



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:29 AM UTC

PDB ID : 1M19 / pdb\_00001m19  
Title : LIGAND BINDING ALTERS THE STRUCTURE AND DYNAMICS OF NUCLEOSOMAL DNA  
Authors : Suto, R.K.; Edayathumangalam, R.S.; White, C.L.; Melander, C.; Gottesfeld, J.M.; Dervan, P.B.; Luger, K.  
Deposited on : 2002-06-18  
Resolution : 2.30 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)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

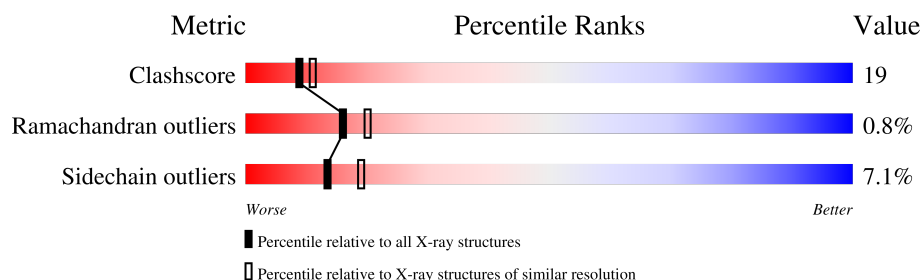
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 6919 (2.30-2.30)                                      |
| Ramachandran outliers | 187476                      | 6854 (2.30-2.30)                                      |
| Sidechain outliers    | 187428                      | 6854 (2.30-2.30)                                      |

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  $\leq 5\%$ .

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | I     | 146    | 45% 54% .        |
| 1   | J     | 146    | 47% 51% .        |
| 2   | A     | 135    | 54% 14% . . 26%  |
| 2   | E     | 135    | 53% 16% . . 27%  |
| 3   | B     | 102    | 64% 10% . 23%    |
| 3   | F     | 102    | 61% 18% 6% 16%   |
| 4   | C     | 129    | 66% 12% . . 17%  |
| 4   | G     | 129    | 60% 16% 5% 19%   |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | D     | 125    |                  |
| 5   | H     | 125    |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 7   | IMT  | I     | 1961 | -         | -        | X       | -                |
| 7   | IMT  | J     | 1901 | -         | -        | X       | -                |
| 7   | IMT  | J     | 1921 | -         | X        | -       | -                |
| 7   | IMT  | J     | 2001 | -         | X        | -       | -                |
| 8   | PYB  | I     | 1962 | -         | -        | X       | -                |
| 8   | PYB  | I     | 1963 | -         | -        | X       | -                |
| 8   | PYB  | I     | 1967 | -         | -        | X       | -                |
| 8   | PYB  | I     | 1968 | -         | -        | X       | -                |
| 8   | PYB  | I     | 1969 | -         | -        | X       | -                |
| 8   | PYB  | I     | 2022 | -         | -        | X       | -                |
| 8   | PYB  | I     | 2023 | -         | -        | X       | -                |
| 8   | PYB  | I     | 2024 | -         | -        | X       | -                |
| 8   | PYB  | I     | 2028 | -         | -        | X       | -                |
| 8   | PYB  | I     | 2029 | -         | -        | X       | -                |
| 8   | PYB  | J     | 1902 | -         | -        | X       | -                |
| 8   | PYB  | J     | 1903 | -         | -        | X       | -                |
| 8   | PYB  | J     | 1906 | -         | -        | X       | -                |
| 8   | PYB  | J     | 1907 | -         | -        | X       | -                |
| 8   | PYB  | J     | 1908 | -         | -        | X       | -                |
| 8   | PYB  | J     | 1927 | -         | -        | X       | -                |
| 8   | PYB  | J     | 1928 | -         | -        | X       | -                |
| 8   | PYB  | J     | 1929 | -         | -        | X       | -                |
| 8   | PYB  | J     | 2003 | -         | -        | X       | -                |
| 8   | PYB  | J     | 2008 | -         | -        | X       | -                |
| 8   | PYB  | J     | 2009 | -         | -        | X       | -                |
| 9   | ABU  | J     | 1905 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 13158 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 DNA chain called Palindromic 146 Base Pair DNA Fragment.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 1   | I     | 146      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2990  | 1430 | 541 | 874 | 145 |         |         |       |
| 1   | J     | 146      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2990  | 1430 | 541 | 874 | 145 |         |         |       |

- Molecule 2 is a protein called Histone H3.3C.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | A     | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 826   | 521 | 160 | 142 | 3 |         |         |       |
| 2   | E     | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 808   | 509 | 156 | 140 | 3 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 486     | SER      | ARG    | conflict | UNP P02302 |
| E     | 686     | SER      | ARG    | conflict | UNP P02302 |

- Molecule 3 is a protein called Histone H4.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | B     | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 627   | 395 | 121 | 110 | 1 |         |         |       |
| 3   | F     | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 694   | 436 | 140 | 117 | 1 |         |         |       |

- Molecule 4 is a protein called Histone H2A type 1.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 4   | C     | 107      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 825   | 520 | 161 | 144 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 4   | G     | 105      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 813   | 513 | 159 | 141 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C     | 899     | ARG      | GLY    | conflict | UNP P06897 |
| G     | 1099    | ARG      | GLY    | conflict | UNP P06897 |

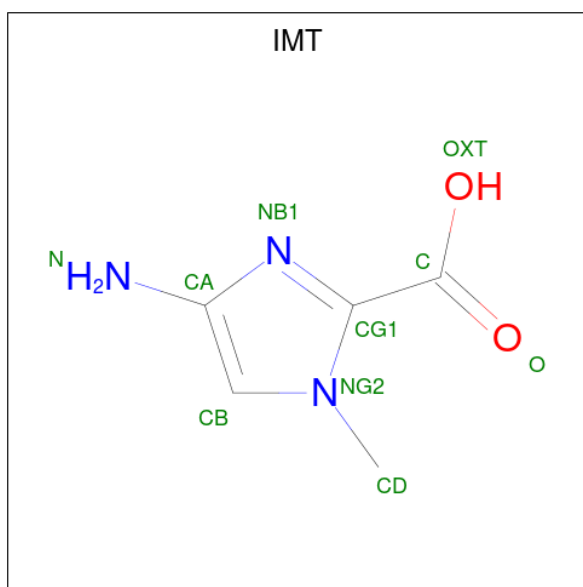
- Molecule 5 is a protein called Histone H2B.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | D     | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 736   | 463 | 132 | 139 | 2 |         |         |       |
| 5   | H     | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 736   | 463 | 132 | 139 | 2 |         |         |       |

- Molecule 6 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

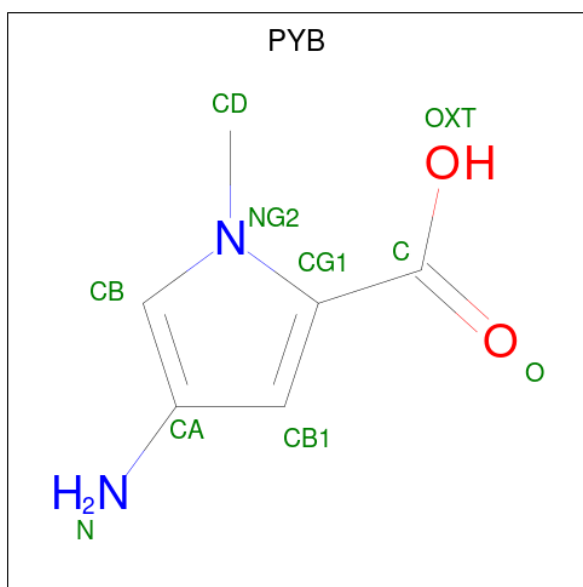
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | I     | 6        | Total | Mn | 0       | 0       |
|     |       |          | 6     | 6  |         |         |
| 6   | J     | 4        | Total | Mn | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 6   | E     | 1        | Total | Mn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 7 is 4-AMINO-(1-METHYLIMIDAZOLE)-2-CARBOXYLIC ACID (CCD ID: IMT) (formula: C<sub>5</sub>H<sub>7</sub>N<sub>3</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 7   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 5 | 2 | 1 |         |         |
| 7   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 5 | 2 | 1 |         |         |
| 7   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 5 | 2 | 1 |         |         |
| 7   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 5 | 2 | 1 |         |         |
| 7   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 8     | 5 | 2 | 1 |         |         |

- Molecule 8 is 4-AMINO-(1-METHYLPYRROLE)-2-CARBOXYLIC ACID (CCD ID: PYB) (formula: C<sub>6</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 8   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |

