331 (94%)  | 20 (6%)  | 0        | 100         | 100 |
| 1   | B     | 351/356 (99%)   | 331 (94%)  | 20 (6%)  | 0        | 100         | 100 |
| 1   | C     | 351/356 (99%)   | 334 (95%)  | 16 (5%)  | 1 (0%)   | 36          | 67  |
| 1   | D     | 351/356 (99%)   | 333 (95%)  | 18 (5%)  | 0        | 100         | 100 |
| 1   | E     | 351/356 (99%)   | 328 (93%)  | 23 (7%)  | 0        | 100         | 100 |
| 1   | F     | 351/356 (99%)   | 331 (94%)  | 20 (6%)  | 0        | 100         | 100 |
| 1   | G     | 351/356 (99%)   | 332 (95%)  | 18 (5%)  | 1 (0%)   | 36          | 67  |
| 1   | H     | 351/356 (99%)   | 334 (95%)  | 17 (5%)  | 0        | 100         | 100 |
| 1   | I     | 351/356 (99%)   | 330 (94%)  | 21 (6%)  | 0        | 100         | 100 |
| 1   | J     | 351/356 (99%)   | 332 (95%)  | 19 (5%)  | 0        | 100         | 100 |
| All | All   | 3510/3560 (99%) | 3316 (94%) | 192 (6%) | 2 (0%)   | 48          | 79  |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 84  | ARG  |
| 1   | C     | 138 | ASP  |

### 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     | 288/290 (99%) | 259 (90%) | 29 (10%) | 7           | 28 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | B     | 288/290 (99%)   | 258 (90%)  | 30 (10%)  | 7           | 27 |
| 1   | C     | 288/290 (99%)   | 258 (90%)  | 30 (10%)  | 7           | 27 |
| 1   | D     | 288/290 (99%)   | 260 (90%)  | 28 (10%)  | 8           | 30 |
| 1   | E     | 288/290 (99%)   | 259 (90%)  | 29 (10%)  | 7           | 28 |
| 1   | F     | 288/290 (99%)   | 260 (90%)  | 28 (10%)  | 8           | 30 |
| 1   | G     | 288/290 (99%)   | 260 (90%)  | 28 (10%)  | 8           | 30 |
| 1   | H     | 288/290 (99%)   | 257 (89%)  | 31 (11%)  | 6           | 26 |
| 1   | I     | 288/290 (99%)   | 262 (91%)  | 26 (9%)   | 9           | 32 |
| 1   | J     | 288/290 (99%)   | 259 (90%)  | 29 (10%)  | 7           | 28 |
| All | All   | 2880/2900 (99%) | 2592 (90%) | 288 (10%) | 7           | 28 |

All (288) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | ASP  |
| 1   | A     | 15  | THR  |
| 1   | A     | 19  | ILE  |
| 1   | A     | 45  | THR  |
| 1   | A     | 66  | GLU  |
| 1   | A     | 79  | LYS  |
| 1   | A     | 104 | THR  |
| 1   | A     | 105 | ASN  |
| 1   | A     | 109 | SER  |
| 1   | A     | 112 | LYS  |
| 1   | A     | 128 | ILE  |
| 1   | A     | 143 | LEU  |
| 1   | A     | 147 | ILE  |
| 1   | A     | 164 | GLU  |
| 1   | A     | 201 | GLN  |
| 1   | A     | 206 | VAL  |
| 1   | A     | 232 | VAL  |
| 1   | A     | 233 | THR  |
| 1   | A     | 265 | VAL  |
| 1   | A     | 279 | GLU  |
| 1   | A     | 288 | ASN  |
| 1   | A     | 289 | GLU  |
| 1   | A     | 301 | ILE  |
| 1   | A     | 321 | THR  |
| 1   | A     | 338 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 344 | THR  |
| 1   | A     | 349 | GLU  |
| 1   | A     | 351 | THR  |
| 1   | A     | 355 | LYS  |
| 1   | B     | 3   | CYS  |
| 1   | B     | 14  | ASP  |
| 1   | B     | 15  | THR  |
| 1   | B     | 19  | ILE  |
| 1   | B     | 45  | THR  |
| 1   | B     | 66  | GLU  |
| 1   | B     | 104 | THR  |
| 1   | B     | 105 | ASN  |
| 1   | B     | 109 | SER  |
| 1   | B     | 112 | LYS  |
| 1   | B     | 123 | GLU  |
| 1   | B     | 128 | ILE  |
| 1   | B     | 143 | LEU  |
| 1   | B     | 147 | ILE  |
| 1   | B     | 164 | GLU  |
| 1   | B     | 201 | GLN  |
| 1   | B     | 206 | VAL  |
| 1   | B     | 232 | VAL  |
| 1   | B     | 233 | THR  |
| 1   | B     | 256 | SER  |
| 1   | B     | 265 | VAL  |
| 1   | B     | 279 | GLU  |
| 1   | B     | 288 | ASN  |
| 1   | B     | 289 | GLU  |
| 1   | B     | 301 | ILE  |
| 1   | B     | 321 | THR  |
| 1   | B     | 338 | MET  |
| 1   | B     | 344 | THR  |
| 1   | B     | 349 | GLU  |
| 1   | B     | 351 | THR  |
| 1   | C     | 3   | CYS  |
| 1   | C     | 14  | ASP  |
| 1   | C     | 15  | THR  |
| 1   | C     | 19  | ILE  |
| 1   | C     | 45  | THR  |
| 1   | C     | 66  | GLU  |
| 1   | C     | 104 | THR  |
| 1   | C     | 105 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 112 | LYS  |
| 1   | C     | 123 | GLU  |
| 1   | C     | 128 | ILE  |
| 1   | C     | 143 | LEU  |
| 1   | C     | 147 | ILE  |
| 1   | C     | 164 | GLU  |
| 1   | C     | 201 | GLN  |
| 1   | C     | 206 | VAL  |
| 1   | C     | 230 | VAL  |
| 1   | C     | 232 | VAL  |
| 1   | C     | 233 | THR  |
| 1   | C     | 265 | VAL  |
| 1   | C     | 279 | GLU  |
| 1   | C     | 288 | ASN  |
| 1   | C     | 289 | GLU  |
| 1   | C     | 301 | ILE  |
| 1   | C     | 321 | THR  |
| 1   | C     | 338 | MET  |
| 1   | C     | 344 | THR  |
| 1   | C     | 349 | GLU  |
| 1   | C     | 351 | THR  |
| 1   | C     | 355 | LYS  |
| 1   | D     | 14  | ASP  |
| 1   | D     | 15  | THR  |
| 1   | D     | 19  | ILE  |
| 1   | D     | 45  | THR  |
| 1   | D     | 66  | GLU  |
| 1   | D     | 79  | LYS  |
| 1   | D     | 104 | THR  |
| 1   | D     | 105 | ASN  |
| 1   | D     | 109 | SER  |
| 1   | D     | 112 | LYS  |
| 1   | D     | 128 | ILE  |
| 1   | D     | 143 | LEU  |
| 1   | D     | 147 | ILE  |
| 1   | D     | 164 | GLU  |
| 1   | D     | 201 | GLN  |
| 1   | D     | 206 | VAL  |
| 1   | D     | 230 | VAL  |
| 1   | D     | 232 | VAL  |
| 1   | D     | 233 | THR  |
| 1   | D     | 265 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 279 | GLU  |
| 1   | D     | 288 | ASN  |
| 1   | D     | 289 | GLU  |
| 1   | D     | 301 | ILE  |
| 1   | D     | 321 | THR  |
| 1   | D     | 344 | THR  |
| 1   | D     | 349 | GLU  |
| 1   | D     | 351 | THR  |
| 1   | E     | 3   | CYS  |
| 1   | E     | 14  | ASP  |
| 1   | E     | 15  | THR  |
| 1   | E     | 19  | ILE  |
| 1   | E     | 45  | THR  |
| 1   | E     | 66  | GLU  |
| 1   | E     | 79  | LYS  |
| 1   | E     | 104 | THR  |
| 1   | E     | 109 | SER  |
| 1   | E     | 112 | LYS  |
| 1   | E     | 128 | ILE  |
| 1   | E     | 143 | LEU  |
| 1   | E     | 147 | ILE  |
| 1   | E     | 164 | GLU  |
| 1   | E     | 201 | GLN  |
| 1   | E     | 206 | VAL  |
| 1   | E     | 232 | VAL  |
| 1   | E     | 233 | THR  |
| 1   | E     | 265 | VAL  |
| 1   | E     | 279 | GLU  |
| 1   | E     | 288 | ASN  |
| 1   | E     | 289 | GLU  |
| 1   | E     | 301 | ILE  |
| 1   | E     | 321 | THR  |
| 1   | E     | 338 | MET  |
| 1   | E     | 344 | THR  |
| 1   | E     | 349 | GLU  |
| 1   | E     | 351 | THR  |
| 1   | E     | 355 | LYS  |
| 1   | F     | 3   | CYS  |
| 1   | F     | 14  | ASP  |
| 1   | F     | 15  | THR  |
| 1   | F     | 19  | ILE  |
| 1   | F     | 45  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 66  | GLU  |
| 1   | F     | 104 | THR  |
| 1   | F     | 105 | ASN  |
| 1   | F     | 109 | SER  |
| 1   | F     | 112 | LYS  |
| 1   | F     | 128 | ILE  |
| 1   | F     | 143 | LEU  |
| 1   | F     | 147 | ILE  |
| 1   | F     | 164 | GLU  |
| 1   | F     | 201 | GLN  |
| 1   | F     | 206 | VAL  |
| 1   | F     | 232 | VAL  |
| 1   | F     | 233 | THR  |
| 1   | F     | 265 | VAL  |
| 1   | F     | 279 | GLU  |
| 1   | F     | 288 | ASN  |
| 1   | F     | 289 | GLU  |
| 1   | F     | 301 | ILE  |
| 1   | F     | 321 | THR  |
| 1   | F     | 344 | THR  |
| 1   | F     | 349 | GLU  |
| 1   | F     | 351 | THR  |
| 1   | F     | 355 | LYS  |
| 1   | G     | 14  | ASP  |
| 1   | G     | 15  | THR  |
| 1   | G     | 19  | ILE  |
| 1   | G     | 45  | THR  |
| 1   | G     | 66  | GLU  |
| 1   | G     | 104 | THR  |
| 1   | G     | 105 | ASN  |
| 1   | G     | 109 | SER  |
| 1   | G     | 112 | LYS  |
| 1   | G     | 128 | ILE  |
| 1   | G     | 143 | LEU  |
| 1   | G     | 147 | ILE  |
| 1   | G     | 164 | GLU  |
| 1   | G     | 201 | GLN  |
| 1   | G     | 206 | VAL  |
| 1   | G     | 232 | VAL  |
| 1   | G     | 233 | THR  |
| 1   | G     | 265 | VAL  |
| 1   | G     | 279 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 288 | ASN  |
| 1   | G     | 289 | GLU  |
| 1   | G     | 301 | ILE  |
| 1   | G     | 321 | THR  |
| 1   | G     | 338 | MET  |
| 1   | G     | 344 | THR  |
| 1   | G     | 349 | GLU  |
| 1   | G     | 351 | THR  |
| 1   | G     | 355 | LYS  |
| 1   | H     | 3   | CYS  |
| 1   | H     | 14  | ASP  |
| 1   | H     | 15  | THR  |
| 1   | H     | 19  | ILE  |
| 1   | H     | 45  | THR  |
| 1   | H     | 66  | GLU  |
| 1   | H     | 79  | LYS  |
| 1   | H     | 104 | THR  |
| 1   | H     | 105 | ASN  |
| 1   | H     | 109 | SER  |
| 1   | H     | 112 | LYS  |
| 1   | H     | 123 | GLU  |
| 1   | H     | 128 | ILE  |
| 1   | H     | 143 | LEU  |
| 1   | H     | 147 | ILE  |
| 1   | H     | 164 | GLU  |
| 1   | H     | 201 | GLN  |
| 1   | H     | 206 | VAL  |
| 1   | H     | 230 | VAL  |
| 1   | H     | 232 | VAL  |
| 1   | H     | 233 | THR  |
| 1   | H     | 265 | VAL  |
| 1   | H     | 279 | GLU  |
| 1   | H     | 288 | ASN  |
| 1   | H     | 289 | GLU  |
| 1   | H     | 301 | ILE  |
| 1   | H     | 321 | THR  |
| 1   | H     | 338 | MET  |
| 1   | H     | 344 | THR  |
| 1   | H     | 349 | GLU  |
| 1   | H     | 351 | THR  |
| 1   | I     | 3   | CYS  |
| 1   | I     | 14  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 15  | THR  |
| 1   | I     | 19  | ILE  |
| 1   | I     | 45  | THR  |
| 1   | I     | 66  | GLU  |
| 1   | I     | 104 | THR  |
| 1   | I     | 105 | ASN  |
| 1   | I     | 112 | LYS  |
| 1   | I     | 128 | ILE  |
| 1   | I     | 143 | LEU  |
| 1   | I     | 147 | ILE  |
| 1   | I     | 164 | GLU  |
| 1   | I     | 201 | GLN  |
| 1   | I     | 206 | VAL  |
| 1   | I     | 232 | VAL  |
| 1   | I     | 233 | THR  |
| 1   | I     | 265 | VAL  |
| 1   | I     | 279 | GLU  |
| 1   | I     | 288 | ASN  |
| 1   | I     | 289 | GLU  |
| 1   | I     | 301 | ILE  |
| 1   | I     | 321 | THR  |
| 1   | I     | 344 | THR  |
| 1   | I     | 349 | GLU  |
| 1   | I     | 351 | THR  |
| 1   | J     | 3   | CYS  |
| 1   | J     | 15  | THR  |
| 1   | J     | 19  | ILE  |
| 1   | J     | 45  | THR  |
| 1   | J     | 66  | GLU  |
| 1   | J     | 79  | LYS  |
| 1   | J     | 104 | THR  |
| 1   | J     | 105 | ASN  |
| 1   | J     | 109 | SER  |
| 1   | J     | 112 | LYS  |
| 1   | J     | 123 | GLU  |
| 1   | J     | 128 | ILE  |
| 1   | J     | 143 | LEU  |
| 1   | J     | 147 | ILE  |
| 1   | J     | 164 | GLU  |
| 1   | J     | 206 | VAL  |
| 1   | J     | 230 | VAL  |
| 1   | J     | 232 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 233 | THR  |
| 1   | J     | 265 | VAL  |
| 1   | J     | 279 | GLU  |
| 1   | J     | 288 | ASN  |
| 1   | J     | 289 | GLU  |
| 1   | J     | 301 | ILE  |
| 1   | J     | 321 | THR  |
| 1   | J     | 338 | MET  |
| 1   | J     | 344 | THR  |
| 1   | J     | 349 | GLU  |
| 1   | J     | 351 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 105 | ASN  |
| 1   | A     | 136 | GLN  |
| 1   | A     | 154 | GLN  |
| 1   | A     | 201 | GLN  |
| 1   | A     | 244 | ASN  |
| 1   | A     | 251 | ASN  |
| 1   | A     | 277 | HIS  |
| 1   | A     | 288 | ASN  |
| 1   | A     | 324 | ASN  |
| 1   | B     | 105 | ASN  |
| 1   | B     | 136 | GLN  |
| 1   | B     | 154 | GLN  |
| 1   | B     | 197 | GLN  |
| 1   | B     | 244 | ASN  |
| 1   | B     | 249 | HIS  |
| 1   | B     | 251 | ASN  |
| 1   | B     | 277 | HIS  |
| 1   | B     | 288 | ASN  |
| 1   | B     | 324 | ASN  |
| 1   | C     | 105 | ASN  |
| 1   | C     | 136 | GLN  |
| 1   | C     | 154 | GLN  |
| 1   | C     | 190 | ASN  |
| 1   | C     | 197 | GLN  |
| 1   | C     | 201 | GLN  |
| 1   | C     | 244 | ASN  |
| 1   | C     | 251 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 277 | HIS  |
| 1   | C     | 288 | ASN  |
| 1   | C     | 324 | ASN  |
| 1   | D     | 105 | ASN  |
| 1   | D     | 136 | GLN  |
| 1   | D     | 140 | ASN  |
| 1   | D     | 154 | GLN  |
| 1   | D     | 190 | ASN  |
| 1   | D     | 201 | GLN  |
| 1   | D     | 277 | HIS  |
| 1   | D     | 288 | ASN  |
| 1   | D     | 324 | ASN  |
| 1   | E     | 105 | ASN  |
| 1   | E     | 136 | GLN  |
| 1   | E     | 154 | GLN  |
| 1   | E     | 190 | ASN  |
| 1   | E     | 197 | GLN  |
| 1   | E     | 201 | GLN  |
| 1   | E     | 244 | ASN  |
| 1   | E     | 251 | ASN  |
| 1   | E     | 277 | HIS  |
| 1   | E     | 288 | ASN  |
| 1   | E     | 324 | ASN  |
| 1   | F     | 105 | ASN  |
| 1   | F     | 136 | GLN  |
| 1   | F     | 154 | GLN  |
| 1   | F     | 190 | ASN  |
| 1   | F     | 197 | GLN  |
| 1   | F     | 201 | GLN  |
| 1   | F     | 249 | HIS  |
| 1   | F     | 251 | ASN  |
| 1   | F     | 277 | HIS  |
| 1   | F     | 288 | ASN  |
| 1   | F     | 324 | ASN  |
| 1   | G     | 11  | ASN  |
| 1   | G     | 105 | ASN  |
| 1   | G     | 136 | GLN  |
| 1   | G     | 154 | GLN  |
| 1   | G     | 197 | GLN  |
| 1   | G     | 277 | HIS  |
| 1   | G     | 288 | ASN  |
| 1   | G     | 324 | ASN  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 105 | ASN  |
| 1   | H     | 154 | GLN  |
| 1   | H     | 190 | ASN  |
| 1   | H     | 197 | GLN  |
| 1   | H     | 201 | GLN  |
| 1   | H     | 244 | ASN  |
| 1   | H     | 251 | ASN  |
| 1   | H     | 277 | HIS  |
| 1   | H     | 288 | ASN  |
| 1   | H     | 324 | ASN  |
| 1   | I     | 105 | ASN  |
| 1   | I     | 136 | GLN  |
| 1   | I     | 154 | GLN  |
| 1   | I     | 190 | ASN  |
| 1   | I     | 197 | GLN  |
| 1   | I     | 201 | GLN  |
| 1   | I     | 244 | ASN  |
| 1   | I     | 251 | ASN  |
| 1   | I     | 277 | HIS  |
| 1   | I     | 288 | ASN  |
| 1   | I     | 324 | ASN  |
| 1   | J     | 11  | ASN  |
| 1   | J     | 105 | ASN  |
| 1   | J     | 154 | GLN  |
| 1   | J     | 190 | ASN  |
| 1   | J     | 201 | GLN  |
| 1   | J     | 244 | ASN  |
| 1   | J     | 277 | HIS  |
| 1   | J     | 288 | ASN  |
| 1   | J     | 324 | 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 30 are monoatomic - leaving 20 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 4   | MSL  | C     | 5010 | 2    | 7,10,10      | 1.46 | 2 (28%)     | 6,14,14     | 1.89 | 3 (50%)     |
| 4   | MSL  | C     | 5007 | 2    | 7,10,10      | 1.46 | 1 (14%)     | 6,14,14     | 3.29 | 3 (50%)     |
| 4   | MSL  | C     | 5005 | 2    | 7,10,10      | 1.05 | 0           | 6,14,14     | 1.41 | 1 (16%)     |
| 4   | MSL  | C     | 5006 | 2    | 7,10,10      | 1.58 | 2 (28%)     | 6,14,14     | 1.40 | 1 (16%)     |
| 3   | ANP  | B     | 6002 | 2    | 33,33,33     | 2.68 | 14 (42%)    | 45,52,52    | 3.37 | 21 (46%)    |
| 4   | MSL  | C     | 5004 | 2    | 7,10,10      | 1.14 | 0           | 6,14,14     | 2.00 | 2 (33%)     |
| 4   | MSL  | C     | 5001 | 2    | 7,10,10      | 1.54 | 1 (14%)     | 6,14,14     | 1.69 | 3 (50%)     |
| 3   | ANP  | F     | 6006 | 2    | 33,33,33     | 3.32 | 14 (42%)    | 45,52,52    | 3.10 | 19 (42%)    |
| 4   | MSL  | C     | 5008 | 2    | 7,10,10      | 1.16 | 0           | 6,14,14     | 1.33 | 1 (16%)     |
| 3   | ANP  | G     | 6007 | 2    | 33,33,33     | 2.46 | 13 (39%)    | 45,52,52    | 2.98 | 17 (37%)    |
| 3   | ANP  | J     | 6010 | 2    | 33,33,33     | 2.58 | 14 (42%)    | 45,52,52    | 3.46 | 23 (51%)    |
| 4   | MSL  | C     | 5009 | 2    | 7,10,10      | 1.08 | 0           | 6,14,14     | 1.59 | 1 (16%)     |
| 3   | ANP  | A     | 6001 | 2    | 33,33,33     | 2.52 | 15 (45%)    | 45,52,52    | 3.13 | 21 (46%)    |
| 4   | MSL  | C     | 5002 | 2    | 7,10,10      | 1.03 | 0           | 6,14,14     | 1.61 | 2 (33%)     |
| 4   | MSL  | C     | 5003 | 2    | 7,10,10      | 1.04 | 0           | 6,14,14     | 2.75 | 3 (50%)     |
| 3   | ANP  | C     | 6003 | 2    | 33,33,33     | 2.50 | 12 (36%)    | 45,52,52    | 3.47 | 19 (42%)    |
| 3   | ANP  | I     | 6009 | 2    | 33,33,33     | 2.51 | 14 (42%)    | 45,52,52    | 3.13 | 20 (44%)    |
| 3   | ANP  | E     | 6005 | 2    | 33,33,33     | 3.30 | 15 (45%)    | 45,52,52    | 3.61 | 21 (46%)    |
| 3   | ANP  | H     | 6008 | 2    | 33,33,33     | 2.51 | 14 (42%)    | 45,52,52    | 3.72 | 20 (44%)    |
| 3   | ANP  | D     | 6004 | 2    | 33,33,33     | 3.20 | 12 (36%)    | 45,52,52    | 3.29 | 20 (44%)    |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|------|------|---------|-------------|---------|
| 4   | MSL  | C     | 5010 | 2    | -       | 5/9/10/10   | -       |
| 4   | MSL  | C     | 5007 | 2    | -       | 8/9/10/10   | -       |
| 4   | MSL  | C     | 5005 | 2    | -       | 7/9/10/10   | -       |
| 4   | MSL  | C     | 5006 | 2    | -       | 4/9/10/10   | -       |
| 3   | ANP  | B     | 6002 | 2    | 2/2/7/8 | 8/18/38/38  | 0/3/3/3 |
| 4   | MSL  | C     | 5004 | 2    | -       | 4/9/10/10   | -       |
| 4   | MSL  | C     | 5001 | 2    | -       | 5/9/10/10   | -       |
| 3   | ANP  | F     | 6006 | 2    | 2/2/7/8 | 6/18/38/38  | 0/3/3/3 |
| 4   | MSL  | C     | 5008 | 2    | -       | 6/9/10/10   | -       |
| 3   | ANP  | G     | 6007 | 2    | 2/2/7/8 | 8/18/38/38  | 0/3/3/3 |
| 3   | ANP  | J     | 6010 | 2    | 2/2/7/8 | 12/18/38/38 | 0/3/3/3 |
| 4   | MSL  | C     | 5009 | 2    | -       | 6/9/10/10   | -       |
| 3   | ANP  | A     | 6001 | 2    | 2/2/7/8 | 10/18/38/38 | 0/3/3/3 |
| 4   | MSL  | C     | 5002 | 2    | -       | 9/9/10/10   | -       |
| 4   | MSL  | C     | 5003 | 2    | -       | 9/9/10/10   | -       |
| 3   | ANP  | C     | 6003 | 2    | 2/2/7/8 | 11/18/38/38 | 0/3/3/3 |
| 3   | ANP  | I     | 6009 | 2    | 2/2/7/8 | 11/18/38/38 | 0/3/3/3 |
| 3   | ANP  | E     | 6005 | 2    | 2/2/7/8 | 10/18/38/38 | 0/3/3/3 |
| 3   | ANP  | H     | 6008 | 2    | 2/2/7/8 | 10/18/38/38 | 0/3/3/3 |
| 3   | ANP  | D     | 6004 | 2    | 2/2/7/8 | 8/18/38/38  | 0/3/3/3 |

All (143) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | E     | 6005 | ANP  | PA-O3A  | 10.57 | 1.70        | 1.59     |
| 3   | F     | 6006 | ANP  | PA-O3A  | 10.12 | 1.70        | 1.59     |
| 3   | D     | 6004 | ANP  | PA-O3A  | 8.89  | 1.69        | 1.59     |
| 3   | D     | 6004 | ANP  | PB-O3A  | 8.38  | 1.69        | 1.59     |
| 3   | E     | 6005 | ANP  | PB-O3A  | 7.62  | 1.68        | 1.59     |
| 3   | F     | 6006 | ANP  | PB-O3A  | 6.96  | 1.67        | 1.59     |
| 3   | H     | 6008 | ANP  | C5'-C4' | -6.47 | 1.32        | 1.51     |
| 3   | F     | 6006 | ANP  | C5'-C4' | -6.26 | 1.32        | 1.51     |
| 3   | G     | 6007 | ANP  | C5'-C4' | -6.23 | 1.32        | 1.51     |
| 3   | F     | 6006 | ANP  | PG-O2G  | 6.18  | 1.73        | 1.56     |
| 3   | A     | 6001 | ANP  | C5'-C4' | -6.17 | 1.33        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | D     | 6004 | ANP  | C5'-C4' | -6.16 | 1.33        | 1.51     |
| 3   | I     | 6009 | ANP  | C5'-C4' | -6.01 | 1.33        | 1.51     |
| 3   | E     | 6005 | ANP  | C5'-C4' | -5.99 | 1.33        | 1.51     |
| 3   | B     | 6002 | ANP  | C5'-C4' | -5.57 | 1.34        | 1.51     |
| 3   | J     | 6010 | ANP  | PG-N3B  | 5.52  | 1.77        | 1.63     |
| 3   | J     | 6010 | ANP  | C5'-C4' | -5.36 | 1.35        | 1.51     |
| 3   | C     | 6003 | ANP  | C5'-C4' | -5.30 | 1.35        | 1.51     |
| 3   | G     | 6007 | ANP  | O2'-C2' | 5.16  | 1.55        | 1.43     |
| 3   | B     | 6002 | ANP  | C4-N3   | 5.13  | 1.44        | 1.34     |
| 3   | B     | 6002 | ANP  | O2'-C2' | 5.05  | 1.55        | 1.43     |
| 3   | C     | 6003 | ANP  | C4-N3   | 4.99  | 1.43        | 1.34     |
| 3   | C     | 6003 | ANP  | C1'-N9  | -4.90 | 1.32        | 1.46     |
| 3   | I     | 6009 | ANP  | O2'-C2' | 4.89  | 1.55        | 1.43     |
| 3   | A     | 6001 | ANP  | C1'-N9  | -4.89 | 1.32        | 1.46     |
| 3   | D     | 6004 | ANP  | C1'-N9  | -4.82 | 1.33        | 1.46     |
| 3   | E     | 6005 | ANP  | C1'-N9  | -4.80 | 1.33        | 1.46     |
| 3   | B     | 6002 | ANP  | C1'-N9  | -4.79 | 1.33        | 1.46     |
| 3   | J     | 6010 | ANP  | C2-N1   | 4.77  | 1.42        | 1.33     |
| 3   | G     | 6007 | ANP  | PB-O2B  | -4.68 | 1.44        | 1.56     |
| 3   | J     | 6010 | ANP  | C1'-N9  | -4.68 | 1.33        | 1.46     |
| 3   | I     | 6009 | ANP  | C1'-N9  | -4.67 | 1.33        | 1.46     |
| 3   | H     | 6008 | ANP  | C1'-N9  | -4.65 | 1.33        | 1.46     |
| 3   | A     | 6001 | ANP  | O2'-C2' | 4.63  | 1.54        | 1.43     |
| 3   | C     | 6003 | ANP  | O2'-C2' | 4.62  | 1.54        | 1.43     |
| 3   | B     | 6002 | ANP  | PB-O2B  | -4.61 | 1.44        | 1.56     |
| 3   | G     | 6007 | ANP  | C1'-N9  | -4.60 | 1.33        | 1.46     |
| 3   | E     | 6005 | ANP  | O2'-C2' | 4.59  | 1.54        | 1.43     |
| 3   | D     | 6004 | ANP  | O2'-C2' | 4.53  | 1.54        | 1.43     |
| 3   | H     | 6008 | ANP  | O2'-C2' | 4.48  | 1.54        | 1.43     |
| 3   | F     | 6006 | ANP  | O2'-C2' | 4.48  | 1.54        | 1.43     |
| 3   | D     | 6004 | ANP  | C4-N3   | 4.44  | 1.42        | 1.34     |
| 3   | J     | 6010 | ANP  | O2'-C2' | 4.43  | 1.53        | 1.43     |
| 3   | I     | 6009 | ANP  | C4-N3   | 4.42  | 1.42        | 1.34     |
| 3   | C     | 6003 | ANP  | C2-N1   | 4.41  | 1.41        | 1.33     |
| 3   | F     | 6006 | ANP  | C4-N3   | 4.40  | 1.42        | 1.34     |
| 3   | F     | 6006 | ANP  | C1'-N9  | -4.23 | 1.34        | 1.46     |
| 3   | J     | 6010 | ANP  | C4-N3   | 4.21  | 1.42        | 1.34     |
| 3   | H     | 6008 | ANP  | PG-O3G  | -4.20 | 1.45        | 1.56     |
| 3   | D     | 6004 | ANP  | C2-N1   | 4.18  | 1.41        | 1.33     |
| 3   | H     | 6008 | ANP  | PB-O2B  | -4.06 | 1.46        | 1.56     |
| 3   | I     | 6009 | ANP  | C2-N1   | 4.05  | 1.41        | 1.33     |
| 3   | G     | 6007 | ANP  | C2-N1   | 4.05  | 1.41        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | H     | 6008 | ANP  | C2-N1   | 4.04  | 1.41        | 1.33     |
| 3   | A     | 6001 | ANP  | C2-N1   | 3.99  | 1.41        | 1.33     |
| 3   | B     | 6002 | ANP  | C2-N1   | 3.94  | 1.40        | 1.33     |
| 3   | A     | 6001 | ANP  | C4-N3   | 3.93  | 1.41        | 1.34     |
| 3   | E     | 6005 | ANP  | C2-N1   | 3.85  | 1.40        | 1.33     |
| 3   | E     | 6005 | ANP  | C4-N3   | 3.83  | 1.41        | 1.34     |
| 3   | E     | 6005 | ANP  | PG-N3B  | 3.83  | 1.73        | 1.63     |
| 3   | C     | 6003 | ANP  | PB-O2B  | -3.79 | 1.46        | 1.56     |
| 3   | B     | 6002 | ANP  | PB-O3A  | 3.72  | 1.63        | 1.59     |
| 3   | F     | 6006 | ANP  | C2-N1   | 3.70  | 1.40        | 1.33     |
| 3   | B     | 6002 | ANP  | PA-O3A  | 3.61  | 1.63        | 1.59     |
| 3   | A     | 6001 | ANP  | PB-O2B  | -3.58 | 1.47        | 1.56     |
| 3   | G     | 6007 | ANP  | C4-N3   | 3.47  | 1.40        | 1.34     |
| 3   | C     | 6003 | ANP  | PA-O3A  | 3.32  | 1.63        | 1.59     |
| 3   | E     | 6005 | ANP  | PG-O1G  | 3.32  | 1.51        | 1.46     |
| 3   | A     | 6001 | ANP  | PA-O3A  | 3.25  | 1.63        | 1.59     |
| 3   | J     | 6010 | ANP  | PB-O2B  | -3.24 | 1.48        | 1.56     |
| 3   | H     | 6008 | ANP  | PG-N3B  | 3.23  | 1.71        | 1.63     |
| 3   | A     | 6001 | ANP  | PG-O1G  | 3.22  | 1.51        | 1.46     |
| 3   | D     | 6004 | ANP  | PB-O1B  | 3.21  | 1.51        | 1.46     |
| 3   | I     | 6009 | ANP  | PB-O1B  | 3.19  | 1.51        | 1.46     |
| 3   | I     | 6009 | ANP  | PB-O2B  | -3.18 | 1.48        | 1.56     |
| 3   | D     | 6004 | ANP  | PG-N3B  | 3.17  | 1.71        | 1.63     |
| 4   | C     | 5006 | MSL  | CB-CG   | 3.10  | 1.55        | 1.52     |
| 4   | C     | 5001 | MSL  | CB-CG   | 3.07  | 1.55        | 1.52     |
| 3   | B     | 6002 | ANP  | PG-N3B  | 3.01  | 1.71        | 1.63     |
| 3   | E     | 6005 | ANP  | PB-O2B  | -3.00 | 1.48        | 1.56     |
| 3   | I     | 6009 | ANP  | C5-N7   | -2.99 | 1.33        | 1.39     |
| 3   | C     | 6003 | ANP  | O5'-C5' | 2.95  | 1.55        | 1.44     |
| 3   | B     | 6002 | ANP  | O5'-C5' | 2.91  | 1.55        | 1.44     |
| 3   | H     | 6008 | ANP  | O5'-C5' | 2.88  | 1.55        | 1.44     |
| 3   | J     | 6010 | ANP  | PA-O3A  | 2.85  | 1.62        | 1.59     |
| 3   | H     | 6008 | ANP  | C4-N3   | 2.84  | 1.39        | 1.34     |
| 3   | G     | 6007 | ANP  | PA-O3A  | 2.84  | 1.62        | 1.59     |
| 3   | J     | 6010 | ANP  | O5'-C5' | 2.80  | 1.55        | 1.44     |
| 3   | A     | 6001 | ANP  | PG-N3B  | 2.76  | 1.70        | 1.63     |
| 3   | E     | 6005 | ANP  | PG-O3G  | -2.76 | 1.49        | 1.56     |
| 3   | B     | 6002 | ANP  | PG-O3G  | -2.76 | 1.49        | 1.56     |
| 3   | I     | 6009 | ANP  | PG-N3B  | 2.74  | 1.70        | 1.63     |
| 3   | A     | 6001 | ANP  | C5-N7   | -2.71 | 1.34        | 1.39     |
| 3   | I     | 6009 | ANP  | C2'-C3' | 2.71  | 1.60        | 1.53     |
| 3   | C     | 6003 | ANP  | PA-O5'  | 2.69  | 1.69        | 1.59     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | H     | 6008 | ANP  | PB-O1B  | 2.67  | 1.50        | 1.46     |
| 3   | J     | 6010 | ANP  | PA-O5'  | 2.63  | 1.69        | 1.59     |
| 3   | I     | 6009 | ANP  | PA-O3A  | 2.58  | 1.62        | 1.59     |
| 3   | I     | 6009 | ANP  | PG-O1G  | 2.55  | 1.50        | 1.46     |
| 3   | F     | 6006 | ANP  | PB-O2B  | -2.54 | 1.50        | 1.56     |
| 3   | B     | 6002 | ANP  | PB-O1B  | 2.54  | 1.50        | 1.46     |
| 3   | J     | 6010 | ANP  | C2'-C3' | 2.52  | 1.60        | 1.53     |
| 3   | F     | 6006 | ANP  | PA-O1A  | 2.47  | 1.59        | 1.50     |
| 3   | A     | 6001 | ANP  | PB-N3B  | -2.47 | 1.56        | 1.63     |
| 3   | D     | 6004 | ANP  | O5'-C5' | 2.41  | 1.53        | 1.44     |
| 3   | F     | 6006 | ANP  | PG-O3G  | 2.40  | 1.63        | 1.56     |
| 3   | A     | 6001 | ANP  | O5'-C5' | 2.39  | 1.53        | 1.44     |
| 3   | C     | 6003 | ANP  | PG-N3B  | 2.39  | 1.69        | 1.63     |
| 3   | H     | 6008 | ANP  | O3'-C3' | -2.38 | 1.37        | 1.43     |
| 3   | F     | 6006 | ANP  | O5'-C5' | 2.38  | 1.53        | 1.44     |
| 3   | G     | 6007 | ANP  | C5-N7   | -2.36 | 1.34        | 1.39     |
| 3   | G     | 6007 | ANP  | PB-N3B  | -2.36 | 1.57        | 1.63     |
| 4   | C     | 5007 | MSL  | CB-CG   | 2.34  | 1.54        | 1.52     |
| 3   | J     | 6010 | ANP  | C5-N7   | -2.32 | 1.34        | 1.39     |
| 3   | G     | 6007 | ANP  | PG-N3B  | 2.31  | 1.69        | 1.63     |
| 3   | H     | 6008 | ANP  | PA-O5'  | 2.29  | 1.68        | 1.59     |
| 3   | E     | 6005 | ANP  | PB-O1B  | 2.29  | 1.49        | 1.46     |
| 3   | F     | 6006 | ANP  | C5-N7   | -2.27 | 1.34        | 1.39     |
| 3   | H     | 6008 | ANP  | C2'-C3' | 2.26  | 1.59        | 1.53     |
| 3   | D     | 6004 | ANP  | PG-O3G  | -2.25 | 1.50        | 1.56     |
| 3   | A     | 6001 | ANP  | C8-N7   | -2.22 | 1.27        | 1.31     |
| 3   | C     | 6003 | ANP  | C5-N7   | -2.19 | 1.35        | 1.39     |
| 4   | C     | 5010 | MSL  | CB-CA   | 2.18  | 1.57        | 1.53     |
| 3   | J     | 6010 | ANP  | C6-N1   | 2.17  | 1.41        | 1.35     |
| 3   | G     | 6007 | ANP  | C2'-C3' | 2.16  | 1.59        | 1.53     |
| 3   | H     | 6008 | ANP  | PA-O3A  | 2.15  | 1.61        | 1.59     |
| 3   | G     | 6007 | ANP  | PG-O3G  | -2.15 | 1.51        | 1.56     |
| 3   | J     | 6010 | ANP  | C5-C4   | 2.14  | 1.42        | 1.39     |
| 3   | B     | 6002 | ANP  | C6-N1   | 2.14  | 1.41        | 1.35     |
| 3   | E     | 6005 | ANP  | C8-N7   | -2.10 | 1.27        | 1.31     |
| 3   | I     | 6009 | ANP  | O5'-C5' | 2.09  | 1.52        | 1.44     |
| 3   | E     | 6005 | ANP  | C2'-C3' | 2.07  | 1.59        | 1.53     |
| 3   | D     | 6004 | ANP  | C6-N1   | 2.06  | 1.41        | 1.35     |
| 4   | C     | 5010 | MSL  | O-C     | 2.06  | 1.28        | 1.22     |
| 3   | E     | 6005 | ANP  | O5'-C5' | 2.05  | 1.52        | 1.44     |
| 3   | A     | 6001 | ANP  | O3'-C3' | -2.05 | 1.37        | 1.43     |
| 3   | I     | 6009 | ANP  | C8-N7   | -2.05 | 1.27        | 1.31     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | G     | 6007 | ANP  | O5'-C5' | 2.05  | 1.52        | 1.44     |
| 3   | B     | 6002 | ANP  | O3'-C3' | -2.04 | 1.37        | 1.43     |
| 3   | A     | 6001 | ANP  | PA-O2A  | -2.03 | 1.45        | 1.55     |
| 4   | C     | 5006 | MSL  | CE-SD   | -2.03 | 1.65        | 1.75     |
| 3   | C     | 6003 | ANP  | C6-N1   | 2.02  | 1.41        | 1.35     |
| 3   | F     | 6006 | ANP  | PA-O5'  | 2.02  | 1.67        | 1.59     |