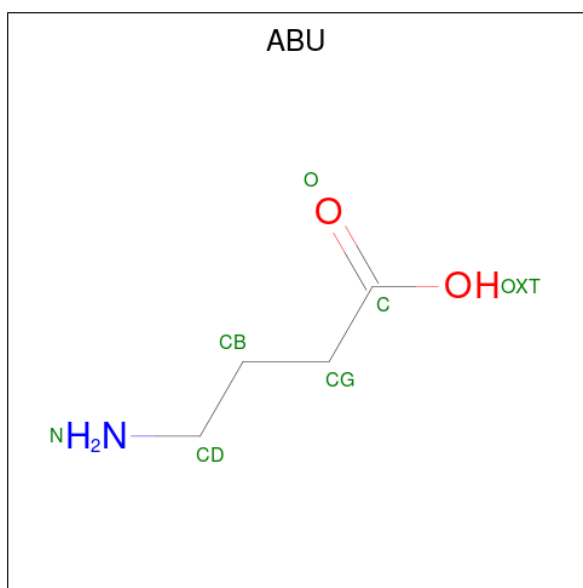
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| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 8   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |
| 8   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 6 | 2 | 1 |         |         |

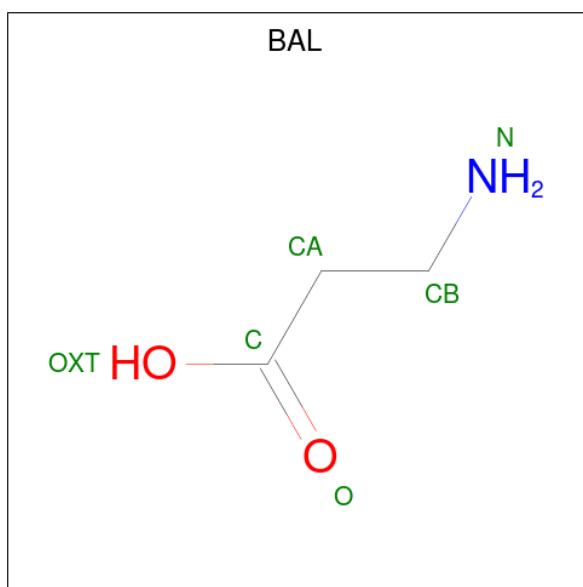


- Molecule 9 is GAMMA-AMINO-BUTANOIC ACID (CCD ID: ABU) (formula:  $C_4H_9NO_2$ ).



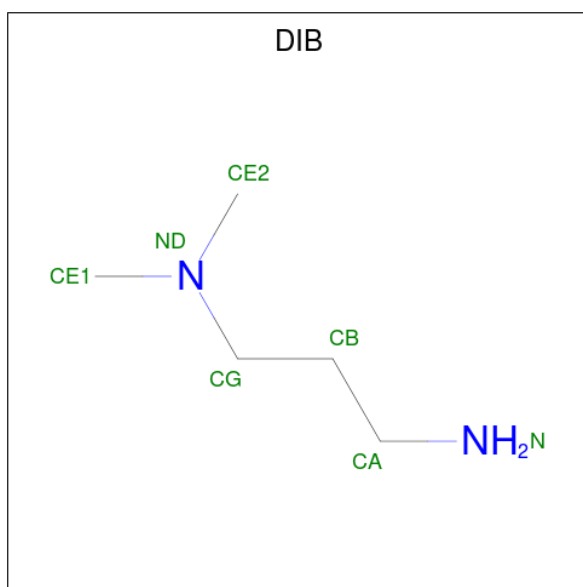
| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 9   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 6     | 4 | 1 | 1 |         |         |
| 9   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 6     | 4 | 1 | 1 |         |         |
| 9   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 6     | 4 | 1 | 1 |         |         |
| 9   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 6     | 4 | 1 | 1 |         |         |
| 9   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 6     | 4 | 1 | 1 |         |         |

- Molecule 10 is BETA-ALANINE (CCD ID: BAL) (formula:  $C_3H_7NO_2$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 10  | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |         |
| 10  | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |         |
| 10  | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |         |
| 10  | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |         |
| 10  | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |         |

- Molecule 11 is 3-AMINO-(DIMETHYLPROPYLAMINE) (CCD ID: DIB) (formula: C<sub>5</sub>H<sub>14</sub>N<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 11  | I     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 7     | 5 | 2 |         |         |
| 11  | I     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 7     | 5 | 2 |         |         |
| 11  | J     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 7     | 5 | 2 |         |         |
| 11  | J     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 7     | 5 | 2 |         |         |
| 11  | J     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 7     | 5 | 2 |         |         |

- Molecule 12 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 12  | I     | 88       | Total | O  | 0       | 0       |
|     |       |          | 88    | 88 |         |         |
| 12  | J     | 67       | Total | O  | 0       | 0       |
|     |       |          | 67    | 67 |         |         |
| 12  | A     | 68       | Total | O  | 0       | 0       |
|     |       |          | 68    | 68 |         |         |
| 12  | B     | 46       | Total | O  | 0       | 0       |
|     |       |          | 46    | 46 |         |         |
| 12  | C     | 79       | Total | O  | 0       | 0       |
|     |       |          | 79    | 79 |         |         |
| 12  | D     | 44       | Total | O  | 0       | 0       |
|     |       |          | 44    | 44 |         |         |
| 12  | E     | 84       | Total | O  | 0       | 0       |
|     |       |          | 84    | 84 |         |         |

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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 12  | F     | 75       | Total<br>75 | O<br>75 | 0       | 0       |
| 12  | G     | 66       | Total<br>66 | O<br>66 | 0       | 0       |
| 12  | H     | 40       | Total<br>40 | O<br>40 | 0       | 0       |

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

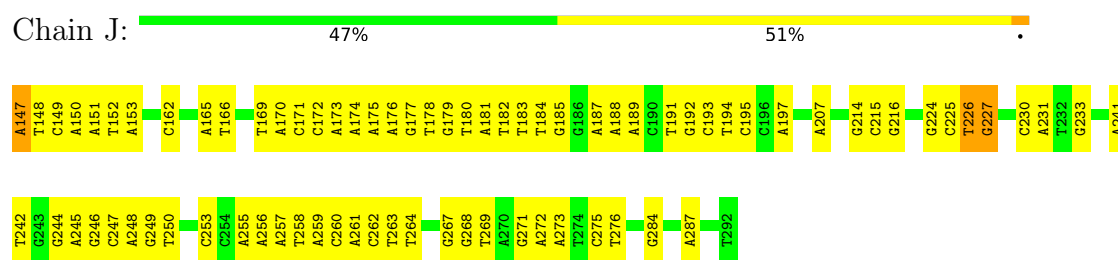
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

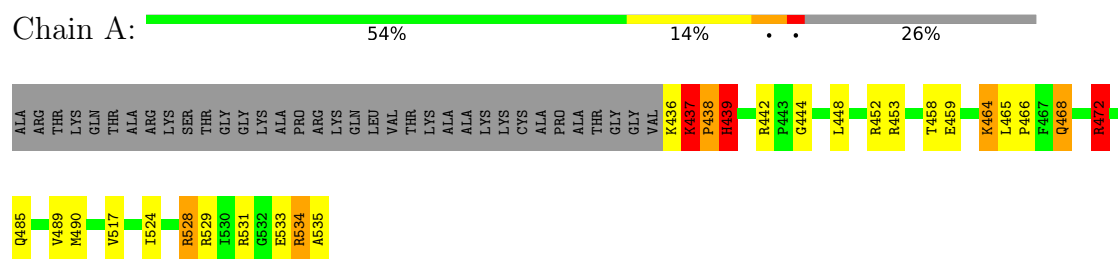
#### • Molecule 1: Palindromic 146 Base Pair DNA Fragment



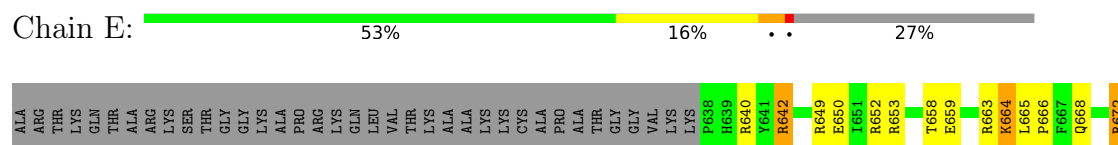
#### • Molecule 1: Palindromic 146 Base Pair DNA Fragment



#### • Molecule 2: Histone H3.3C



#### • Molecule 2: Histone H3.3C





• Molecule 3: Histone H4

Chain B: 64% 10% 23%



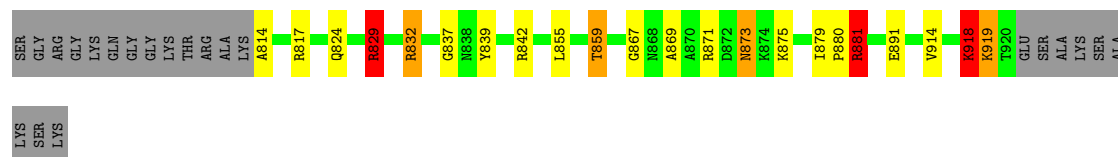
• Molecule 3: Histone H4

Chain F: 61% 18% 6% 16%



• Molecule 4: Histone H2A type 1

Chain C: 66% 12% 17%



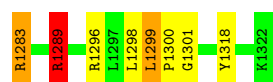
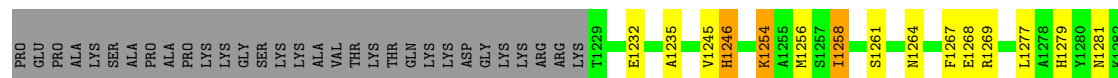
• Molecule 4: Histone H2A type 1

Chain G: 60% 16% 5% 19%



• Molecule 5: Histone H2B

Chain D: 57% 14% 25%



• Molecule 5: Histone H2B

Chain H: 58% 14% 25%

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| PRO | GLU | PRO | ALA | LYS | SER | ALA | PRO | ALA | PRO | LYS | LYS | GLY | SER | LYS | LYS | ALA | VAL | THR | LYS | THR | GLN | LYS | LYS | ASP | GLY | LYS | LYS | ARG | ARG | LYS | TI429 | R1430 | E1432 | S1433 | Y1438 | L1442 | K1443 | Q1444 | V1445 | H1446 | TI449 | I1458 | N1464 | E1468 | R1483 | S1484 | R1489 | R1496 | L1497 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|

|       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|
| L1498 | L1499 | P1500 | G1501 | E1502 | L1503 | K1522 |
|-------|-------|-------|-------|-------|-------|-------|

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                           | Source    |
|----------------------------------------------------------|-------------------------------------------------|-----------|
| Space group                                              | P 21 21 21                                      | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 107.05Å 109.66Å 183.02Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 80.00 – 2.30                                    | Depositor |
| % Data completeness<br>(in resolution range)             | 97.1 (80.00-2.30)                               | Depositor |
| $R_{merge}$                                              | 0.07                                            | Depositor |
| $R_{sym}$                                                | (Not available)                                 | Depositor |
| Refinement program                                       | CNS                                             | Depositor |
| R, $R_{free}$                                            | 0.214 , 0.253                                   | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 13158                                           | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 70.0                                            | wwPDB-VP  |



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BAL, IMT, MN, ABU, PYB, DIB

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   | I     | 0.34         | 0/3354         | 0.75        | 0/5175          |
| 1   | J     | 0.35         | 0/3354         | 0.78        | 1/5175 (0.0%)   |
| 2   | A     | 0.89         | 0/838          | 1.23        | 8/1122 (0.7%)   |
| 2   | E     | 1.05         | 0/820          | 1.19        | 5/1099 (0.5%)   |
| 3   | B     | 0.91         | 0/634          | 1.18        | 3/848 (0.4%)    |
| 3   | F     | 1.04         | 1/702 (0.1%)   | 1.23        | 5/937 (0.5%)    |
| 4   | C     | 0.98         | 0/835          | 1.13        | 4/1127 (0.4%)   |
| 4   | G     | 0.85         | 0/823          | 1.07        | 4/1110 (0.4%)   |
| 5   | D     | 1.01         | 2/747 (0.3%)   | 1.15        | 6/1004 (0.6%)   |
| 5   | H     | 0.82         | 0/747          | 1.09        | 5/1004 (0.5%)   |
| All | All   | 0.70         | 3/12854 (0.0%) | 0.96        | 41/18601 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | I     | 0                   | 4                   |
| 1   | J     | 0                   | 3                   |
| 2   | A     | 0                   | 2                   |
| 2   | E     | 0                   | 2                   |
| 3   | B     | 0                   | 2                   |
| 3   | F     | 0                   | 2                   |
| 4   | C     | 0                   | 1                   |
| 4   | G     | 0                   | 2                   |
| 5   | D     | 0                   | 1                   |
| All | All   | 0                   | 19                  |

All (3) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 5   | D     | 1256 | MET  | SD-CE | 8.38 | 2.00        | 1.79     |
| 3   | F     | 250  | ILE  | CA-CB | 6.12 | 1.62        | 1.54     |
| 5   | D     | 1258 | ILE  | CA-C  | 5.95 | 1.60        | 1.52     |

All (41) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 464  | LYS  | N-CA-C      | 8.76  | 120.44      | 111.07   |
| 4   | C     | 918  | LYS  | N-CA-C      | 8.47  | 121.26      | 110.24   |
| 2   | A     | 437  | LYS  | CA-C-N      | 8.29  | 130.21      | 119.84   |
| 2   | A     | 437  | LYS  | C-N-CA      | 8.29  | 130.21      | 119.84   |
| 2   | A     | 439  | HIS  | N-CA-C      | 8.27  | 128.41      | 110.80   |
| 2   | E     | 664  | LYS  | N-CA-C      | 7.87  | 119.64      | 111.14   |
| 3   | B     | 25   | ASN  | N-CA-C      | 7.73  | 119.49      | 111.14   |
| 3   | B     | 30   | THR  | N-CA-C      | 7.65  | 120.88      | 110.55   |
| 4   | G     | 1025 | PHE  | CA-C-N      | 7.62  | 129.37      | 119.84   |
| 4   | G     | 1025 | PHE  | C-N-CA      | 7.62  | 129.37      | 119.84   |
| 2   | A     | 485  | GLN  | N-CA-C      | -7.38 | 100.10      | 110.50   |
| 1   | J     | 227  | DG   | C5'-C4'-C3' | -7.32 | 103.92      | 114.90   |
| 2   | E     | 717  | VAL  | N-CA-C      | -7.32 | 106.00      | 113.10   |
| 2   | A     | 517  | VAL  | N-CA-C      | -6.68 | 106.62      | 113.10   |
| 3   | F     | 228  | GLY  | N-CA-C      | -6.63 | 107.38      | 114.67   |
| 2   | E     | 685  | GLN  | N-CA-C      | -6.27 | 101.14      | 110.23   |
| 3   | F     | 230  | THR  | N-CA-C      | 6.06  | 118.53      | 110.53   |
| 2   | E     | 652  | ARG  | CB-CG-CD    | 6.03  | 125.17      | 111.30   |
| 4   | C     | 881  | ARG  | CB-CG-CD    | 5.95  | 124.99      | 111.30   |
| 4   | G     | 1092 | GLU  | N-CA-C      | 5.92  | 117.81      | 111.36   |
| 5   | D     | 1235 | ALA  | N-CA-C      | 5.91  | 118.49      | 111.33   |
| 2   | E     | 683  | ARG  | N-CA-C      | -5.73 | 101.72      | 110.14   |
| 5   | H     | 1499 | LEU  | CA-C-N      | 5.71  | 125.47      | 119.76   |
| 5   | H     | 1499 | LEU  | C-N-CA      | 5.71  | 125.47      | 119.76   |
| 3   | B     | 93   | GLN  | N-CA-C      | -5.69 | 106.20      | 113.02   |
| 5   | D     | 1298 | LEU  | N-CA-C      | 5.63  | 120.27      | 112.45   |
| 2   | A     | 437  | LYS  | N-CA-C      | 5.59  | 118.58      | 110.14   |
| 4   | C     | 891  | GLU  | N-CA-C      | 5.57  | 118.07      | 111.33   |
| 5   | D     | 1299 | LEU  | CA-C-N      | 5.40  | 125.31      | 119.85   |
| 5   | D     | 1299 | LEU  | C-N-CA      | 5.40  | 125.31      | 119.85   |
| 5   | D     | 1246 | HIS  | CA-C-N      | 5.34  | 125.41      | 119.32   |
| 5   | D     | 1246 | HIS  | C-N-CA      | 5.34  | 125.41      | 119.32   |
| 4   | G     | 1023 | LEU  | N-CA-C      | 5.34  | 118.29      | 109.85   |
| 3   | F     | 229  | ILE  | CB-CA-C     | -5.29 | 106.65      | 112.68   |
| 3   | F     | 283  | ALA  | N-CA-C      | -5.29 | 105.62      | 111.71   |
| 3   | F     | 301  | GLY  | N-CA-C      | -5.22 | 107.49      | 115.00   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 5   | H     | 1438 | VAL  | N-CA-C | -5.10 | 105.57      | 110.72   |
| 5   | H     | 1501 | GLY  | N-CA-C | 5.10  | 125.27      | 113.18   |
| 5   | H     | 1498 | LEU  | N-CA-C | 5.09  | 119.53      | 112.45   |
| 2   | A     | 489  | VAL  | N-CA-C | -5.06 | 105.61      | 110.72   |
| 4   | C     | 824  | GLN  | N-CA-C | -5.03 | 106.31      | 112.90   |

There are no chirality outliers.