All (221) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 3   | E     | 6005 | ANP  | C2'-C3'-C4' | -11.86 | 79.70       | 102.61   |
| 3   | H     | 6008 | ANP  | C2'-C3'-C4' | -11.38 | 80.62       | 102.61   |
| 3   | B     | 6002 | ANP  | O4'-C1'-N9  | 11.30  | 129.79      | 108.09   |
| 3   | J     | 6010 | ANP  | O4'-C1'-N9  | 11.21  | 129.61      | 108.09   |
| 3   | C     | 6003 | ANP  | C2'-C3'-C4' | -11.09 | 81.18       | 102.61   |
| 3   | C     | 6003 | ANP  | O4'-C1'-N9  | 10.71  | 128.66      | 108.09   |
| 3   | J     | 6010 | ANP  | C2'-C3'-C4' | -10.57 | 82.19       | 102.61   |
| 3   | H     | 6008 | ANP  | O4'-C1'-N9  | 10.28  | 127.83      | 108.09   |
| 3   | D     | 6004 | ANP  | C2'-C3'-C4' | -10.26 | 82.79       | 102.61   |
| 3   | E     | 6005 | ANP  | O4'-C1'-N9  | 9.96   | 127.22      | 108.09   |
| 3   | A     | 6001 | ANP  | O4'-C1'-N9  | 9.94   | 127.18      | 108.09   |
| 3   | B     | 6002 | ANP  | C2'-C3'-C4' | -9.34  | 84.57       | 102.61   |
| 3   | F     | 6006 | ANP  | C2'-C3'-C4' | -9.06  | 85.11       | 102.61   |
| 3   | I     | 6009 | ANP  | C2'-C3'-C4' | -8.85  | 85.51       | 102.61   |
| 3   | E     | 6005 | ANP  | O1G-PG-N3B  | 8.78   | 124.69      | 111.77   |
| 3   | F     | 6006 | ANP  | O4'-C1'-N9  | 8.68   | 124.75      | 108.09   |
| 3   | G     | 6007 | ANP  | O4'-C1'-N9  | 8.55   | 124.51      | 108.09   |
| 3   | D     | 6004 | ANP  | O4'-C1'-N9  | 8.49   | 124.39      | 108.09   |
| 3   | A     | 6001 | ANP  | C2'-C3'-C4' | -8.43  | 86.32       | 102.61   |
| 3   | I     | 6009 | ANP  | O4'-C1'-N9  | 7.88   | 123.22      | 108.09   |
| 3   | B     | 6002 | ANP  | C4'-O4'-C1' | -7.83  | 92.17       | 109.47   |
| 3   | G     | 6007 | ANP  | C2'-C3'-C4' | -7.49  | 88.14       | 102.61   |
| 3   | E     | 6005 | ANP  | C4'-O4'-C1' | -7.45  | 93.02       | 109.47   |
| 3   | D     | 6004 | ANP  | C4'-O4'-C1' | -7.06  | 93.87       | 109.47   |
| 3   | H     | 6008 | ANP  | C4'-O4'-C1' | -6.98  | 94.06       | 109.47   |
| 3   | C     | 6003 | ANP  | C4'-O4'-C1' | -6.96  | 94.10       | 109.47   |
| 4   | C     | 5007 | MSL  | OE-SD-CE    | -6.90  | 97.94       | 109.10   |
| 3   | H     | 6008 | ANP  | O2'-C2'-C3' | -6.65  | 90.51       | 111.82   |
| 3   | A     | 6001 | ANP  | C4'-O4'-C1' | -6.54  | 95.02       | 109.47   |
| 3   | F     | 6006 | ANP  | C5'-C4'-C3' | 6.53   | 138.70      | 115.21   |
| 3   | I     | 6009 | ANP  | C2'-C1'-N9  | 6.35   | 129.08      | 113.30   |
| 3   | J     | 6010 | ANP  | C5'-C4'-C3' | 6.27   | 137.77      | 115.21   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | H     | 6008 | ANP  | O2B-PB-O3A  | -6.26 | 83.74       | 104.64   |
| 3   | I     | 6009 | ANP  | C5'-C4'-C3' | 5.89  | 136.41      | 115.21   |
| 3   | D     | 6004 | ANP  | C5'-C4'-C3' | 5.88  | 136.39      | 115.21   |
| 3   | C     | 6003 | ANP  | C5'-C4'-C3' | 5.78  | 136.02      | 115.21   |
| 3   | E     | 6005 | ANP  | C5'-C4'-C3' | 5.73  | 135.84      | 115.21   |
| 3   | G     | 6007 | ANP  | C5'-C4'-C3' | 5.60  | 135.36      | 115.21   |
| 3   | D     | 6004 | ANP  | C2'-C1'-N9  | 5.57  | 127.15      | 113.30   |
| 3   | B     | 6002 | ANP  | O2'-C2'-C3' | -5.56 | 93.98       | 111.82   |
| 3   | F     | 6006 | ANP  | C2'-C1'-N9  | 5.53  | 127.04      | 113.30   |
| 3   | H     | 6008 | ANP  | C2'-C1'-N9  | 5.34  | 126.57      | 113.30   |
| 3   | J     | 6010 | ANP  | C4'-O4'-C1' | -5.34 | 97.68       | 109.47   |
| 3   | G     | 6007 | ANP  | C4'-O4'-C1' | -5.30 | 97.76       | 109.47   |
| 3   | E     | 6005 | ANP  | O2'-C2'-C3' | -5.25 | 95.00       | 111.82   |
| 3   | G     | 6007 | ANP  | C2'-C1'-N9  | 5.11  | 125.99      | 113.30   |
| 3   | I     | 6009 | ANP  | O3A-PB-N3B  | 5.10  | 120.75      | 106.59   |
| 3   | A     | 6001 | ANP  | C5'-C4'-C3' | 5.08  | 133.49      | 115.21   |
| 3   | G     | 6007 | ANP  | O1G-PG-N3B  | 5.07  | 119.23      | 111.77   |
| 3   | H     | 6008 | ANP  | C5'-C4'-C3' | 5.03  | 133.33      | 115.21   |
| 3   | H     | 6008 | ANP  | O4'-C4'-C5' | 5.03  | 125.43      | 109.33   |
| 3   | B     | 6002 | ANP  | C5'-C4'-C3' | 4.96  | 133.06      | 115.21   |
| 3   | F     | 6006 | ANP  | O1G-PG-N3B  | 4.95  | 119.06      | 111.77   |
| 3   | I     | 6009 | ANP  | C4'-O4'-C1' | -4.95 | 98.53       | 109.47   |
| 3   | F     | 6006 | ANP  | C4'-O4'-C1' | -4.88 | 98.69       | 109.47   |
| 3   | D     | 6004 | ANP  | O1B-PB-N3B  | -4.85 | 104.62      | 111.77   |
| 4   | C     | 5003 | MSL  | OE-SD-CE    | -4.84 | 101.27      | 109.10   |
| 3   | A     | 6001 | ANP  | O2'-C2'-C3' | -4.82 | 96.37       | 111.82   |
| 3   | H     | 6008 | ANP  | C5-C6-N6    | 4.78  | 135.11      | 123.29   |
| 3   | C     | 6003 | ANP  | O2'-C2'-C3' | -4.74 | 96.64       | 111.82   |
| 3   | D     | 6004 | ANP  | O3A-PB-N3B  | 4.73  | 119.70      | 106.59   |
| 3   | H     | 6008 | ANP  | N6-C6-N1    | -4.70 | 107.90      | 118.38   |
| 3   | E     | 6005 | ANP  | C2'-C1'-N9  | 4.70  | 124.99      | 113.30   |
| 3   | I     | 6009 | ANP  | O2B-PB-O1B  | 4.65  | 119.84      | 109.87   |
| 3   | H     | 6008 | ANP  | O3A-PB-N3B  | 4.61  | 119.39      | 106.59   |
| 3   | C     | 6003 | ANP  | O4'-C4'-C5' | 4.52  | 123.83      | 109.33   |
| 3   | B     | 6002 | ANP  | O4'-C4'-C5' | 4.46  | 123.61      | 109.33   |
| 3   | C     | 6003 | ANP  | O1G-PG-N3B  | 4.44  | 118.31      | 111.77   |
| 3   | B     | 6002 | ANP  | O5'-PA-O1A  | -4.36 | 91.64       | 108.94   |
| 3   | J     | 6010 | ANP  | N9-C8-N7    | 4.34  | 120.10      | 113.94   |
| 3   | J     | 6010 | ANP  | C2'-C1'-N9  | 4.29  | 123.96      | 113.30   |
| 3   | J     | 6010 | ANP  | C4-N9-C8    | -4.26 | 101.26      | 105.74   |
| 3   | D     | 6004 | ANP  | O2'-C2'-C3' | -4.26 | 98.16       | 111.82   |
| 3   | B     | 6002 | ANP  | O3A-PB-N3B  | 4.22  | 118.30      | 106.59   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | G     | 6007 | ANP  | O2'-C2'-C3' | -4.18 | 98.42       | 111.82   |
| 3   | A     | 6001 | ANP  | O1B-PB-N3B  | -4.16 | 105.64      | 111.77   |
| 3   | D     | 6004 | ANP  | O4'-C4'-C5' | 4.11  | 122.50      | 109.33   |
| 3   | H     | 6008 | ANP  | O3G-PG-O1G  | -4.10 | 103.17      | 113.45   |
| 3   | C     | 6003 | ANP  | C2'-C1'-N9  | 4.07  | 123.42      | 113.30   |
| 3   | A     | 6001 | ANP  | O4'-C4'-C5' | 4.04  | 122.27      | 109.33   |
| 3   | C     | 6003 | ANP  | O2B-PB-O1B  | 4.03  | 118.51      | 109.87   |
| 3   | A     | 6001 | ANP  | C2'-C1'-N9  | 4.01  | 123.27      | 113.30   |
| 3   | J     | 6010 | ANP  | O4'-C4'-C5' | 4.00  | 122.14      | 109.33   |
| 3   | C     | 6003 | ANP  | C4-N9-C8    | -4.00 | 101.54      | 105.74   |
| 3   | G     | 6007 | ANP  | C4-N9-C8    | -3.98 | 101.56      | 105.74   |
| 3   | E     | 6005 | ANP  | O4'-C4'-C5' | 3.91  | 121.86      | 109.33   |
| 3   | C     | 6003 | ANP  | O3'-C3'-C4' | 3.91  | 122.31      | 111.08   |
| 3   | I     | 6009 | ANP  | O4'-C4'-C5' | 3.90  | 121.84      | 109.33   |
| 3   | F     | 6006 | ANP  | C4-N9-C8    | -3.87 | 101.67      | 105.74   |
| 3   | I     | 6009 | ANP  | O1G-PG-N3B  | 3.85  | 117.43      | 111.77   |
| 3   | G     | 6007 | ANP  | N9-C8-N7    | 3.79  | 119.31      | 113.94   |
| 3   | H     | 6008 | ANP  | C4-N9-C8    | -3.75 | 101.80      | 105.74   |
| 3   | C     | 6003 | ANP  | N9-C8-N7    | 3.73  | 119.22      | 113.94   |
| 3   | J     | 6010 | ANP  | O2B-PB-O1B  | 3.72  | 117.85      | 109.87   |
| 3   | F     | 6006 | ANP  | N9-C8-N7    | 3.61  | 119.06      | 113.94   |
| 4   | C     | 5004 | MSL  | OE-SD-CE    | -3.60 | 103.27      | 109.10   |
| 3   | B     | 6002 | ANP  | O3'-C3'-C4' | 3.60  | 121.41      | 111.08   |
| 3   | J     | 6010 | ANP  | O3'-C3'-C4' | 3.60  | 121.41      | 111.08   |
| 4   | C     | 5003 | MSL  | CE-SD-CG    | 3.59  | 117.21      | 105.22   |
| 3   | I     | 6009 | ANP  | O2'-C2'-C3' | -3.58 | 100.34      | 111.82   |
| 3   | F     | 6006 | ANP  | O3'-C3'-C4' | 3.58  | 121.36      | 111.08   |
| 3   | J     | 6010 | ANP  | O3A-PB-N3B  | 3.57  | 116.50      | 106.59   |
| 3   | I     | 6009 | ANP  | C4-N9-C8    | -3.57 | 101.99      | 105.74   |
| 3   | A     | 6001 | ANP  | C4-N9-C8    | -3.56 | 102.00      | 105.74   |
| 3   | A     | 6001 | ANP  | O5'-PA-O1A  | -3.52 | 95.00       | 108.94   |
| 3   | E     | 6005 | ANP  | O3'-C3'-C4' | 3.51  | 121.16      | 111.08   |
| 3   | A     | 6001 | ANP  | N9-C8-N7    | 3.50  | 118.91      | 113.94   |
| 3   | H     | 6008 | ANP  | O2B-PB-O1B  | 3.47  | 117.31      | 109.87   |
| 3   | G     | 6007 | ANP  | O4'-C4'-C5' | 3.45  | 120.38      | 109.33   |
| 3   | I     | 6009 | ANP  | N9-C8-N7    | 3.41  | 118.78      | 113.94   |
| 3   | F     | 6006 | ANP  | O2'-C2'-C3' | -3.40 | 100.93      | 111.82   |
| 3   | F     | 6006 | ANP  | O2A-PA-O3A  | 3.34  | 116.29      | 107.27   |
| 3   | J     | 6010 | ANP  | O2'-C2'-C3' | -3.33 | 101.14      | 111.82   |
| 3   | G     | 6007 | ANP  | O3'-C3'-C4' | 3.31  | 120.58      | 111.08   |
| 3   | H     | 6008 | ANP  | N9-C8-N7    | 3.26  | 118.57      | 113.94   |
| 3   | F     | 6006 | ANP  | O1B-PB-N3B  | -3.24 | 106.99      | 111.77   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | E     | 6005 | ANP  | O5'-PA-O1A  | -3.23 | 96.15       | 108.94   |
| 3   | J     | 6010 | ANP  | O3G-PG-O1G  | -3.22 | 105.38      | 113.45   |
| 3   | C     | 6003 | ANP  | O2G-PG-O1G  | -3.22 | 105.38      | 113.45   |
| 3   | G     | 6007 | ANP  | O2B-PB-O3A  | -3.20 | 93.95       | 104.64   |
| 3   | J     | 6010 | ANP  | O5'-PA-O1A  | -3.15 | 96.45       | 108.94   |
| 3   | B     | 6002 | ANP  | O2B-PB-O1B  | 3.13  | 116.59      | 109.87   |
| 4   | C     | 5007 | MSL  | CE-SD-CG    | 3.13  | 115.67      | 105.22   |
| 3   | D     | 6004 | ANP  | N9-C8-N7    | 3.13  | 118.38      | 113.94   |
| 4   | C     | 5005 | MSL  | CE-SD-CG    | 3.11  | 115.59      | 105.22   |
| 3   | J     | 6010 | ANP  | C6-C5-N7    | -3.11 | 126.10      | 132.09   |
| 3   | F     | 6006 | ANP  | O5'-PA-O1A  | -3.09 | 96.67       | 108.94   |
| 3   | B     | 6002 | ANP  | C4-N9-C1'   | 3.03  | 133.72      | 126.63   |
| 3   | G     | 6007 | ANP  | O3G-PG-O1G  | -3.02 | 105.87      | 113.45   |
| 3   | D     | 6004 | ANP  | C4-N9-C8    | -3.01 | 102.58      | 105.74   |
| 3   | E     | 6005 | ANP  | N9-C8-N7    | 2.99  | 118.17      | 113.94   |
| 3   | J     | 6010 | ANP  | O4'-C4'-C3' | -2.96 | 99.27       | 105.15   |
| 3   | D     | 6004 | ANP  | O5'-PA-O1A  | -2.95 | 97.24       | 108.94   |
| 3   | C     | 6003 | ANP  | O4'-C4'-C3' | -2.95 | 99.30       | 105.15   |
| 3   | C     | 6003 | ANP  | C4-N9-C1'   | 2.95  | 133.53      | 126.63   |
| 3   | G     | 6007 | ANP  | C5-C6-N6    | 2.94  | 130.56      | 123.29   |
| 3   | A     | 6001 | ANP  | O3A-PB-N3B  | 2.87  | 114.56      | 106.59   |
| 3   | A     | 6001 | ANP  | C6-C5-N7    | -2.86 | 126.57      | 132.09   |
| 3   | H     | 6008 | ANP  | O3'-C3'-C4' | 2.86  | 119.30      | 111.08   |
| 3   | D     | 6004 | ANP  | O1G-PG-N3B  | 2.86  | 115.98      | 111.77   |
| 3   | E     | 6005 | ANP  | C4-N9-C8    | -2.86 | 102.74      | 105.74   |
| 3   | B     | 6002 | ANP  | N9-C8-N7    | 2.85  | 117.99      | 113.94   |
| 3   | J     | 6010 | ANP  | C4-N9-C1'   | 2.85  | 133.30      | 126.63   |
| 4   | C     | 5009 | MSL  | OE-SD-CE    | -2.84 | 104.50      | 109.10   |
| 3   | H     | 6008 | ANP  | O2G-PG-O1G  | 2.83  | 120.55      | 113.45   |
| 3   | F     | 6006 | ANP  | O2B-PB-O1B  | 2.83  | 115.94      | 109.87   |
| 3   | G     | 6007 | ANP  | C6-C5-N7    | -2.83 | 126.64      | 132.09   |
| 3   | D     | 6004 | ANP  | O3'-C3'-C4' | 2.81  | 119.14      | 111.08   |
| 3   | E     | 6005 | ANP  | O1B-PB-N3B  | -2.80 | 107.64      | 111.77   |
| 3   | D     | 6004 | ANP  | O2A-PA-O3A  | 2.80  | 114.85      | 107.27   |
| 3   | B     | 6002 | ANP  | O3G-PG-O1G  | -2.80 | 106.44      | 113.45   |
| 3   | I     | 6009 | ANP  | O3'-C3'-C2' | 2.79  | 120.76      | 111.82   |
| 3   | J     | 6010 | ANP  | O2B-PB-O3A  | -2.78 | 95.38       | 104.64   |
| 3   | B     | 6002 | ANP  | C4-N9-C8    | -2.77 | 102.83      | 105.74   |
| 4   | C     | 5003 | MSL  | OXT-C-O     | -2.76 | 117.82      | 124.08   |
| 3   | E     | 6005 | ANP  | O3A-PB-N3B  | 2.72  | 114.14      | 106.59   |
| 3   | H     | 6008 | ANP  | O4'-C4'-C3' | -2.72 | 99.75       | 105.15   |
| 3   | I     | 6009 | ANP  | C6-C5-N7    | -2.71 | 126.87      | 132.09   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | D     | 6004 | ANP  | C5-C6-N6    | 2.70  | 129.97      | 123.29   |
| 3   | A     | 6001 | ANP  | O3'-C3'-C4' | 2.69  | 118.80      | 111.08   |
| 3   | I     | 6009 | ANP  | O1B-PB-N3B  | -2.67 | 107.84      | 111.77   |
| 3   | C     | 6003 | ANP  | N6-C6-N1    | -2.67 | 112.44      | 118.38   |
| 3   | J     | 6010 | ANP  | O1B-PB-N3B  | -2.62 | 107.92      | 111.77   |
| 3   | A     | 6001 | ANP  | C5-C6-N6    | 2.60  | 129.73      | 123.29   |
| 3   | B     | 6002 | ANP  | C6-C5-N7    | -2.60 | 127.08      | 132.09   |
| 3   | J     | 6010 | ANP  | C6-C5-C4    | 2.59  | 120.72      | 117.18   |
| 3   | F     | 6006 | ANP  | C6-C5-N7    | -2.55 | 127.17      | 132.09   |
| 3   | H     | 6008 | ANP  | O2'-C2'-C1' | -2.54 | 101.35      | 110.10   |
| 3   | C     | 6003 | ANP  | C5-C6-N6    | 2.54  | 129.57      | 123.29   |
| 3   | J     | 6010 | ANP  | C5-C6-N6    | 2.54  | 129.57      | 123.29   |
| 3   | B     | 6002 | ANP  | C4-C5-N7    | 2.51  | 113.46      | 110.58   |
| 3   | A     | 6001 | ANP  | O2B-PB-O1B  | 2.51  | 115.25      | 109.87   |
| 3   | F     | 6006 | ANP  | C4-C5-N7    | 2.50  | 113.44      | 110.58   |
| 3   | B     | 6002 | ANP  | C2'-C1'-N9  | 2.50  | 119.51      | 113.30   |
| 3   | E     | 6005 | ANP  | C5-C6-N6    | 2.48  | 129.43      | 123.29   |
| 3   | A     | 6001 | ANP  | C4-C5-N7    | 2.48  | 113.42      | 110.58   |
| 4   | C     | 5001 | MSL  | CB-CA-C     | 2.46  | 116.97      | 110.45   |
| 4   | C     | 5004 | MSL  | CE-SD-CG    | 2.45  | 113.41      | 105.22   |
| 3   | G     | 6007 | ANP  | C6-C5-C4    | 2.45  | 120.52      | 117.18   |
| 4   | C     | 5002 | MSL  | OXT-C-O     | -2.45 | 118.53      | 124.08   |
| 4   | C     | 5010 | MSL  | OXT-C-O     | -2.43 | 118.58      | 124.08   |
| 3   | D     | 6004 | ANP  | O4'-C4'-C3' | -2.42 | 100.35      | 105.15   |
| 3   | F     | 6006 | ANP  | C5-C6-N6    | 2.42  | 129.27      | 123.29   |
| 4   | C     | 5010 | MSL  | CB-CA-C     | 2.41  | 116.84      | 110.45   |
| 3   | E     | 6005 | ANP  | C6-C5-N7    | -2.39 | 127.49      | 132.09   |
| 3   | G     | 6007 | ANP  | O5'-PA-O1A  | -2.37 | 99.54       | 108.94   |
| 3   | A     | 6001 | ANP  | O1G-PG-N3B  | 2.37  | 115.25      | 111.77   |
| 3   | J     | 6010 | ANP  | O3'-C3'-C2' | 2.36  | 119.38      | 111.82   |
| 3   | I     | 6009 | ANP  | O3'-C3'-C4' | 2.35  | 117.84      | 111.08   |
| 3   | B     | 6002 | ANP  | O2B-PB-O3A  | -2.35 | 96.81       | 104.64   |
| 4   | C     | 5001 | MSL  | CE-SD-CG    | 2.32  | 112.97      | 105.22   |
| 3   | D     | 6004 | ANP  | O3G-PG-O1G  | -2.30 | 107.67      | 113.45   |
| 4   | C     | 5001 | MSL  | OXT-C-O     | -2.30 | 118.86      | 124.08   |
| 3   | D     | 6004 | ANP  | N6-C6-N1    | -2.30 | 113.25      | 118.38   |
| 3   | I     | 6009 | ANP  | C4-C5-N7    | 2.29  | 113.20      | 110.58   |
| 3   | B     | 6002 | ANP  | N3-C4-N9    | 2.28  | 131.05      | 127.17   |
| 3   | E     | 6005 | ANP  | O3G-PG-O1G  | -2.27 | 107.75      | 113.45   |
| 3   | J     | 6010 | ANP  | C4-C5-N7    | 2.27  | 113.18      | 110.58   |
| 3   | E     | 6005 | ANP  | O2G-PG-O3G  | -2.26 | 101.51      | 107.59   |
| 3   | F     | 6006 | ANP  | O4'-C4'-C5' | 2.25  | 116.56      | 109.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | E     | 6005 | ANP  | O2A-PA-O1A  | -2.25 | 101.99      | 112.44   |
| 3   | B     | 6002 | ANP  | PA-O5'-C5'  | 2.24  | 134.17      | 121.35   |
| 3   | I     | 6009 | ANP  | C5-C6-N6    | 2.23  | 128.81      | 123.29   |
| 4   | C     | 5006 | MSL  | OE-SD-CE    | -2.22 | 105.51      | 109.10   |
| 3   | E     | 6005 | ANP  | C4-C5-N7    | 2.20  | 113.09      | 110.58   |
| 3   | B     | 6002 | ANP  | O3'-C3'-C2' | 2.19  | 118.85      | 111.82   |
| 4   | C     | 5010 | MSL  | OE-SD-CE    | 2.16  | 112.60      | 109.10   |
| 3   | A     | 6001 | ANP  | O3'-C3'-C2' | 2.16  | 118.73      | 111.82   |
| 3   | F     | 6006 | ANP  | O3A-PB-N3B  | 2.15  | 112.56      | 106.59   |
| 3   | C     | 6003 | ANP  | C6-C5-N7    | -2.12 | 128.00      | 132.09   |
| 4   | C     | 5007 | MSL  | OXT-C-O     | -2.11 | 119.30      | 124.08   |
| 3   | A     | 6001 | ANP  | O2B-PB-O3A  | -2.10 | 97.62       | 104.64   |
| 4   | C     | 5002 | MSL  | CB-CA-C     | 2.09  | 116.00      | 110.45   |
| 3   | E     | 6005 | ANP  | O4'-C4'-C3' | -2.09 | 101.01      | 105.15   |
| 3   | A     | 6001 | ANP  | C6-C5-C4    | 2.08  | 120.02      | 117.18   |
| 3   | H     | 6008 | ANP  | N3-C2-N1    | 2.06  | 131.70      | 128.58   |
| 4   | C     | 5008 | MSL  | CE-SD-CG    | 2.06  | 112.09      | 105.22   |
| 3   | C     | 6003 | ANP  | C6-C5-C4    | 2.05  | 119.98      | 117.18   |
| 3   | I     | 6009 | ANP  | O4'-C4'-C3' | -2.05 | 101.09      | 105.15   |
| 3   | I     | 6009 | ANP  | C6-C5-C4    | 2.02  | 119.93      | 117.18   |
| 3   | D     | 6004 | ANP  | O3'-C3'-C2' | 2.01  | 118.26      | 111.82   |