All (19) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 2   | A     | 472  | ARG  | Sidechain |
| 2   | A     | 531  | ARG  | Sidechain |
| 3   | B     | 39   | ARG  | Sidechain |
| 3   | B     | 45   | ARG  | Sidechain |
| 4   | C     | 829  | ARG  | Sidechain |
| 5   | D     | 1289 | ARG  | Sidechain |
| 2   | E     | 672  | ARG  | Sidechain |
| 2   | E     | 731  | ARG  | Sidechain |
| 3   | F     | 239  | ARG  | Sidechain |
| 3   | F     | 245  | ARG  | Sidechain |
| 4   | G     | 1081 | ARG  | Sidechain |
| 4   | G     | 1088 | ARG  | Sidechain |
| 1   | I     | 131  | DG   | Sidechain |
| 1   | I     | 135  | DG   | Sidechain |
| 1   | I     | 67   | DA   | Sidechain |
| 1   | I     | 77   | DC   | Sidechain |
| 1   | J     | 147  | DA   | Sidechain |
| 1   | J     | 214  | DG   | Sidechain |
| 1   | J     | 226  | DT   | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | I     | 2990  | 0        | 1651     | 131     | 0            |
| 1   | J     | 2990  | 0        | 1651     | 127     | 0            |
| 2   | A     | 826   | 0        | 871      | 18      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | E     | 808   | 0        | 846      | 23      | 0            |
| 3   | B     | 627   | 0        | 663      | 9       | 0            |
| 3   | F     | 694   | 0        | 742      | 17      | 0            |
| 4   | C     | 825   | 0        | 884      | 23      | 0            |
| 4   | G     | 813   | 0        | 872      | 33      | 0            |
| 5   | D     | 736   | 0        | 760      | 16      | 0            |
| 5   | H     | 736   | 0        | 760      | 15      | 0            |
| 6   | E     | 1     | 0        | 0        | 0       | 0            |
| 6   | I     | 6     | 0        | 0        | 0       | 0            |
| 6   | J     | 4     | 0        | 0        | 0       | 0            |
| 7   | I     | 16    | 0        | 8        | 7       | 0            |
| 7   | J     | 24    | 0        | 12       | 7       | 0            |
| 8   | I     | 126   | 0        | 84       | 40      | 0            |
| 8   | J     | 189   | 0        | 126      | 58      | 0            |
| 9   | I     | 12    | 0        | 0        | 2       | 0            |
| 9   | J     | 18    | 0        | 0        | 7       | 0            |
| 10  | I     | 10    | 0        | 8        | 3       | 0            |
| 10  | J     | 15    | 0        | 12       | 2       | 0            |
| 11  | I     | 14    | 0        | 25       | 5       | 0            |
| 11  | J     | 21    | 0        | 37       | 8       | 0            |
| 12  | A     | 68    | 0        | 0        | 1       | 0            |
| 12  | B     | 46    | 0        | 0        | 3       | 0            |
| 12  | C     | 79    | 0        | 0        | 3       | 0            |
| 12  | D     | 44    | 0        | 0        | 4       | 0            |
| 12  | E     | 84    | 0        | 0        | 5       | 0            |
| 12  | F     | 75    | 0        | 0        | 2       | 0            |
| 12  | G     | 66    | 0        | 0        | 1       | 0            |
| 12  | H     | 40    | 0        | 0        | 0       | 0            |
| 12  | I     | 88    | 0        | 0        | 6       | 0            |
| 12  | J     | 67    | 0        | 0        | 5       | 0            |
| All | All   | 13158 | 0        | 10012    | 415     | 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 19.