All (20) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 3   | A     | 6001 | ANP  | C4'  |
| 3   | A     | 6001 | ANP  | C1'  |
| 3   | B     | 6002 | ANP  | C4'  |
| 3   | B     | 6002 | ANP  | C1'  |
| 3   | C     | 6003 | ANP  | C4'  |
| 3   | C     | 6003 | ANP  | C1'  |
| 3   | D     | 6004 | ANP  | C4'  |
| 3   | D     | 6004 | ANP  | C1'  |
| 3   | E     | 6005 | ANP  | C4'  |
| 3   | E     | 6005 | ANP  | C1'  |
| 3   | F     | 6006 | ANP  | C4'  |
| 3   | F     | 6006 | ANP  | C1'  |
| 3   | G     | 6007 | ANP  | C4'  |
| 3   | G     | 6007 | ANP  | C1'  |
| 3   | H     | 6008 | ANP  | C4'  |
| 3   | H     | 6008 | ANP  | C1'  |
| 3   | I     | 6009 | ANP  | C4'  |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 3   | I     | 6009 | ANP  | C1'  |
| 3   | J     | 6010 | ANP  | C4'  |
| 3   | J     | 6010 | ANP  | C1'  |

All (157) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 3   | A     | 6001 | ANP  | PG-N3B-PB-O1B  |
| 3   | A     | 6001 | ANP  | PG-N3B-PB-O3A  |
| 3   | A     | 6001 | ANP  | C5'-O5'-PA-O2A |
| 3   | A     | 6001 | ANP  | C5'-O5'-PA-O3A |
| 3   | A     | 6001 | ANP  | O4'-C1'-N9-C8  |
| 3   | A     | 6001 | ANP  | O4'-C1'-N9-C4  |
| 3   | A     | 6001 | ANP  | C2'-C1'-N9-C8  |
| 3   | A     | 6001 | ANP  | C2'-C1'-N9-C4  |
| 3   | B     | 6002 | ANP  | PB-N3B-PG-O1G  |
| 3   | B     | 6002 | ANP  | PG-N3B-PB-O1B  |
| 3   | B     | 6002 | ANP  | O4'-C1'-N9-C8  |
| 3   | B     | 6002 | ANP  | O4'-C1'-N9-C4  |
| 3   | B     | 6002 | ANP  | C2'-C1'-N9-C8  |
| 3   | C     | 6003 | ANP  | PB-N3B-PG-O1G  |
| 3   | C     | 6003 | ANP  | PG-N3B-PB-O1B  |
| 3   | C     | 6003 | ANP  | PG-N3B-PB-O3A  |
| 3   | C     | 6003 | ANP  | C5'-O5'-PA-O1A |
| 3   | C     | 6003 | ANP  | C5'-O5'-PA-O2A |
| 3   | C     | 6003 | ANP  | C5'-O5'-PA-O3A |
| 3   | C     | 6003 | ANP  | O4'-C1'-N9-C8  |
| 3   | C     | 6003 | ANP  | O4'-C1'-N9-C4  |
| 3   | C     | 6003 | ANP  | C2'-C1'-N9-C8  |
| 3   | C     | 6003 | ANP  | C2'-C1'-N9-C4  |
| 3   | D     | 6004 | ANP  | C5'-O5'-PA-O1A |
| 3   | D     | 6004 | ANP  | C5'-O5'-PA-O2A |
| 3   | D     | 6004 | ANP  | O4'-C1'-N9-C8  |
| 3   | D     | 6004 | ANP  | O4'-C1'-N9-C4  |
| 3   | D     | 6004 | ANP  | C2'-C1'-N9-C8  |
| 3   | D     | 6004 | ANP  | C2'-C1'-N9-C4  |
| 3   | E     | 6005 | ANP  | PG-N3B-PB-O1B  |
| 3   | E     | 6005 | ANP  | C5'-O5'-PA-O1A |
| 3   | E     | 6005 | ANP  | C5'-O5'-PA-O2A |
| 3   | E     | 6005 | ANP  | C5'-O5'-PA-O3A |
| 3   | E     | 6005 | ANP  | O4'-C1'-N9-C8  |
| 3   | E     | 6005 | ANP  | O4'-C1'-N9-C4  |

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| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 3   | E     | 6005 | ANP  | C2'-C1'-N9-C8  |
| 3   | E     | 6005 | ANP  | C2'-C1'-N9-C4  |
| 3   | F     | 6006 | ANP  | O4'-C1'-N9-C8  |
| 3   | F     | 6006 | ANP  | O4'-C1'-N9-C4  |
| 3   | F     | 6006 | ANP  | C2'-C1'-N9-C8  |
| 3   | F     | 6006 | ANP  | C2'-C1'-N9-C4  |
| 3   | G     | 6007 | ANP  | C5'-O5'-PA-O1A |
| 3   | G     | 6007 | ANP  | C5'-O5'-PA-O2A |
| 3   | G     | 6007 | ANP  | O4'-C1'-N9-C8  |
| 3   | G     | 6007 | ANP  | O4'-C1'-N9-C4  |
| 3   | G     | 6007 | ANP  | C2'-C1'-N9-C8  |
| 3   | G     | 6007 | ANP  | C2'-C1'-N9-C4  |
| 3   | H     | 6008 | ANP  | PB-N3B-PG-O1G  |
| 3   | H     | 6008 | ANP  | PG-N3B-PB-O1B  |
| 3   | H     | 6008 | ANP  | PG-N3B-PB-O3A  |
| 3   | H     | 6008 | ANP  | C5'-O5'-PA-O2A |
| 3   | H     | 6008 | ANP  | O4'-C1'-N9-C8  |
| 3   | H     | 6008 | ANP  | O4'-C1'-N9-C4  |
| 3   | H     | 6008 | ANP  | C2'-C1'-N9-C8  |
| 3   | I     | 6009 | ANP  | PB-N3B-PG-O1G  |
| 3   | I     | 6009 | ANP  | PG-N3B-PB-O1B  |
| 3   | I     | 6009 | ANP  | PG-N3B-PB-O3A  |
| 3   | I     | 6009 | ANP  | O4'-C1'-N9-C8  |
| 3   | I     | 6009 | ANP  | O4'-C1'-N9-C4  |
| 3   | I     | 6009 | ANP  | C2'-C1'-N9-C8  |
| 3   | I     | 6009 | ANP  | C2'-C1'-N9-C4  |
| 3   | J     | 6010 | ANP  | PB-N3B-PG-O1G  |
| 3   | J     | 6010 | ANP  | PG-N3B-PB-O1B  |
| 3   | J     | 6010 | ANP  | C5'-O5'-PA-O2A |
| 3   | J     | 6010 | ANP  | C5'-O5'-PA-O3A |
| 3   | J     | 6010 | ANP  | O4'-C1'-N9-C8  |
| 3   | J     | 6010 | ANP  | O4'-C1'-N9-C4  |
| 3   | J     | 6010 | ANP  | C2'-C1'-N9-C8  |
| 3   | J     | 6010 | ANP  | C2'-C1'-N9-C4  |
| 4   | C     | 5001 | MSL  | O-C-CA-N       |
| 4   | C     | 5002 | MSL  | O-C-CA-N       |
| 4   | C     | 5002 | MSL  | CB-CG-SD-OE    |
| 4   | C     | 5002 | MSL  | CB-CG-SD-CE    |
| 4   | C     | 5003 | MSL  | O-C-CA-N       |
| 4   | C     | 5003 | MSL  | C-CA-CB-CG     |
| 4   | C     | 5003 | MSL  | N-CA-CB-CG     |
| 4   | C     | 5003 | MSL  | CB-CG-SD-OE    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 4   | C     | 5003 | MSL  | CB-CG-SD-CE     |
| 4   | C     | 5004 | MSL  | O-C-CA-N        |
| 4   | C     | 5005 | MSL  | C-CA-CB-CG      |
| 4   | C     | 5005 | MSL  | CB-CG-SD-OE     |
| 4   | C     | 5005 | MSL  | CB-CG-SD-CE     |
| 4   | C     | 5006 | MSL  | O-C-CA-N        |
| 4   | C     | 5007 | MSL  | O-C-CA-N        |
| 4   | C     | 5007 | MSL  | CB-CG-SD-OE     |
| 4   | C     | 5007 | MSL  | CB-CG-SD-CE     |
| 4   | C     | 5008 | MSL  | O-C-CA-N        |
| 4   | C     | 5008 | MSL  | CB-CG-SD-OE     |
| 4   | C     | 5008 | MSL  | CB-CG-SD-CE     |
| 4   | C     | 5009 | MSL  | O-C-CA-N        |
| 4   | C     | 5009 | MSL  | CB-CG-SD-OE     |
| 4   | C     | 5009 | MSL  | CB-CG-SD-CE     |
| 4   | C     | 5010 | MSL  | N-CA-CB-CG      |
| 4   | C     | 5002 | MSL  | OXT-C-CA-N      |
| 4   | C     | 5007 | MSL  | OXT-C-CA-N      |
| 4   | C     | 5010 | MSL  | OXT-C-CA-N      |
| 3   | A     | 6001 | ANP  | C3'-C4'-C5'-O5' |
| 3   | B     | 6002 | ANP  | C3'-C4'-C5'-O5' |
| 3   | C     | 6003 | ANP  | C3'-C4'-C5'-O5' |
| 3   | D     | 6004 | ANP  | C3'-C4'-C5'-O5' |
| 3   | E     | 6005 | ANP  | C3'-C4'-C5'-O5' |
| 3   | F     | 6006 | ANP  | C3'-C4'-C5'-O5' |
| 3   | G     | 6007 | ANP  | C3'-C4'-C5'-O5' |
| 3   | H     | 6008 | ANP  | C3'-C4'-C5'-O5' |
| 3   | I     | 6009 | ANP  | C3'-C4'-C5'-O5' |
| 3   | J     | 6010 | ANP  | C3'-C4'-C5'-O5' |
| 4   | C     | 5006 | MSL  | OXT-C-CA-N      |
| 4   | C     | 5009 | MSL  | OXT-C-CA-N      |
| 3   | B     | 6002 | ANP  | C2'-C1'-N9-C4   |
| 3   | H     | 6008 | ANP  | C2'-C1'-N9-C4   |
| 4   | C     | 5001 | MSL  | OXT-C-CA-N      |
| 4   | C     | 5003 | MSL  | OXT-C-CA-N      |
| 4   | C     | 5008 | MSL  | OXT-C-CA-N      |
| 4   | C     | 5004 | MSL  | OXT-C-CA-N      |
| 3   | B     | 6002 | ANP  | PB-O3A-PA-O1A   |
| 4   | C     | 5002 | MSL  | C-CA-CB-CG      |
| 4   | C     | 5001 | MSL  | OXT-C-CA-CB     |
| 4   | C     | 5001 | MSL  | N-CA-CB-CG      |
| 4   | C     | 5005 | MSL  | N-CA-CB-CG      |

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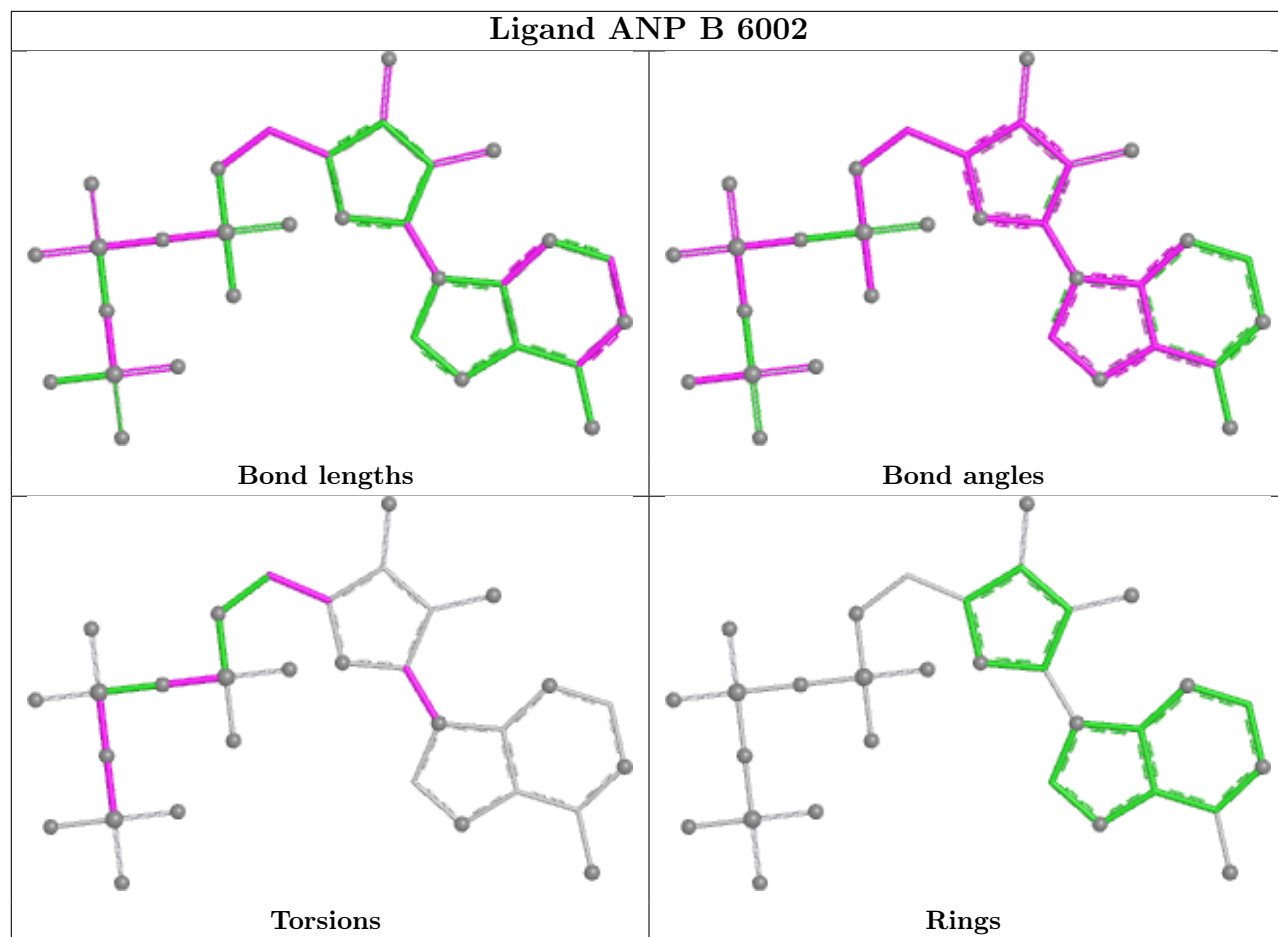
| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 4   | C     | 5004 | MSL  | OXT-C-CA-CB    |
| 4   | C     | 5005 | MSL  | OXT-C-CA-CB    |
| 4   | C     | 5008 | MSL  | OXT-C-CA-CB    |
| 3   | E     | 6005 | ANP  | PG-N3B-PB-O3A  |
| 3   | J     | 6010 | ANP  | PG-N3B-PB-O3A  |
| 4   | C     | 5001 | MSL  | O-C-CA-CB      |
| 4   | C     | 5003 | MSL  | O-C-CA-CB      |
| 4   | C     | 5006 | MSL  | OXT-C-CA-CB    |
| 3   | D     | 6004 | ANP  | C5'-O5'-PA-O3A |
| 3   | F     | 6006 | ANP  | C5'-O5'-PA-O1A |
| 3   | G     | 6007 | ANP  | C5'-O5'-PA-O3A |
| 3   | H     | 6008 | ANP  | C5'-O5'-PA-O3A |
| 3   | I     | 6009 | ANP  | C5'-O5'-PA-O1A |
| 3   | I     | 6009 | ANP  | C5'-O5'-PA-O2A |
| 3   | I     | 6009 | ANP  | C5'-O5'-PA-O3A |
| 4   | C     | 5002 | MSL  | CA-CB-CG-SD    |
| 4   | C     | 5003 | MSL  | CA-CB-CG-SD    |
| 4   | C     | 5005 | MSL  | CA-CB-CG-SD    |
| 4   | C     | 5007 | MSL  | CA-CB-CG-SD    |
| 4   | C     | 5002 | MSL  | O-C-CA-CB      |
| 4   | C     | 5003 | MSL  | OXT-C-CA-CB    |
| 4   | C     | 5004 | MSL  | O-C-CA-CB      |
| 4   | C     | 5005 | MSL  | O-C-CA-CB      |
| 4   | C     | 5006 | MSL  | O-C-CA-CB      |
| 4   | C     | 5008 | MSL  | O-C-CA-CB      |
| 4   | C     | 5002 | MSL  | OXT-C-CA-CB    |
| 4   | C     | 5007 | MSL  | C-CA-CB-CG     |
| 3   | J     | 6010 | ANP  | PB-O3A-PA-O2A  |
| 4   | C     | 5009 | MSL  | OXT-C-CA-CB    |
| 4   | C     | 5009 | MSL  | O-C-CA-CB      |
| 4   | C     | 5007 | MSL  | OXT-C-CA-CB    |
| 4   | C     | 5010 | MSL  | OXT-C-CA-CB    |
| 4   | C     | 5002 | MSL  | N-CA-CB-CG     |
| 4   | C     | 5007 | MSL  | O-C-CA-CB      |
| 3   | A     | 6001 | ANP  | PA-O3A-PB-O1B  |
| 3   | J     | 6010 | ANP  | PA-O3A-PB-O1B  |
| 4   | C     | 5010 | MSL  | O-C-CA-CB      |
| 4   | C     | 5010 | MSL  | O-C-CA-N       |

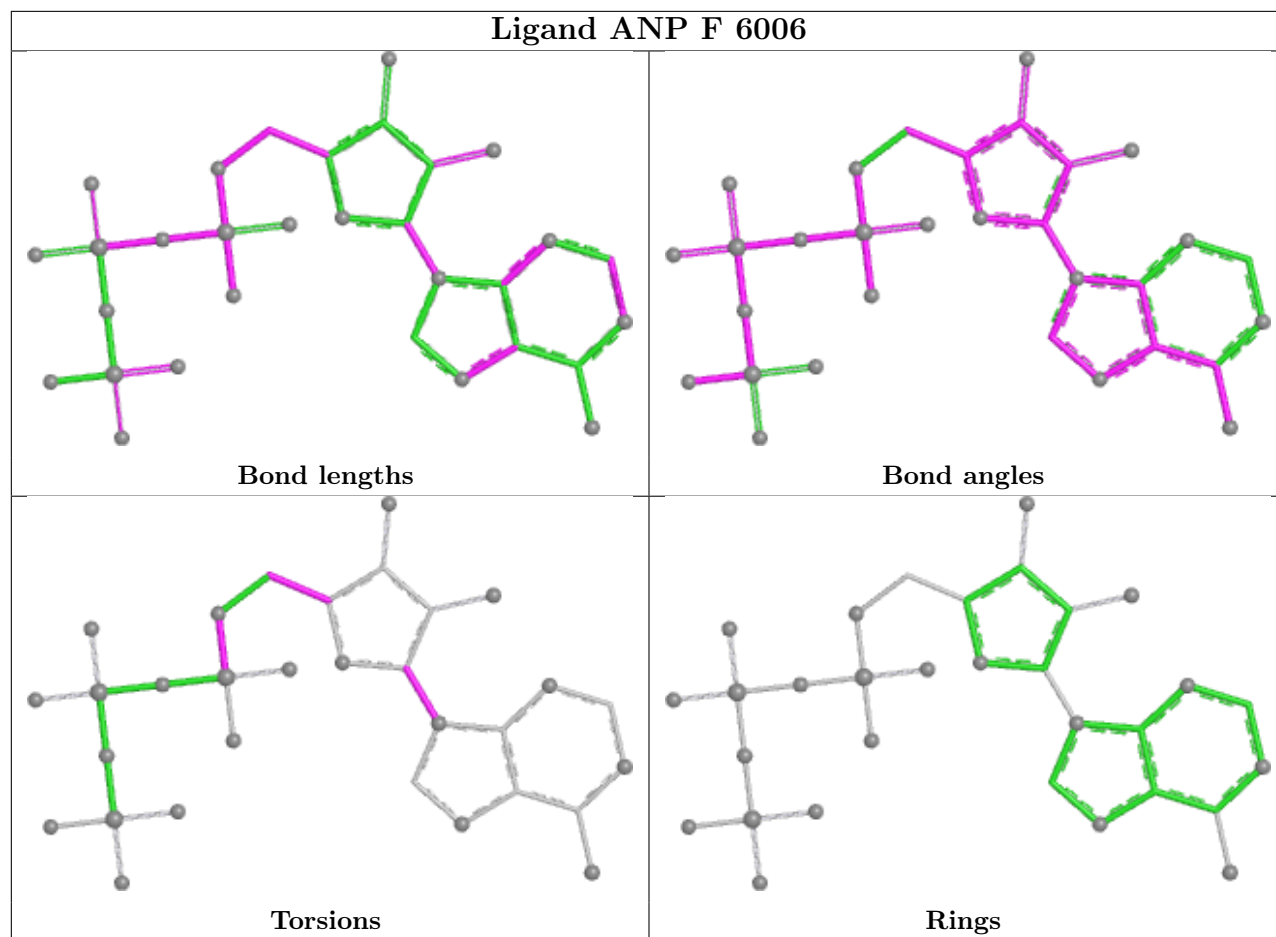
There are no ring outliers.