All (415) 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:J:249:DG:N2      | 8:J:1929:PYB:HB1 | 1.68                     | 1.08              |
| 11:J:1911:DIB:HE22 | 4:C:814:ALA:HB3  | 1.36                     | 1.08              |
| 1:J:174:DA:H2''    | 1:J:175:DA:H5''  | 1.38                     | 1.05              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:I:93:DT:H2''    | 1:I:94:DG:H5''     | 1.43                     | 0.99              |
| 1:I:125:DG:H1'    | 1:I:126:DA:H5'     | 1.49                     | 0.94              |
| 1:J:249:DG:H21    | 8:J:1929:PYB:HB1   | 1.30                     | 0.92              |
| 3:F:287:VAL:HG11  | 3:F:302:GLY:HA3    | 1.51                     | 0.92              |
| 1:J:188:DA:N3     | 8:J:2006:PYB:HB1   | 1.86                     | 0.90              |
| 1:J:287:DA:H5''   | 12:J:2055:HOH:O    | 1.75                     | 0.85              |
| 12:I:2045:HOH:O   | 4:G:1075:LYS:HE2   | 1.78                     | 0.84              |
| 1:J:259:DA:H4'    | 9:J:1905:ABU:CG    | 2.07                     | 0.83              |
| 1:J:174:DA:C2'    | 1:J:175:DA:H5''    | 2.08                     | 0.82              |
| 4:G:1017:ARG:HH22 | 4:G:1031:HIS:CD2   | 1.98                     | 0.81              |
| 1:I:37:DT:H2''    | 1:I:38:DT:C6       | 2.15                     | 0.81              |
| 2:E:664:LYS:HB2   | 12:E:802:HOH:O     | 1.80                     | 0.81              |
| 1:J:194:DT:H4'    | 11:J:2011:DIB:HE13 | 1.63                     | 0.80              |
| 1:I:47:DC:H4'     | 11:J:1931:DIB:HG2  | 1.65                     | 0.79              |
| 11:J:1911:DIB:CE2 | 4:C:814:ALA:HB3    | 2.11                     | 0.79              |
| 1:I:5:DA:H2''     | 1:I:6:DT:H5'       | 1.66                     | 0.78              |
| 1:J:192:DG:N3     | 10:J:2010:BAL:HA2  | 1.99                     | 0.78              |
| 1:I:126:DA:OP2    | 1:I:126:DA:H3'     | 1.85                     | 0.77              |
| 1:J:149:DC:H2'    | 1:J:150:DA:C8      | 2.21                     | 0.76              |
| 1:J:260:DC:O2     | 8:J:1907:PYB:N     | 2.16                     | 0.76              |
| 2:A:528:ARG:HB2   | 2:A:535:ALA:OXT    | 1.85                     | 0.76              |
| 1:J:259:DA:C4'    | 9:J:1905:ABU:CG    | 2.64                     | 0.75              |
| 1:J:147:DA:H2'    | 1:J:148:DT:H72     | 1.69                     | 0.75              |
| 1:I:68:DG:H1      | 1:J:225:DC:H42     | 1.35                     | 0.74              |
| 1:I:115:DA:C2     | 8:I:2029:PYB:HB1   | 2.22                     | 0.74              |
| 1:I:125:DG:H2''   | 1:I:126:DA:OP2     | 1.85                     | 0.74              |
| 2:A:448:LEU:HD11  | 3:B:44:LYS:HD2     | 1.69                     | 0.74              |
| 1:J:249:DG:H21    | 8:J:1929:PYB:CB1   | 2.01                     | 0.74              |
| 1:J:175:DA:H2''   | 1:J:176:DA:C8      | 2.23                     | 0.74              |
| 2:E:668:GLN:O     | 2:E:672:ARG:HG2    | 1.88                     | 0.74              |
| 11:I:2031:DIB:HA2 | 1:J:177:DG:N3      | 2.02                     | 0.73              |
| 5:D:1264:ASN:O    | 5:D:1268:GLU:HG3   | 1.89                     | 0.73              |
| 12:B:141:HOH:O    | 4:G:1099:ARG:HD3   | 1.89                     | 0.72              |
| 1:I:111:DA:H4'    | 4:G:1042:ARG:HH11  | 1.54                     | 0.72              |
| 1:I:133:DA:H2''   | 1:I:134:DG:H5'     | 1.72                     | 0.72              |
| 1:I:71:DG:H21     | 8:I:1969:PYB:HB1   | 1.54                     | 0.72              |
| 4:C:918:LYS:O     | 4:C:919:LYS:HB2    | 1.89                     | 0.72              |
| 4:G:1017:ARG:HH22 | 4:G:1031:HIS:HD2   | 1.37                     | 0.72              |
| 1:J:275:DC:C6     | 1:J:276:DT:H72     | 2.25                     | 0.71              |
| 1:J:244:DG:H1'    | 1:J:245:DA:H5'     | 1.73                     | 0.71              |
| 1:J:188:DA:H2''   | 1:J:189:DA:O5'     | 1.89                     | 0.70              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:C:855:LEU:O     | 4:C:859:THR:HG23 | 1.92                     | 0.70              |
| 3:B:95:ARG:HD3    | 12:B:142:HOH:O   | 1.92                     | 0.69              |
| 1:I:125:DG:H1'    | 1:I:126:DA:C5'   | 2.22                     | 0.69              |
| 11:I:1971:DIB:HG2 | 1:J:226:DT:H4'   | 1.75                     | 0.69              |
| 1:J:227:DG:N7     | 12:J:2021:HOH:O  | 2.25                     | 0.69              |
| 1:I:133:DA:H2''   | 1:I:134:DG:C5'   | 2.23                     | 0.69              |
| 1:J:172:DC:H1'    | 1:J:173:DA:C5    | 2.28                     | 0.69              |
| 1:I:9:DC:H42      | 1:J:284:DG:H1    | 1.41                     | 0.69              |
| 1:I:31:DG:H2''    | 1:I:32:DT:H5'    | 1.74                     | 0.69              |
| 2:A:534:ARG:O     | 2:A:534:ARG:HG2  | 1.93                     | 0.68              |
| 2:E:663:ARG:NH1   | 12:E:774:HOH:O   | 2.27                     | 0.67              |
| 1:I:66:DC:H42     | 1:J:227:DG:H1    | 1.42                     | 0.67              |
| 1:J:174:DA:H2''   | 1:J:175:DA:C5'   | 2.19                     | 0.67              |
| 1:I:48:DT:H2''    | 1:I:49:DC:C5     | 2.30                     | 0.67              |
| 3:B:30:THR:HB     | 3:B:32:PRO:HD2   | 1.78                     | 0.66              |
| 1:J:151:DA:H2''   | 1:J:152:DT:C5'   | 2.26                     | 0.66              |
| 4:C:832:ARG:NH2   | 5:D:1232:GLU:OE2 | 2.27                     | 0.66              |
| 2:E:664:LYS:HE2   | 12:E:801:HOH:O   | 1.95                     | 0.66              |
| 1:I:125:DG:C1'    | 1:I:126:DA:H5'   | 2.25                     | 0.65              |
| 1:J:149:DC:H5''   | 1:J:149:DC:H6    | 1.60                     | 0.65              |
| 5:H:1445:VAL:HG12 | 5:H:1446:HIS:CD2 | 2.32                     | 0.65              |
| 1:J:253:DC:H4'    | 8:J:1924:PYB:CB  | 2.26                     | 0.65              |
| 1:I:129:DC:H2'    | 1:I:130:DT:H71   | 1.79                     | 0.65              |
| 1:J:181:DA:H2''   | 1:J:182:DT:OP2   | 1.95                     | 0.65              |
| 1:I:37:DT:H2''    | 1:I:38:DT:C5     | 2.32                     | 0.64              |
| 3:F:230:THR:HB    | 3:F:232:PRO:HD2  | 1.79                     | 0.64              |
| 1:I:68:DG:H1      | 1:J:225:DC:N4    | 1.96                     | 0.64              |
| 1:I:60:DC:H42     | 1:J:233:DG:H1    | 1.44                     | 0.64              |
| 1:J:249:DG:H22    | 8:J:1929:PYB:HB1 | 1.62                     | 0.64              |
| 1:I:93:DT:C2'     | 1:I:94:DG:H5''   | 2.22                     | 0.64              |
| 1:I:100:DG:OP1    | 3:F:279:LYS:HE2  | 1.97                     | 0.64              |
| 1:J:149:DC:H2''   | 1:J:150:DA:O5'   | 1.97                     | 0.64              |
| 1:J:182:DT:H2''   | 1:J:183:DT:C5'   | 2.28                     | 0.64              |
| 5:D:1281:ASN:O    | 5:D:1283:ARG:HD3 | 1.97                     | 0.64              |
| 1:I:31:DG:N2      | 1:I:32:DT:C2     | 2.67                     | 0.63              |
| 1:J:215:DC:OP1    | 2:E:642:ARG:NH1  | 2.26                     | 0.63              |
| 1:I:119:DT:H2''   | 1:I:120:DT:C5    | 2.34                     | 0.63              |
| 1:I:5:DA:H2''     | 1:I:6:DT:C5'     | 2.29                     | 0.63              |
| 1:I:116:DC:H4'    | 8:I:2029:PYB:NG2 | 2.13                     | 0.63              |
| 2:A:468:GLN:O     | 2:A:472:ARG:HG2  | 1.99                     | 0.63              |
| 3:F:287:VAL:CG1   | 3:F:302:GLY:HA3  | 2.28                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:J:182:DT:H1'   | 1:J:183:DT:H5''   | 1.81                     | 0.63              |
| 2:E:725:GLN:HB3  | 2:E:734:ARG:NH2   | 2.13                     | 0.62              |
| 1:J:149:DC:C2'   | 1:J:150:DA:C8     | 2.83                     | 0.62              |
| 1:I:22:DC:H2''   | 1:I:23:DT:O5'     | 2.00                     | 0.62              |
| 8:I:1962:PYB:O   | 8:I:1963:PYB:HB   | 2.01                     | 0.61              |
| 1:I:115:DA:H2    | 8:I:2029:PYB:HB1  | 1.66                     | 0.61              |
| 1:J:247:DC:H5    | 12:J:2019:HOH:O   | 1.82                     | 0.61              |
| 1:J:173:DA:H1'   | 1:J:174:DA:H5'    | 1.81                     | 0.60              |
| 3:F:277:LYS:HE2  | 5:H:1489:ARG:NH2  | 2.16                     | 0.60              |
| 1:J:151:DA:H2''  | 1:J:152:DT:H5''   | 1.83                     | 0.60              |
| 1:J:193:DC:H2''  | 1:J:194:DT:H71    | 1.83                     | 0.60              |
| 8:J:1927:PYB:O   | 8:J:1928:PYB:HB   | 2.01                     | 0.60              |
| 1:I:52:DT:H2''   | 1:I:53:DC:C5      | 2.37                     | 0.60              |
| 1:I:71:DG:N2     | 8:I:1969:PYB:HB1  | 2.16                     | 0.59              |
| 8:J:1902:PYB:O   | 8:J:1903:PYB:HB   | 2.02                     | 0.59              |
| 1:I:131:DG:H3'   | 4:G:1076:THR:HG22 | 1.84                     | 0.59              |
| 5:D:1289:ARG:HD3 | 12:D:406:HOH:O    | 2.03                     | 0.59              |
| 1:I:21:DT:H6     | 1:I:21:DT:H5'     | 1.67                     | 0.59              |
| 1:I:99:DA:H2''   | 1:I:100:DG:C5'    | 2.33                     | 0.59              |
| 1:J:184:DT:H2''  | 1:J:185:DG:N7     | 2.18                     | 0.59              |
| 1:I:58:DG:H2''   | 1:I:59:DG:O5'     | 2.02                     | 0.59              |
| 2:A:465:LEU:HB3  | 2:A:466:PRO:HD3   | 1.85                     | 0.59              |
| 1:I:44:DC:H4'    | 8:J:1928:PYB:CG1  | 2.34                     | 0.58              |
| 8:I:2022:PYB:O   | 8:I:2023:PYB:HB   | 2.03                     | 0.58              |
| 5:H:1464:ASN:O   | 5:H:1468:GLU:HG3  | 2.03                     | 0.58              |
| 1:I:32:DT:O4'    | 7:J:1901:IMT:NB1  | 2.37                     | 0.58              |
| 1:I:35:DA:H2''   | 1:I:36:DT:OP2     | 2.02                     | 0.57              |
| 1:J:260:DC:H2''  | 1:J:261:DA:C8     | 2.40                     | 0.57              |
| 1:I:31:DG:H2''   | 1:I:32:DT:C5'     | 2.33                     | 0.57              |
| 1:I:35:DA:H1'    | 1:I:36:DT:H5'     | 1.86                     | 0.57              |
| 1:J:248:DA:N3    | 10:J:1930:BAL:HA2 | 2.19                     | 0.57              |
| 1:J:170:DA:H2''  | 1:J:171:DC:OP2    | 2.05                     | 0.57              |
| 1:I:103:DG:N2    | 8:J:2009:PYB:HB1  | 2.19                     | 0.56              |
| 1:J:247:DC:C5    | 12:J:2019:HOH:O   | 2.52                     | 0.56              |
| 1:J:183:DT:H2'   | 1:J:184:DT:H71    | 1.87                     | 0.56              |
| 1:J:192:DG:H4'   | 8:J:2009:PYB:HD2  | 1.86                     | 0.56              |
| 1:I:99:DA:H2''   | 1:I:100:DG:H5'    | 1.88                     | 0.56              |
| 8:I:1963:PYB:O   | 8:I:1964:PYB:HB   | 2.05                     | 0.56              |
| 9:J:1905:ABU:OXT | 8:J:1906:PYB:HB   | 2.06                     | 0.56              |
| 1:I:114:DC:O2    | 8:I:2028:PYB:HB1  | 2.05                     | 0.56              |
| 4:C:855:LEU:O    | 4:C:859:THR:CG2   | 2.53                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:G:1063:LEU:HD13  | 5:H:1442:LEU:HB2  | 1.87                     | 0.56              |
| 4:G:1016:THR:HG23  | 4:G:1019:SER:OG   | 2.06                     | 0.56              |
| 3:F:289:ALA:O      | 3:F:293:GLN:HG3   | 2.06                     | 0.56              |
| 8:J:2002:PYB:O     | 8:J:2003:PYB:HB   | 2.06                     | 0.55              |
| 1:I:38:DT:H4'      | 4:C:842:ARG:HH21  | 1.71                     | 0.55              |
| 3:F:230:THR:CB     | 3:F:232:PRO:HD2   | 2.36                     | 0.55              |
| 8:I:1966:PYB:O     | 8:I:1967:PYB:HB   | 2.06                     | 0.55              |
| 2:A:458:THR:CG2    | 4:G:1081:ARG:HD3  | 2.37                     | 0.55              |
| 1:J:151:DA:C2'     | 1:J:152:DT:H5''   | 2.37                     | 0.55              |
| 3:B:84:MET:HE1     | 3:B:102:GLY:HA3   | 1.88                     | 0.55              |
| 1:J:284:DG:OP2     | 1:J:284:DG:H2'    | 2.07                     | 0.55              |
| 1:I:27:DA:H2''     | 1:I:28:DA:O5'     | 2.07                     | 0.54              |
| 1:J:182:DT:C2'     | 1:J:183:DT:H5''   | 2.37                     | 0.54              |
| 4:C:914:VAL:HG13   | 12:C:294:HOH:O    | 2.06                     | 0.54              |
| 7:I:1961:IMT:O     | 8:I:1962:PYB:HB   | 2.08                     | 0.54              |
| 1:J:197:DA:C5'     | 2:E:683:ARG:HD2   | 2.37                     | 0.54              |
| 2:E:680:THR:O      | 2:E:681:ASP:HB2   | 2.08                     | 0.54              |
| 1:I:74:DT:H2'      | 12:I:2085:HOH:O   | 2.08                     | 0.54              |
| 1:I:7:DA:C2        | 1:J:287:DA:C2     | 2.96                     | 0.54              |
| 8:I:1967:PYB:O     | 8:I:1968:PYB:HB   | 2.07                     | 0.54              |
| 2:E:729:ARG:HD2    | 2:E:729:ARG:O     | 2.08                     | 0.54              |
| 3:F:268:ASP:OD2    | 3:F:292:ARG:HD3   | 2.07                     | 0.54              |
| 1:I:126:DA:H1'     | 1:I:127:DA:O4'    | 2.07                     | 0.54              |
| 8:I:1968:PYB:O     | 8:I:1969:PYB:HB   | 2.06                     | 0.54              |
| 3:B:31:LYS:HB3     | 3:B:32:PRO:HD3    | 1.89                     | 0.53              |
| 3:F:231:LYS:O      | 3:F:235:ARG:HG2   | 2.08                     | 0.53              |
| 1:I:115:DA:N3      | 8:I:2029:PYB:HB1  | 2.23                     | 0.53              |
| 8:J:1902:PYB:O     | 8:J:1903:PYB:CB   | 2.56                     | 0.53              |
| 1:J:260:DC:O4'     | 8:J:1906:PYB:CB1  | 2.56                     | 0.53              |
| 8:J:1928:PYB:O     | 8:J:1929:PYB:HB   | 2.07                     | 0.53              |
| 8:J:2008:PYB:O     | 8:J:2009:PYB:HB   | 2.08                     | 0.53              |
| 1:J:147:DA:H2'     | 1:J:148:DT:C7     | 2.37                     | 0.53              |
| 1:J:180:DT:H2''    | 1:J:181:DA:C8     | 2.44                     | 0.52              |
| 11:J:1911:DIB:HE22 | 4:C:814:ALA:CB    | 2.26                     | 0.52              |
| 7:J:1901:IMT:O     | 8:J:1902:PYB:HB   | 2.09                     | 0.52              |
| 1:J:197:DA:H5''    | 2:E:683:ARG:CD    | 2.40                     | 0.52              |
| 1:I:72:DA:O4'      | 7:I:1961:IMT:CA   | 2.58                     | 0.52              |
| 8:J:2003:PYB:O     | 8:J:2004:PYB:HB   | 2.10                     | 0.52              |
| 1:I:117:DT:O4'     | 10:I:2030:BAL:HA1 | 2.10                     | 0.52              |
| 8:J:1928:PYB:O     | 8:J:1929:PYB:CB   | 2.57                     | 0.52              |
| 4:C:918:LYS:HE2    | 12:C:626:HOH:O    | 2.10                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:182:DT:H2''   | 1:J:183:DT:H5'    | 1.90                     | 0.51              |
| 3:F:277:LYS:HE2   | 5:H:1489:ARG:HH22 | 1.75                     | 0.51              |
| 1:I:116:DC:H4'    | 8:I:2029:PYB:HD2  | 1.92                     | 0.51              |
| 1:J:151:DA:H2''   | 1:J:152:DT:H5'    | 1.93                     | 0.51              |
| 1:J:255:DA:H2''   | 1:J:256:DA:OP2    | 2.09                     | 0.51              |
| 8:J:1927:PYB:O    | 8:J:1928:PYB:CB   | 2.57                     | 0.51              |
| 2:E:729:ARG:HD2   | 2:E:729:ARG:C     | 2.35                     | 0.51              |
| 4:C:837:GLY:HA3   | 4:C:839:TYR:CE2   | 2.46                     | 0.51              |
| 1:I:83:DA:H5''    | 2:E:640:ARG:HD3   | 1.92                     | 0.51              |
| 1:J:151:DA:OP2    | 2:A:436:LYS:HE2   | 2.11                     | 0.51              |
| 1:J:230:DC:H2''   | 1:J:231:DA:C8     | 2.46                     | 0.51              |
| 1:J:263:DT:H2''   | 1:J:264:DT:H72    | 1.93                     | 0.51              |
| 8:I:2022:PYB:O    | 8:I:2023:PYB:CB   | 2.54                     | 0.51              |
| 1:J:169:DT:C2     | 1:J:170:DA:C6     | 2.99                     | 0.51              |
| 1:J:268:DG:H8     | 1:J:268:DG:H5''   | 1.75                     | 0.51              |