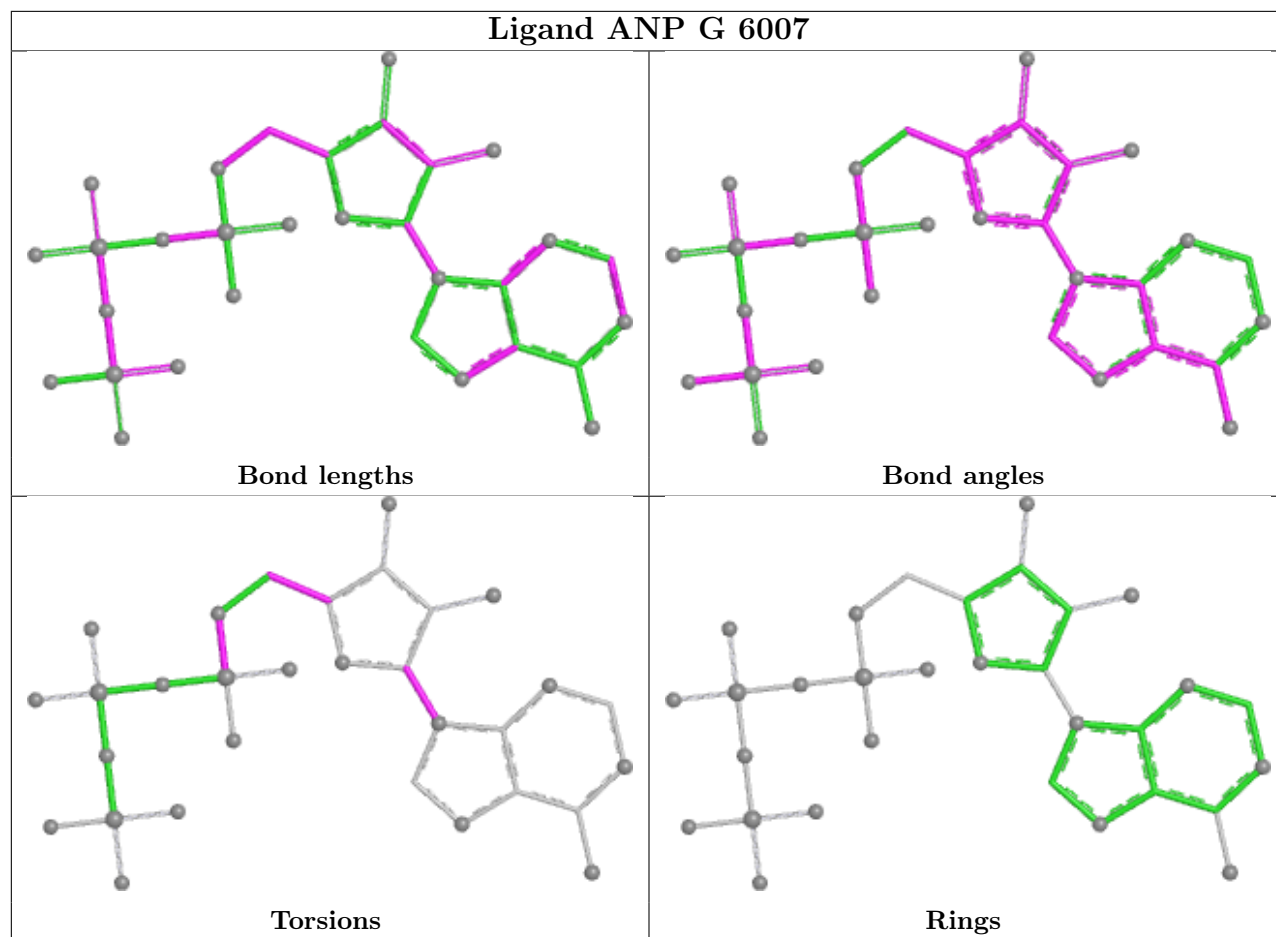
20 monomers are involved in 67 short contacts:

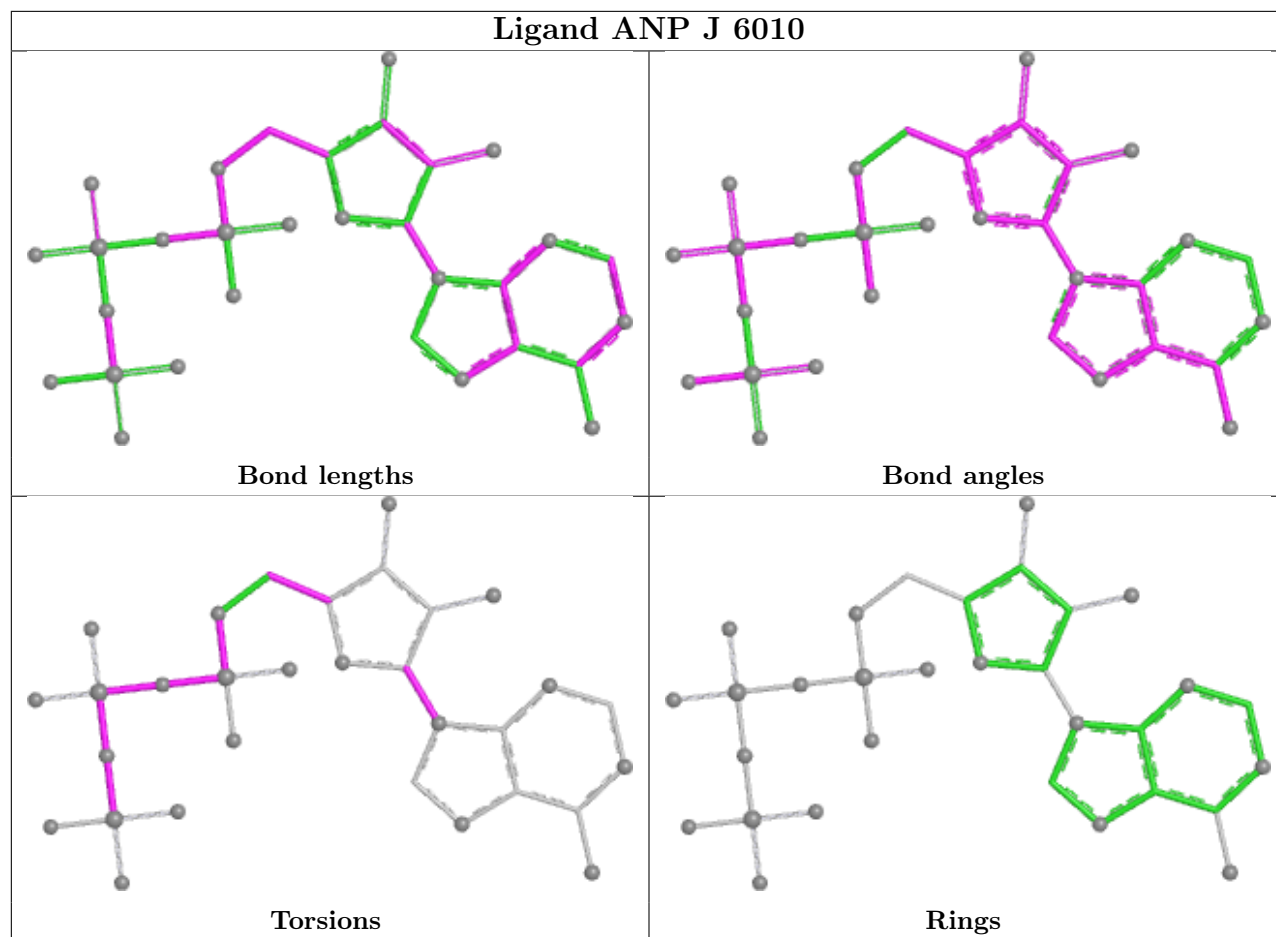
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | C     | 5010 | MSL  | 2       | 0            |
| 4   | C     | 5007 | MSL  | 7       | 0            |
| 4   | C     | 5005 | MSL  | 7       | 0            |
| 4   | C     | 5006 | MSL  | 3       | 0            |
| 3   | B     | 6002 | ANP  | 3       | 0            |
| 4   | C     | 5004 | MSL  | 3       | 0            |
| 4   | C     | 5001 | MSL  | 2       | 0            |
| 3   | F     | 6006 | ANP  | 4       | 0            |
| 4   | C     | 5008 | MSL  | 3       | 0            |
| 3   | G     | 6007 | ANP  | 5       | 0            |
| 3   | J     | 6010 | ANP  | 3       | 0            |
| 4   | C     | 5009 | MSL  | 3       | 0            |
| 3   | A     | 6001 | ANP  | 7       | 0            |
| 4   | C     | 5002 | MSL  | 6       | 0            |
| 4   | C     | 5003 | MSL  | 6       | 0            |
| 3   | C     | 6003 | ANP  | 4       | 0            |
| 3   | I     | 6009 | ANP  | 3       | 0            |
| 3   | E     | 6005 | ANP  | 6       | 0            |
| 3   | H     | 6008 | ANP  | 3       | 0            |
| 3   | D     | 6004 | ANP  | 6       | 0            |

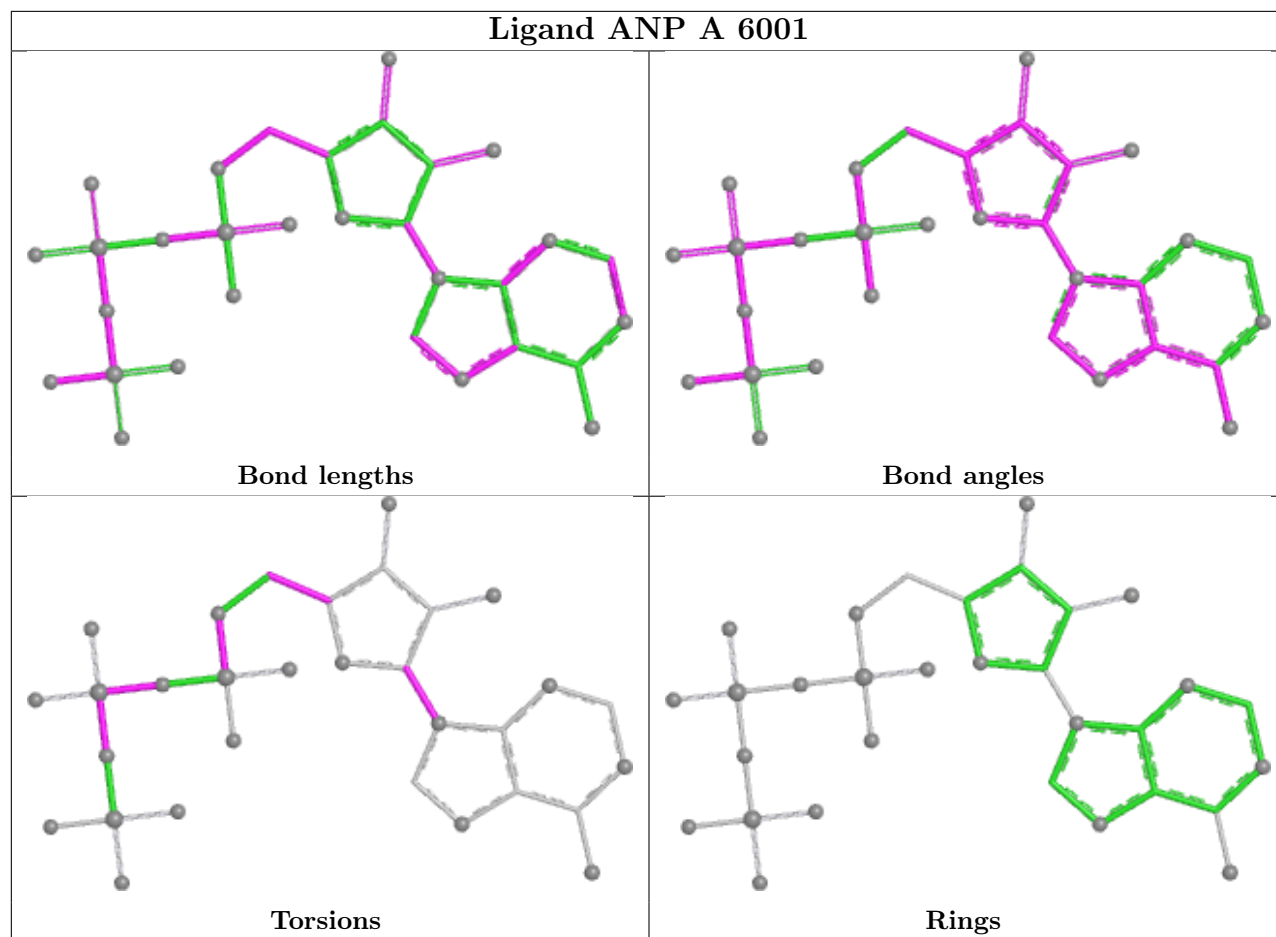
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