| 8:I:2027:PYB:O    | 8:I:2028:PYB:HB   | 2.10                     | 0.50              |
| 1:J:241:DA:H2''   | 1:J:242:DT:O5'    | 2.12                     | 0.50              |
| 1:J:249:DG:H2''   | 1:J:250:DT:H71    | 1.93                     | 0.50              |
| 4:C:914:VAL:HG11  | 12:E:817:HOH:O    | 2.11                     | 0.50              |
| 4:G:1064:GLU:OE1  | 5:H:1445:VAL:HG13 | 2.11                     | 0.50              |
| 1:I:112:DT:H4'    | 9:I:2025:ABU:CG   | 2.41                     | 0.50              |
| 1:I:138:DG:H2''   | 1:I:139:DA:OP2    | 2.11                     | 0.50              |
| 1:I:116:DC:H4'    | 8:I:2029:PYB:CD   | 2.41                     | 0.50              |
| 3:B:24:ASP:CG     | 3:B:25:ASN:H      | 2.19                     | 0.50              |
| 1:I:48:DT:H2''    | 1:I:49:DC:H5      | 1.77                     | 0.50              |
| 1:J:172:DC:H1'    | 1:J:173:DA:N7     | 2.27                     | 0.50              |
| 8:I:1963:PYB:O    | 8:I:1964:PYB:CB   | 2.59                     | 0.50              |
| 1:J:197:DA:H5''   | 2:E:683:ARG:HD2   | 1.93                     | 0.50              |
| 11:I:1971:DIB:HA2 | 1:J:224:DG:H21    | 1.76                     | 0.50              |
| 2:E:728:ARG:HD2   | 2:E:733:GLU:OE1   | 2.12                     | 0.50              |
| 8:J:2007:PYB:O    | 8:J:2008:PYB:HB   | 2.12                     | 0.49              |
| 3:B:24:ASP:OD1    | 3:B:25:ASN:N      | 2.45                     | 0.49              |
| 2:E:665:LEU:HB3   | 2:E:666:PRO:HD3   | 1.94                     | 0.49              |
| 1:J:182:DT:H2''   | 1:J:183:DT:H5''   | 1.91                     | 0.49              |
| 1:I:24:DA:H2''    | 1:I:25:DC:OP2     | 2.11                     | 0.49              |
| 8:I:1968:PYB:O    | 8:I:1969:PYB:CB   | 2.59                     | 0.49              |
| 1:I:130:DT:C4     | 1:J:162:DC:N4     | 2.80                     | 0.49              |
| 7:I:2021:IMT:O    | 8:I:2022:PYB:HB   | 2.13                     | 0.49              |
| 2:A:438:PRO:HD2   | 2:A:439:HIS:H     | 1.78                     | 0.49              |
| 1:I:83:DA:C5'     | 2:E:640:ARG:HD3   | 2.43                     | 0.49              |
| 1:J:275:DC:N1     | 1:J:276:DT:H72    | 2.28                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:J:1903:PYB:O    | 8:J:1904:PYB:HB    | 2.13                     | 0.49              |
| 1:I:47:DC:O3'     | 11:J:1931:DIB:HE13 | 2.13                     | 0.48              |
| 3:B:24:ASP:CG     | 3:B:25:ASN:N       | 2.71                     | 0.48              |
| 4:C:869:ALA:O     | 4:C:873:ASN:ND2    | 2.41                     | 0.48              |
| 1:I:111:DA:C4'    | 4:G:1042:ARG:HH11  | 2.24                     | 0.48              |
| 8:J:2002:PYB:O    | 8:J:2003:PYB:CB    | 2.60                     | 0.48              |
| 4:G:1112:GLN:OE1  | 12:G:643:HOH:O     | 2.20                     | 0.48              |
| 4:C:867:GLY:HA3   | 5:D:1246:HIS:CD2   | 2.48                     | 0.48              |
| 4:G:1016:THR:HG23 | 4:G:1019:SER:CB    | 2.43                     | 0.48              |
| 4:G:1032:ARG:HH22 | 5:H:1432:GLU:CD    | 2.21                     | 0.48              |
| 1:I:21:DT:H5'     | 1:I:21:DT:C6       | 2.48                     | 0.48              |
| 1:I:114:DC:H42    | 1:J:179:DG:H1      | 1.61                     | 0.48              |
| 1:I:45:DT:O2      | 8:J:1929:PYB:C     | 2.62                     | 0.48              |
| 3:B:30:THR:CB     | 3:B:32:PRO:HD2     | 2.42                     | 0.48              |
| 1:I:8:DT:OP1      | 2:E:649:ARG:HD2    | 2.14                     | 0.48              |
| 1:I:5:DA:H1'      | 1:I:6:DT:H5''      | 1.95                     | 0.48              |
| 1:I:35:DA:H1'     | 1:I:36:DT:C5'      | 2.44                     | 0.48              |
| 1:I:38:DT:C4      | 1:I:39:DG:C6       | 3.02                     | 0.48              |
| 1:J:269:DT:OP1    | 4:C:829:ARG:NH2    | 2.47                     | 0.48              |
| 1:I:47:DC:N4      | 1:J:245:DA:N6      | 2.62                     | 0.47              |
| 1:I:124:DA:H2''   | 1:I:125:DG:N7      | 2.29                     | 0.47              |
| 1:I:128:DT:H1'    | 1:I:129:DC:H5'     | 1.97                     | 0.47              |
| 1:J:194:DT:H4'    | 11:J:2011:DIB:CE1  | 2.39                     | 0.47              |
| 1:J:207:DA:H5''   | 12:F:314:HOH:O     | 2.13                     | 0.47              |
| 1:J:259:DA:O4'    | 9:J:1905:ABU:CG    | 2.61                     | 0.47              |
| 2:A:444:GLY:O     | 2:A:448:LEU:HD13   | 2.14                     | 0.47              |
| 3:F:231:LYS:N     | 3:F:232:PRO:CD     | 2.78                     | 0.47              |
| 1:I:33:DG:H21     | 8:J:1903:PYB:H     | 1.61                     | 0.47              |
| 8:J:1923:PYB:O    | 8:J:1924:PYB:HB    | 2.13                     | 0.47              |
| 1:I:23:DT:O2      | 1:J:271:DG:N2      | 2.48                     | 0.47              |
| 8:J:1926:PYB:O    | 8:J:1927:PYB:HB    | 2.15                     | 0.47              |
| 1:I:77:DC:H42     | 1:J:216:DG:H1      | 1.63                     | 0.47              |
| 1:I:131:DG:H3'    | 4:G:1076:THR:CG2   | 2.45                     | 0.47              |
| 1:J:260:DC:O4'    | 8:J:1906:PYB:CA    | 2.63                     | 0.47              |
| 1:J:261:DA:H2''   | 1:J:262:DC:H5'     | 1.97                     | 0.47              |
| 1:J:263:DT:H2''   | 1:J:264:DT:C7      | 2.45                     | 0.47              |
| 3:F:220:LYS:HG2   | 3:F:221:VAL:N      | 2.30                     | 0.47              |
| 8:I:2023:PYB:O    | 8:I:2024:PYB:HB    | 2.14                     | 0.47              |
| 1:J:148:DT:H2''   | 1:J:149:DC:O5'     | 2.15                     | 0.47              |
| 1:J:245:DA:H2''   | 1:J:246:DG:OP2     | 2.15                     | 0.47              |
| 9:I:2025:ABU:OXT  | 8:I:2026:PYB:HB    | 2.15                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:F:231:LYS:HB3   | 3:F:232:PRO:HD3    | 1.97                     | 0.47              |
| 1:I:111:DA:H4'    | 4:G:1042:ARG:NH1   | 2.27                     | 0.47              |
| 4:G:1079:ILE:HG12 | 4:G:1082:HIS:CE1   | 2.50                     | 0.47              |
| 1:I:112:DT:H5'    | 4:G:1042:ARG:HD3   | 1.96                     | 0.46              |
| 4:G:1064:GLU:HA   | 5:H:1445:VAL:HG11  | 1.95                     | 0.46              |
| 1:I:45:DT:H2''    | 1:I:46:DG:C8       | 2.50                     | 0.46              |
| 1:I:44:DC:H4'     | 8:J:1928:PYB:NG2   | 2.29                     | 0.46              |
| 1:I:32:DT:O4'     | 7:J:1901:IMT:CA    | 2.64                     | 0.46              |
| 8:I:1966:PYB:O    | 8:I:1967:PYB:CB    | 2.60                     | 0.46              |
| 1:J:149:DC:H2'    | 1:J:150:DA:H8      | 1.77                     | 0.46              |
| 1:J:259:DA:H2''   | 1:J:260:DC:C6      | 2.51                     | 0.46              |
| 1:I:94:DG:H2''    | 1:I:95:DA:O5'      | 2.15                     | 0.46              |
| 8:J:1908:PYB:O    | 8:J:1909:PYB:HB    | 2.16                     | 0.46              |
| 8:J:2008:PYB:O    | 8:J:2009:PYB:CB    | 2.62                     | 0.46              |
| 4:G:1076:THR:O    | 5:H:1449:THR:HG23  | 2.15                     | 0.46              |
| 4:G:1079:ILE:HB   | 4:G:1080:PRO:CD    | 2.46                     | 0.46              |
| 1:I:27:DA:H5''    | 12:I:2086:HOH:O    | 2.16                     | 0.46              |
| 8:I:2027:PYB:O    | 8:I:2028:PYB:CB    | 2.63                     | 0.46              |
| 7:J:1921:IMT:O    | 8:J:1922:PYB:HB    | 2.15                     | 0.46              |
| 1:I:72:DA:O4'     | 7:I:1961:IMT:NB1   | 2.49                     | 0.46              |
| 1:I:127:DA:N3     | 1:I:128:DT:C2      | 2.83                     | 0.46              |
| 1:J:191:DT:H5'    | 8:J:2008:PYB:C     | 2.46                     | 0.46              |
| 1:I:125:DG:C6     | 1:I:126:DA:C5      | 3.05                     | 0.45              |
| 1:I:133:DA:C2'    | 1:I:134:DG:H5''    | 2.46                     | 0.45              |