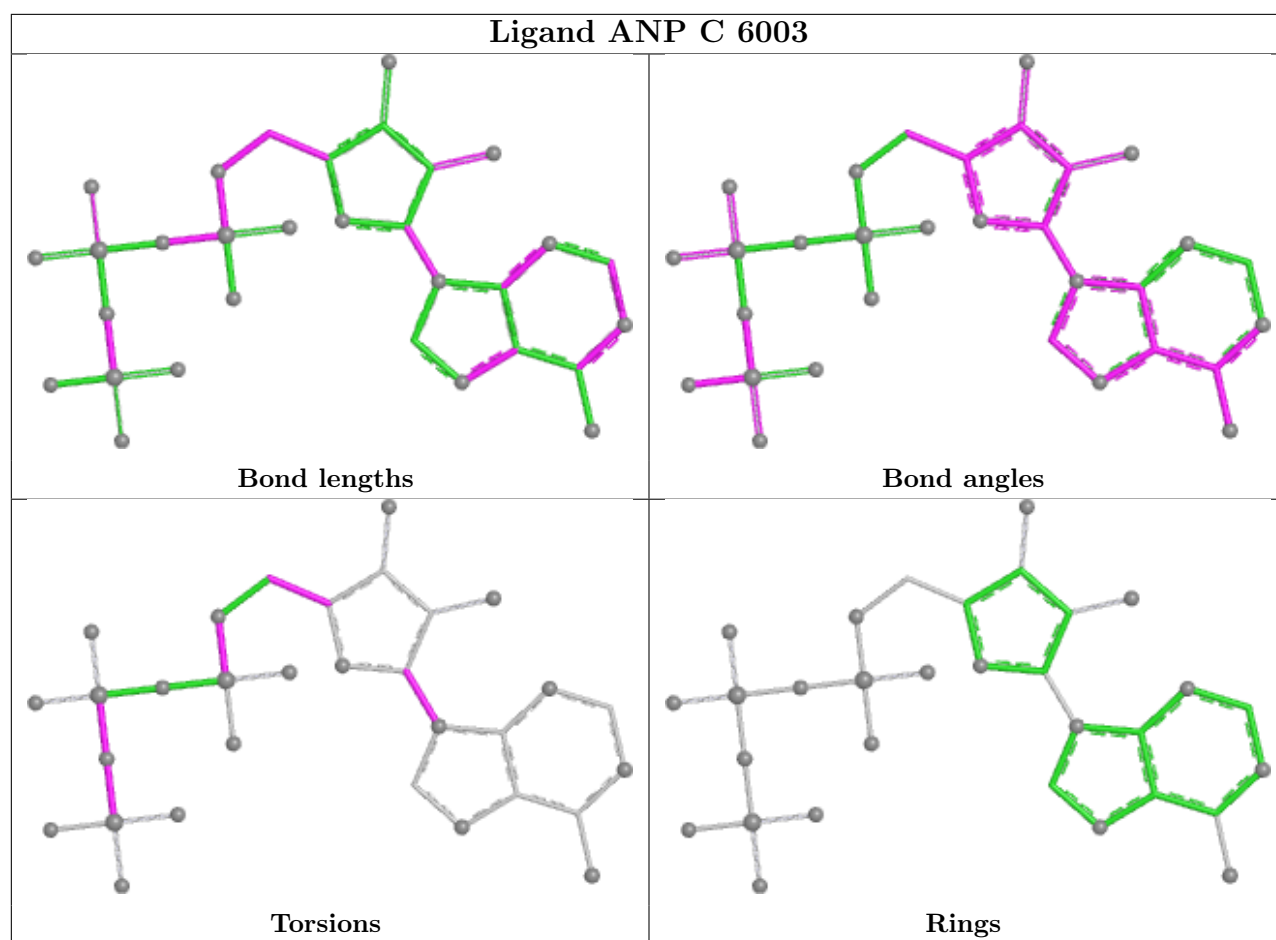


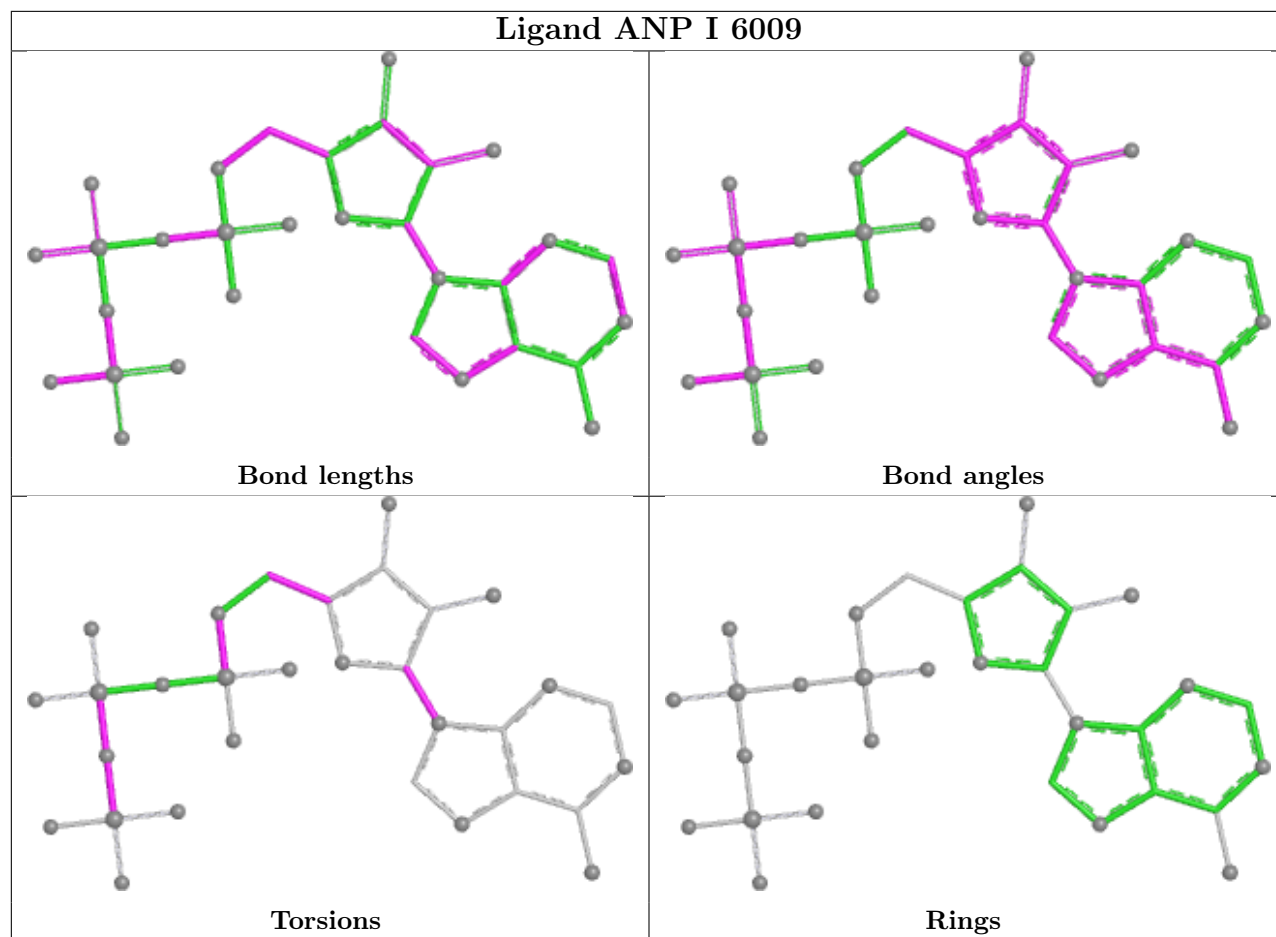


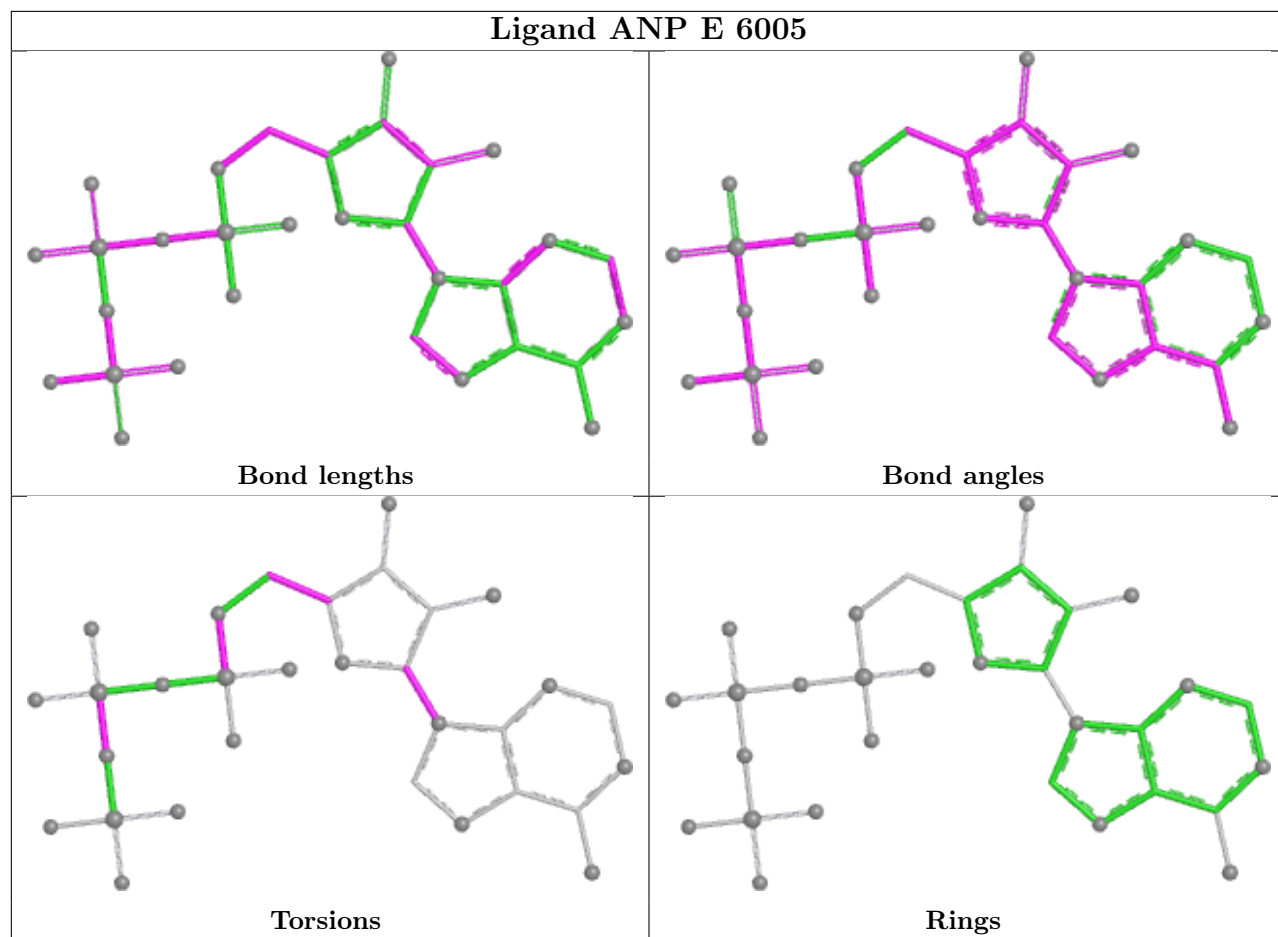


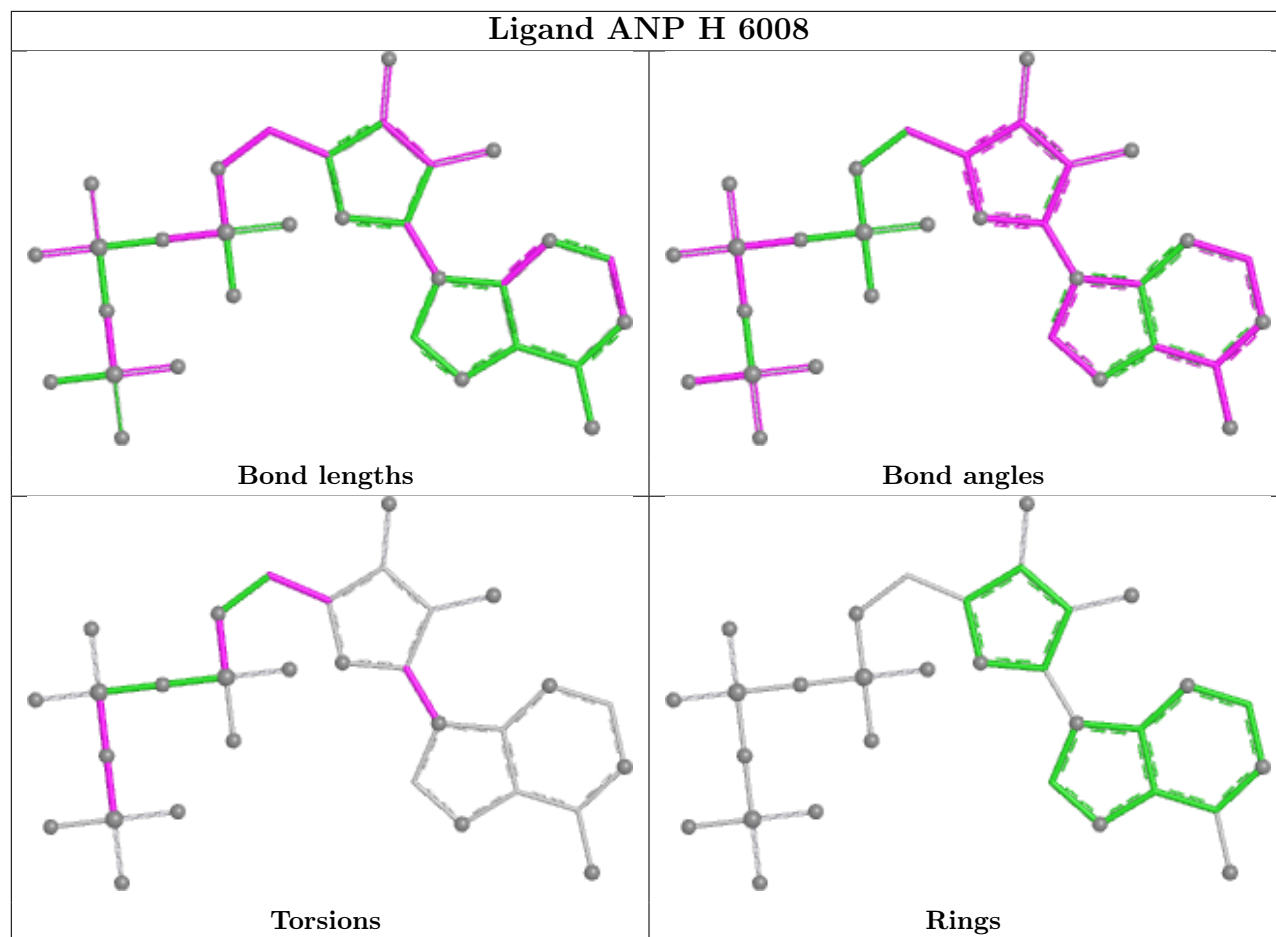


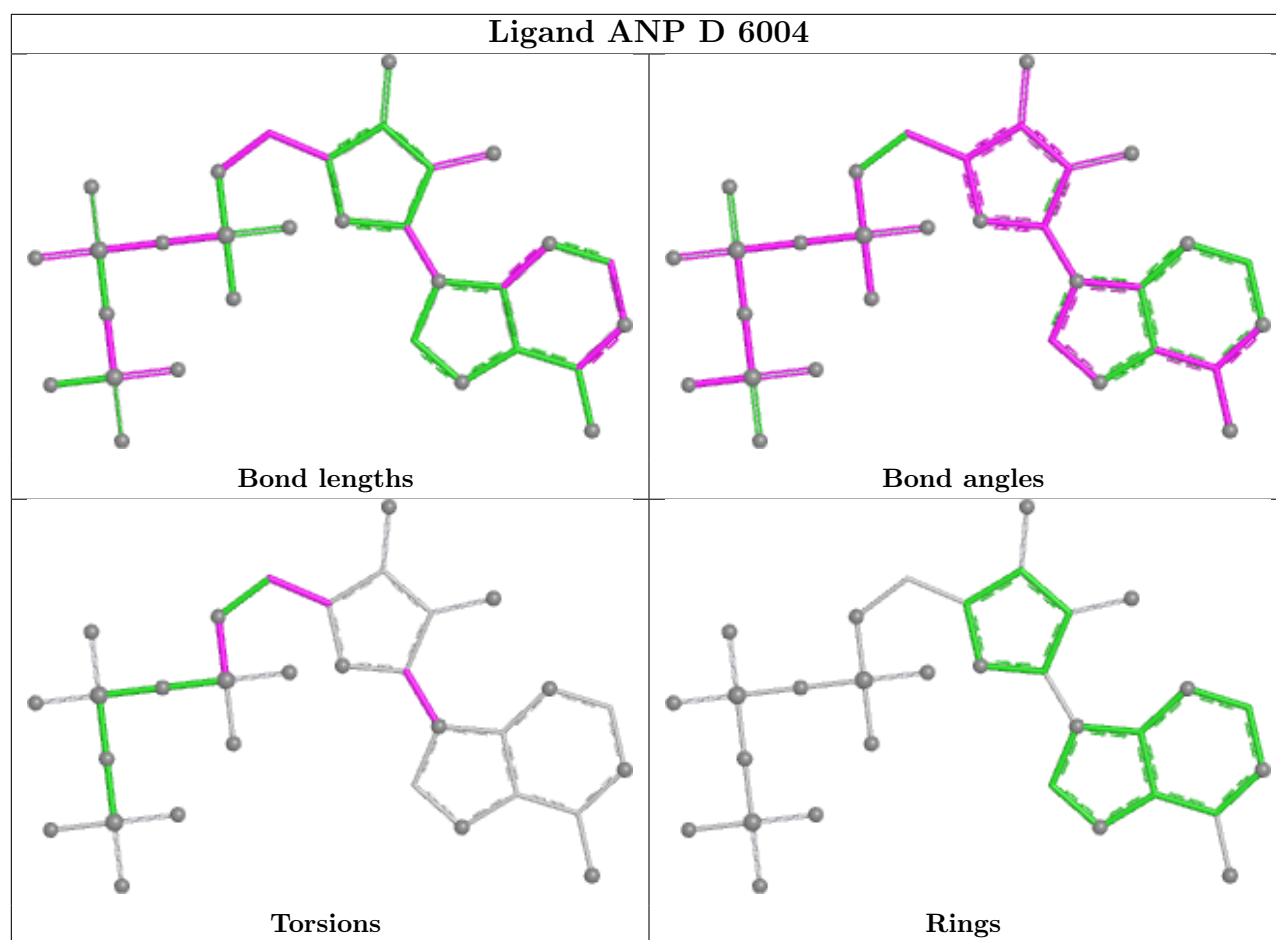












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 353/356 (99%)   | -0.77  | 0 100 100      | 55, 73, 96, 108       | 0     |
| 1   | B     | 353/356 (99%)   | -0.65  | 0 100 100      | 55, 73, 96, 108       | 0     |
| 1   | C     | 353/356 (99%)   | -0.75  | 0 100 100      | 55, 73, 96, 108       | 0     |
| 1   | D     | 353/356 (99%)   | -0.71  | 0 100 100      | 55, 73, 96, 108       | 0     |
| 1   | E     | 353/356 (99%)   | -0.74  | 0 100 100      | 55, 73, 96, 108       | 0     |
| 1   | F     | 353/356 (99%)   | -0.68  | 0 100 100      | 55, 73, 96, 108       | 0     |
| 1   | G     | 353/356 (99%)   | -0.72  | 0 100 100      | 55, 73, 96, 108       | 0     |
| 1   | H     | 353/356 (99%)   | -0.61  | 1 (0%) 90 76   | 55, 73, 96, 108       | 0     |
| 1   | I     | 353/356 (99%)   | -0.79  | 0 100 100      | 55, 73, 96, 108       | 0     |
| 1   | J     | 353/356 (99%)   | -0.70  | 0 100 100      | 55, 73, 96, 108       | 0     |
| All | All   | 3530/3560 (99%) | -0.71  | 1 (0%) 100 100 | 55, 73, 96, 108       | 0     |

All (1) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 118 | GLU  | 2.5  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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.

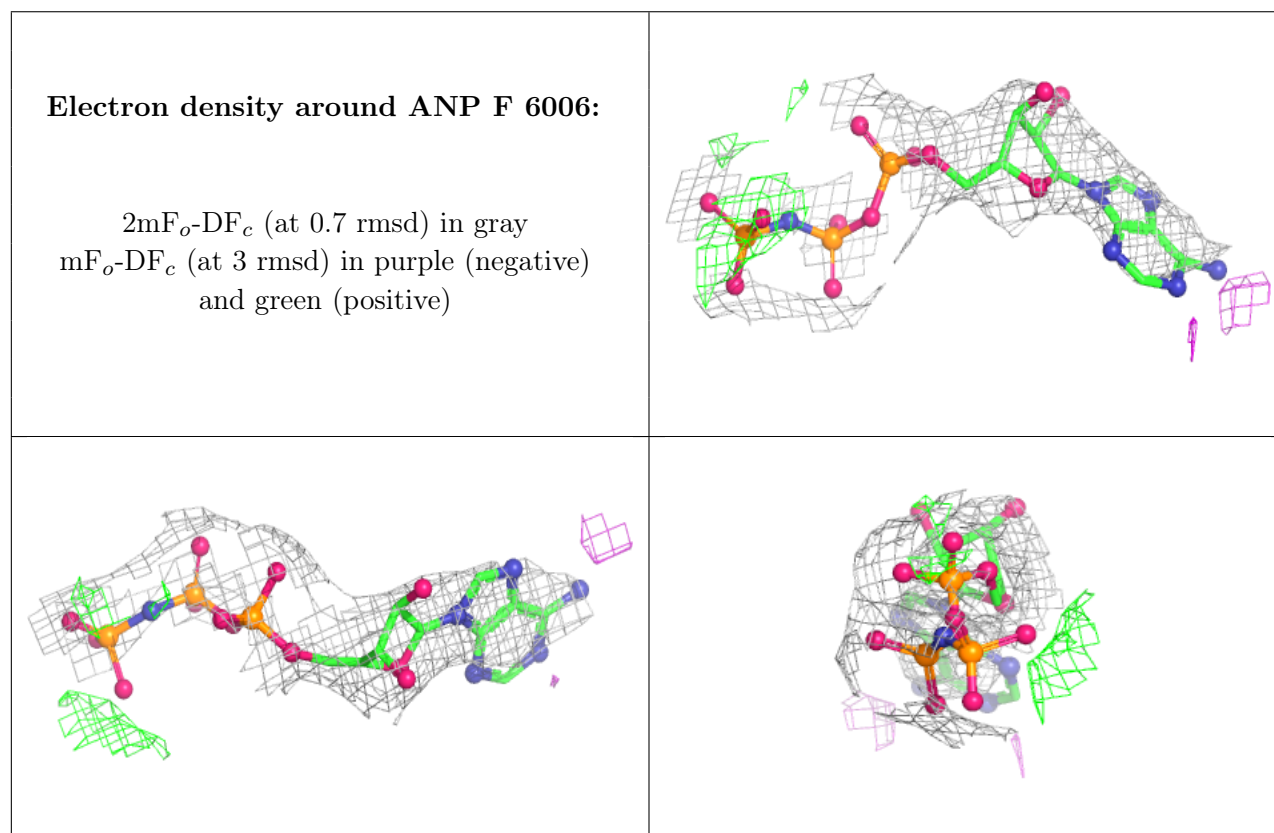
| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 2   | MN   | J     | 1091 | 1/1   | 0.81 | 0.09 | 62,62,62,62                | 0     |
| 2   | MN   | B     | 1011 | 1/1   | 0.87 | 0.09 | 62,62,62,62                | 0     |
| 2   | MN   | A     | 1001 | 1/1   | 0.89 | 0.07 | 68,68,68,68                | 0     |
| 2   | MN   | C     | 1021 | 1/1   | 0.90 | 0.07 | 66,66,66,66                | 0     |
| 2   | MN   | I     | 1081 | 1/1   | 0.92 | 0.05 | 68,68,68,68                | 0     |
| 2   | MN   | E     | 1041 | 1/1   | 0.93 | 0.06 | 73,73,73,73                | 0     |
| 2   | MN   | H     | 1071 | 1/1   | 0.94 | 0.06 | 57,57,57,57                | 0     |
| 2   | MN   | F     | 1053 | 1/1   | 0.94 | 0.05 | 69,69,69,69                | 0     |
| 2   | MN   | G     | 1061 | 1/1   | 0.94 | 0.05 | 66,66,66,66                | 0     |
| 2   | MN   | E     | 1043 | 1/1   | 0.95 | 0.05 | 61,61,61,61                | 0     |
| 3   | ANP  | F     | 6006 | 31/31 | 0.95 | 0.07 | 78,91,100,101              | 0     |
| 4   | MSL  | C     | 5007 | 11/11 | 0.95 | 0.07 | 62,68,77,77                | 0     |
| 2   | MN   | F     | 1051 | 1/1   | 0.96 | 0.04 | 69,69,69,69                | 0     |
| 4   | MSL  | C     | 5003 | 11/11 | 0.96 | 0.07 | 63,64,66,66                | 0     |
| 4   | MSL  | C     | 5005 | 11/11 | 0.96 | 0.07 | 75,78,79,79                | 0     |
| 2   | MN   | D     | 1031 | 1/1   | 0.96 | 0.04 | 65,65,65,65                | 0     |
| 3   | ANP  | A     | 6001 | 31/31 | 0.97 | 0.06 | 60,76,82,82                | 0     |
| 3   | ANP  | G     | 6007 | 31/31 | 0.97 | 0.06 | 65,86,95,96                | 0     |
| 3   | ANP  | I     | 6009 | 31/31 | 0.97 | 0.05 | 69,78,84,85                | 0     |
| 3   | ANP  | C     | 6003 | 31/31 | 0.97 | 0.07 | 64,76,92,93                | 0     |
| 3   | ANP  | D     | 6004 | 31/31 | 0.97 | 0.06 | 83,95,105,106              | 0     |
| 4   | MSL  | C     | 5006 | 11/11 | 0.97 | 0.07 | 73,79,85,85                | 0     |
| 3   | ANP  | E     | 6005 | 31/31 | 0.97 | 0.06 | 79,95,105,106              | 0     |
| 4   | MSL  | C     | 5008 | 11/11 | 0.97 | 0.07 | 63,65,66,67                | 0     |
| 3   | ANP  | J     | 6010 | 31/31 | 0.98 | 0.04 | 47,58,64,67                | 0     |
| 4   | MSL  | C     | 5001 | 11/11 | 0.98 | 0.06 | 51,54,57,58                | 0     |
| 4   | MSL  | C     | 5002 | 11/11 | 0.98 | 0.06 | 37,41,46,48                | 0     |
| 2   | MN   | B     | 1013 | 1/1   | 0.98 | 0.03 | 56,56,56,56                | 0     |
| 4   | MSL  | C     | 5004 | 11/11 | 0.98 | 0.06 | 71,73,75,77                | 0     |
| 3   | ANP  | B     | 6002 | 31/31 | 0.98 | 0.04 | 42,50,60,65                | 0     |
| 2   | MN   | E     | 1042 | 1/1   | 0.98 | 0.03 | 65,65,65,65                | 0     |
| 3   | ANP  | H     | 6008 | 31/31 | 0.98 | 0.05 | 40,48,59,67                | 0     |
| 2   | MN   | D     | 1033 | 1/1   | 0.98 | 0.03 | 56,56,56,56                | 0     |
| 4   | MSL  | C     | 5009 | 11/11 | 0.98 | 0.04 | 53,56,64,65                | 0     |
| 4   | MSL  | C     | 5010 | 11/11 | 0.98 | 0.05 | 38,42,49,49                | 0     |
| 2   | MN   | F     | 1052 | 1/1   | 0.99 | 0.03 | 70,70,70,70                | 0     |
| 2   | MN   | J     | 1093 | 1/1   | 0.99 | 0.05 | 57,57,57,57                | 0     |

*Continued on next page...*

*Continued from previous page...*

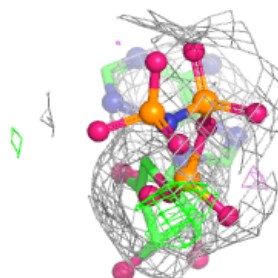
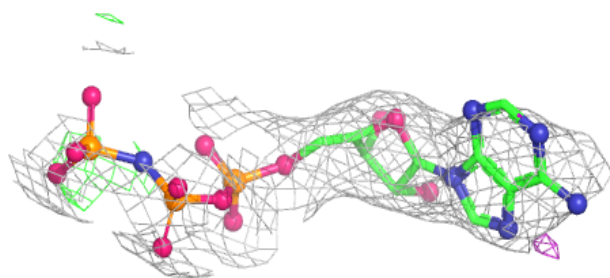
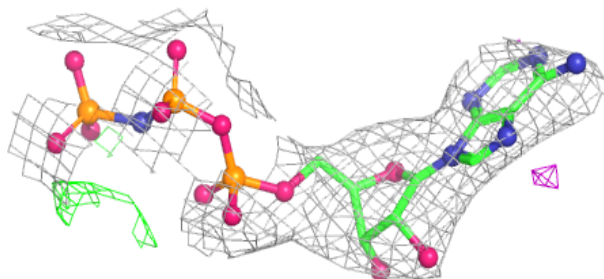
| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2   | MN   | C     | 1023 | 1/1   | 0.99 | 0.03 | 63,63,63,63                 | 0     |
| 2   | MN   | A     | 1003 | 1/1   | 0.99 | 0.03 | 57,57,57,57                 | 0     |
| 2   | MN   | G     | 1062 | 1/1   | 0.99 | 0.03 | 65,65,65,65                 | 0     |
| 2   | MN   | G     | 1063 | 1/1   | 0.99 | 0.03 | 63,63,63,63                 | 0     |
| 2   | MN   | D     | 1032 | 1/1   | 0.99 | 0.02 | 70,70,70,70                 | 0     |
| 2   | MN   | H     | 1072 | 1/1   | 0.99 | 0.02 | 57,57,57,57                 | 0     |
| 2   | MN   | H     | 1073 | 1/1   | 0.99 | 0.04 | 48,48,48,48                 | 0     |
| 2   | MN   | B     | 1012 | 1/1   | 0.99 | 0.03 | 60,60,60,60                 | 0     |
| 2   | MN   | I     | 1083 | 1/1   | 0.99 | 0.02 | 62,62,62,62                 | 0     |
| 2   | MN   | C     | 1022 | 1/1   | 1.00 | 0.01 | 66,66,66,66                 | 0     |
| 2   | MN   | A     | 1002 | 1/1   | 1.00 | 0.02 | 62,62,62,62                 | 0     |
| 2   | MN   | J     | 1092 | 1/1   | 1.00 | 0.03 | 62,62,62,62                 | 0     |
| 2   | MN   | I     | 1082 | 1/1   | 1.00 | 0.02 | 67,67,67,67                 | 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.

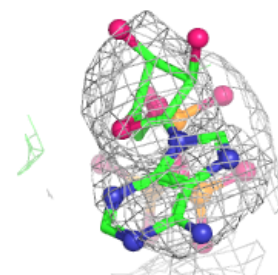
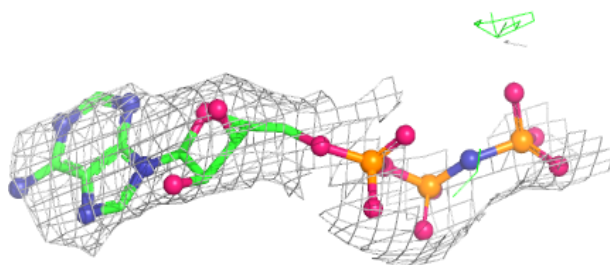


**Electron density around ANP A 6001:**

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

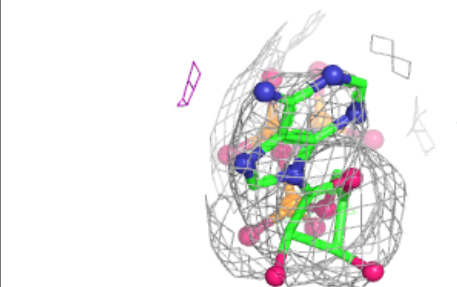
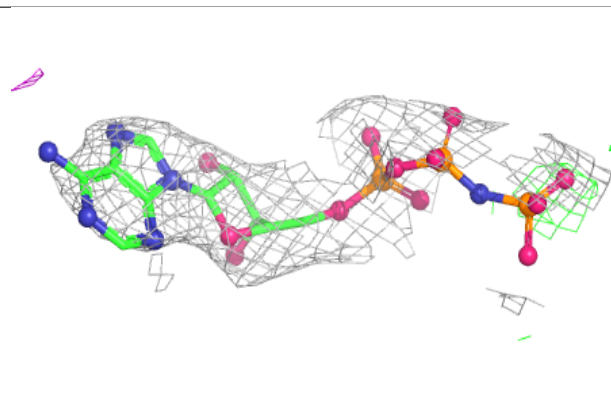
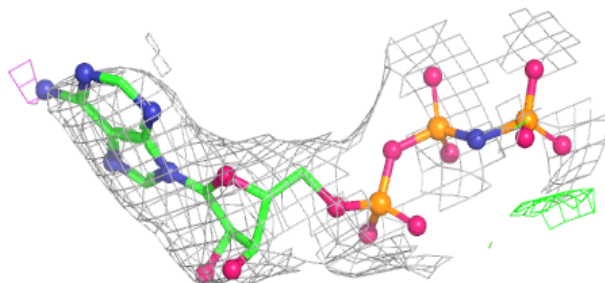
**Electron density around ANP G 6007:**

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

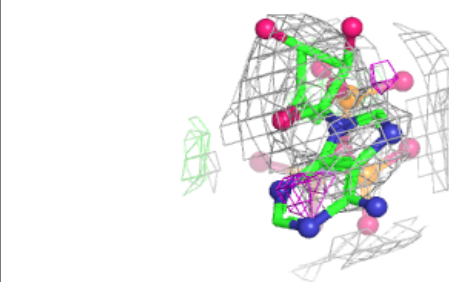
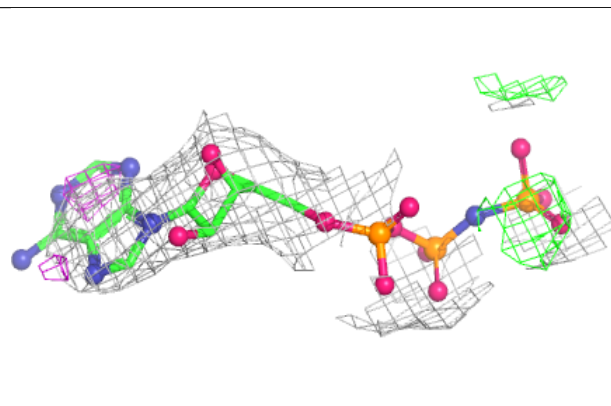
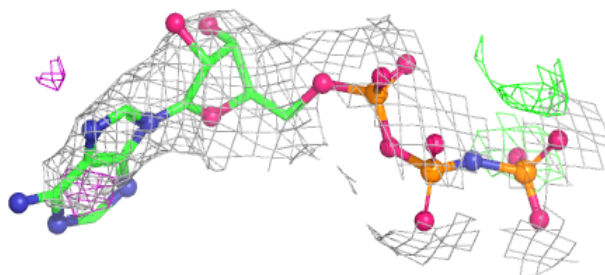


**Electron density around ANP I 6009:**

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

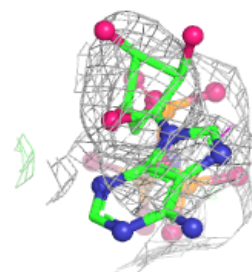
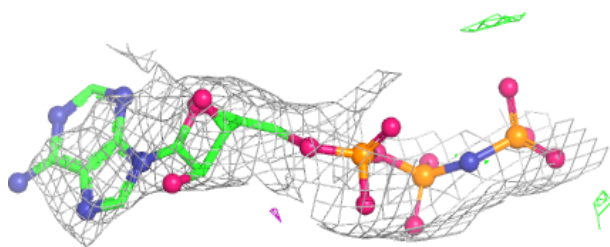
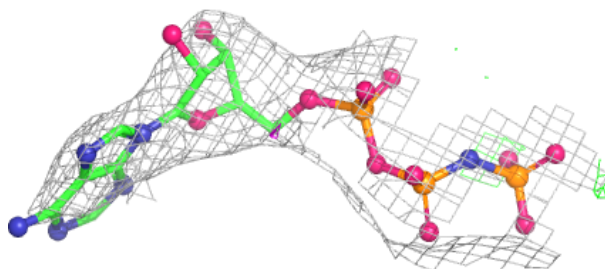
**Electron density around ANP C 6003:**

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

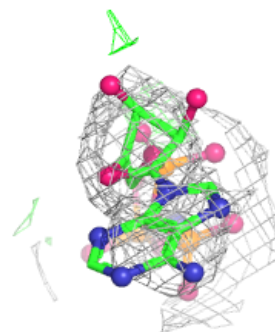
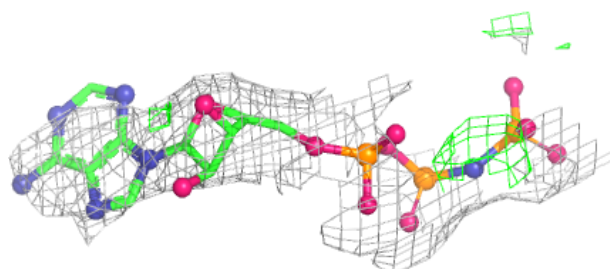
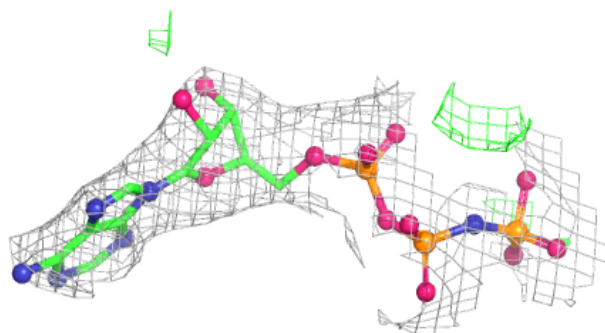


**Electron density around ANP D 6004:**

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

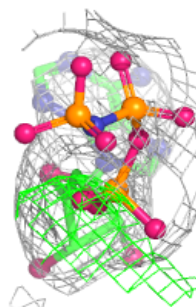
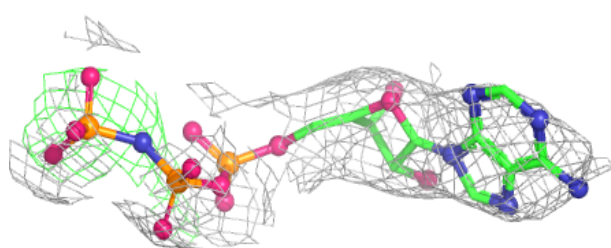
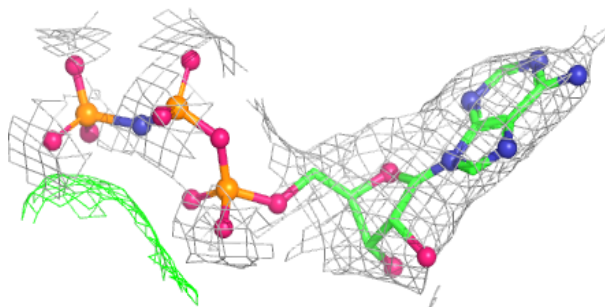
**Electron density around ANP E 6005:**

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

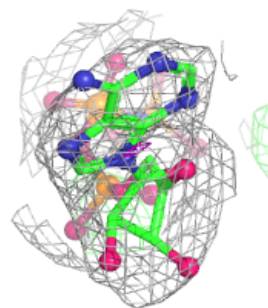
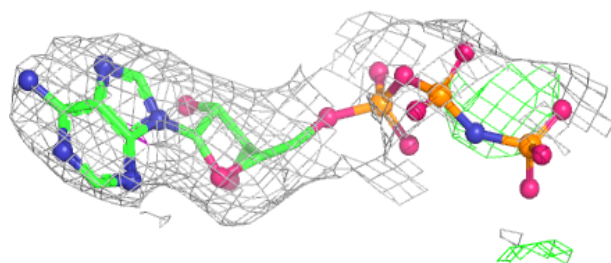
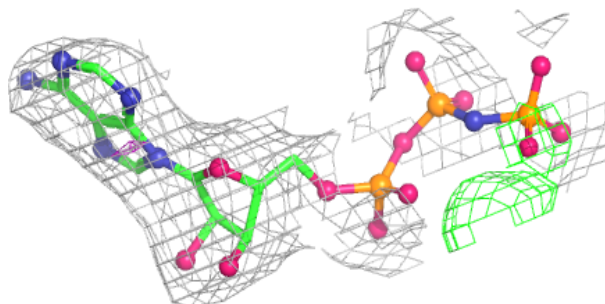


**Electron density around ANP J 6010:**

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

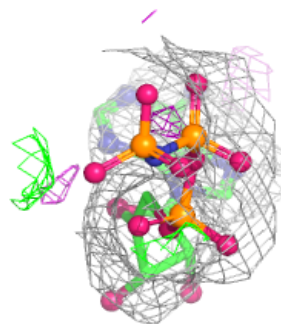
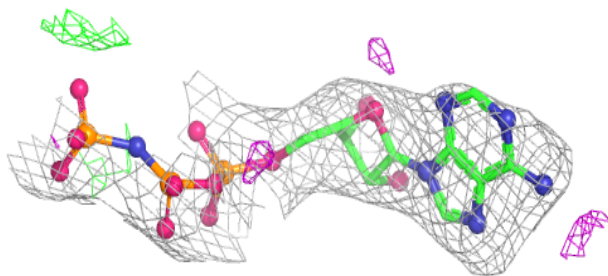
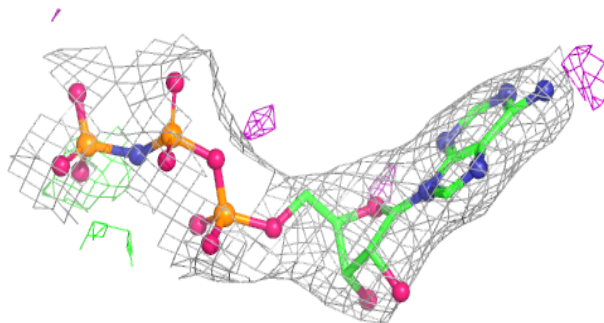
**Electron density around ANP B 6002:**

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



**Electron density around ANP H 6008:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.