| 1:J:257:DA:C8     | 1:J:258:DT:H72     | 2.52                     | 0.45              |
| 5:D:1300:PRO:HG3  | 12:D:476:HOH:O     | 2.16                     | 0.45              |
| 1:I:127:DA:C4     | 1:I:128:DT:C4      | 3.03                     | 0.45              |
| 8:I:2028:PYB:O    | 8:I:2029:PYB:HB    | 2.16                     | 0.45              |
| 1:J:271:DG:H2''   | 1:J:272:DA:OP2     | 2.16                     | 0.45              |
| 5:D:1279:HIS:HB3  | 12:D:422:HOH:O     | 2.15                     | 0.45              |
| 4:G:1087:VAL:HG12 | 4:G:1088:ARG:HD3   | 1.97                     | 0.45              |
| 8:J:1907:PYB:O    | 8:J:1908:PYB:HB    | 2.16                     | 0.45              |
| 3:F:287:VAL:HG11  | 3:F:302:GLY:CA     | 2.35                     | 0.45              |
| 1:I:47:DC:C3'     | 11:J:1931:DIB:HE13 | 2.47                     | 0.45              |
| 1:I:127:DA:C2     | 1:I:128:DT:N3      | 2.85                     | 0.45              |
| 8:J:1923:PYB:O    | 8:J:1924:PYB:CB    | 2.64                     | 0.45              |
| 4:G:1037:GLY:O    | 4:G:1038:ASN:HB2   | 2.15                     | 0.45              |
| 1:I:66:DC:N4      | 1:J:227:DG:H1      | 2.10                     | 0.45              |
| 1:J:268:DG:H5''   | 1:J:268:DG:C8      | 2.52                     | 0.45              |
| 2:A:464:LYS:HE2   | 2:A:490:MET:HE1    | 1.99                     | 0.45              |
| 5:D:1245:VAL:HG23 | 5:D:1246:HIS:CD2   | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:111:DA:C2'    | 1:I:112:DT:H71    | 2.46                     | 0.45              |
| 1:J:197:DA:H5'    | 2:E:683:ARG:HD2   | 1.99                     | 0.45              |
| 2:A:437:LYS:HA    | 2:A:438:PRO:HD3   | 1.53                     | 0.45              |
| 12:B:120:HOH:O    | 5:D:1296:ARG:HD3  | 2.16                     | 0.45              |
| 4:G:1016:THR:HG23 | 4:G:1019:SER:HG   | 1.81                     | 0.45              |
| 5:D:1299:LEU:HA   | 5:D:1300:PRO:HD3  | 1.77                     | 0.45              |
| 5:H:1443:LYS:HA   | 5:H:1443:LYS:HD3  | 1.57                     | 0.45              |
| 1:I:21:DT:C2      | 1:J:273:DA:C2     | 3.05                     | 0.44              |
| 7:J:2001:IMT:O    | 8:J:2002:PYB:HB   | 2.17                     | 0.44              |
| 8:J:2003:PYB:O    | 8:J:2004:PYB:CB   | 2.63                     | 0.44              |
| 1:J:192:DG:H2''   | 1:J:193:DC:O5'    | 2.18                     | 0.44              |
| 8:J:1907:PYB:O    | 8:J:1908:PYB:CB   | 2.63                     | 0.44              |
| 2:E:663:ARG:CD    | 12:E:774:HOH:O    | 2.65                     | 0.44              |
| 4:G:1092:GLU:HB3  | 5:H:1503:LEU:HD22 | 1.98                     | 0.44              |
| 7:I:1961:IMT:O    | 8:I:1962:PYB:CB   | 2.61                     | 0.44              |
| 7:I:2021:IMT:CA   | 1:J:179:DG:O4'    | 2.66                     | 0.44              |
| 1:I:36:DT:H2''    | 1:I:37:DT:H5''    | 1.98                     | 0.44              |
| 1:J:165:DA:C2     | 1:J:166:DT:N3     | 2.85                     | 0.44              |
| 5:D:1254:LYS:O    | 5:D:1258:ILE:HG12 | 2.17                     | 0.44              |
| 1:J:147:DA:C2'    | 1:J:148:DT:H72    | 2.43                     | 0.44              |
| 8:J:1922:PYB:O    | 8:J:1923:PYB:CB   | 2.65                     | 0.44              |
| 1:I:127:DA:H2''   | 1:I:128:DT:C6     | 2.52                     | 0.44              |
| 1:J:169:DT:H2''   | 1:J:170:DA:C8     | 2.53                     | 0.44              |
| 1:I:46:DG:H2''    | 1:I:47:DC:C5      | 2.53                     | 0.44              |
| 1:I:46:DG:H1'     | 1:I:47:DC:C5      | 2.52                     | 0.44              |
| 8:I:1962:PYB:O    | 8:I:1963:PYB:CB   | 2.56                     | 0.44              |
| 9:J:1905:ABU:OXT  | 8:J:1906:PYB:CB   | 2.60                     | 0.44              |
| 2:A:438:PRO:CD    | 2:A:439:HIS:H     | 2.31                     | 0.44              |
| 1:I:75:DT:H4'     | 8:I:1964:PYB:CB   | 2.48                     | 0.43              |
| 2:A:534:ARG:C     | 2:A:535:ALA:OXT   | 2.61                     | 0.43              |
| 7:J:1901:IMT:O    | 8:J:1902:PYB:CB   | 2.63                     | 0.43              |
| 8:J:2007:PYB:O    | 8:J:2008:PYB:CB   | 2.65                     | 0.43              |
| 8:I:1968:PYB:O    | 8:I:1968:PYB:HD1  | 2.17                     | 0.43              |
| 8:J:2006:PYB:O    | 8:J:2007:PYB:HB   | 2.18                     | 0.43              |
| 1:J:177:DG:OP1    | 4:G:1017:ARG:HG3  | 2.19                     | 0.43              |
| 2:A:437:LYS:H     | 2:A:437:LYS:HD2   | 1.82                     | 0.43              |
| 5:D:1269:ARG:HD3  | 12:D:275:HOH:O    | 2.16                     | 0.43              |
| 1:I:59:DG:H2''    | 1:I:60:DC:C6      | 2.53                     | 0.43              |
| 1:I:102:DA:H2''   | 1:I:103:DG:C8     | 2.54                     | 0.43              |
| 1:I:120:DT:H2''   | 1:I:121:DG:C8     | 2.54                     | 0.43              |
| 1:I:124:DA:H2''   | 1:I:125:DG:C8     | 2.54                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:173:DA:C1'    | 1:J:174:DA:H5'    | 2.47                     | 0.43              |
| 1:J:182:DT:C1'    | 1:J:183:DT:H5''   | 2.47                     | 0.43              |
| 1:J:267:DG:H2''   | 1:J:268:DG:O5'    | 2.18                     | 0.43              |
| 3:F:228:GLY:HA3   | 12:F:326:HOH:O    | 2.18                     | 0.43              |
| 8:I:1967:PYB:O    | 8:I:1968:PYB:CB   | 2.59                     | 0.43              |
| 8:J:1903:PYB:O    | 8:J:1904:PYB:CB   | 2.64                     | 0.43              |
| 2:A:524:ILE:O     | 2:A:528:ARG:HG3   | 2.18                     | 0.43              |
| 4:C:817:ARG:HD2   | 5:D:1318:TYR:OH   | 2.18                     | 0.43              |
| 4:G:1016:THR:HG23 | 4:G:1019:SER:HB3  | 2.00                     | 0.43              |
| 1:I:38:DT:H4'     | 4:C:842:ARG:NH2   | 2.34                     | 0.43              |
| 1:I:61:DA:N6      | 12:I:2076:HOH:O   | 2.51                     | 0.43              |
| 2:A:438:PRO:HD2   | 2:A:439:HIS:N     | 2.34                     | 0.43              |
| 4:G:1017:ARG:NH2  | 4:G:1031:HIS:HD2  | 2.12                     | 0.43              |
| 1:I:37:DT:C2'     | 1:I:38:DT:C5      | 3.00                     | 0.43              |
| 1:I:100:DG:H2''   | 1:I:101:DC:C6     | 2.54                     | 0.43              |
| 12:J:2027:HOH:O   | 4:C:875:LYS:HE2   | 2.18                     | 0.43              |
| 1:I:28:DA:H1'     | 1:I:29:DA:C8      | 2.54                     | 0.43              |
| 8:I:2023:PYB:O    | 8:I:2024:PYB:CB   | 2.66                     | 0.43              |
| 11:I:2031:DIB:HA2 | 1:J:177:DG:H21    | 1.83                     | 0.43              |
| 1:J:183:DT:H2''   | 1:J:184:DT:C6     | 2.53                     | 0.43              |
| 1:J:192:DG:C4'    | 8:J:2009:PYB:HD2  | 2.49                     | 0.43              |
| 12:A:582:HOH:O    | 2:E:722:LYS:HE3   | 2.19                     | 0.43              |
| 4:G:1032:ARG:NH2  | 5:H:1432:GLU:OE2  | 2.52                     | 0.42              |
| 8:I:2028:PYB:O    | 8:I:2029:PYB:CB   | 2.67                     | 0.42              |
| 1:J:174:DA:H4'    | 5:H:1430:ARG:HD3  | 2.01                     | 0.42              |
| 4:G:1015:LYS:C    | 4:G:1016:THR:HG22 | 2.44                     | 0.42              |
| 1:J:260:DC:H2''   | 1:J:261:DA:H8     | 1.85                     | 0.42              |
| 4:G:1016:THR:O    | 4:G:1020:ARG:HG2  | 2.19                     | 0.42              |
| 5:H:1499:LEU:HA   | 5:H:1500:PRO:HD3  | 1.81                     | 0.42              |
| 1:I:21:DT:O2      | 1:J:273:DA:C2     | 2.73                     | 0.42              |
| 1:I:101:DC:H2''   | 1:I:102:DA:C8     | 2.54                     | 0.42              |
| 8:I:2024:PYB:CD   | 1:J:183:DT:H4'    | 2.50                     | 0.42              |
| 1:I:116:DC:H4'    | 8:I:2029:PYB:CB   | 2.49                     | 0.42              |
| 10:I:2030:BAL:HB3 | 1:J:178:DT:O2     | 2.20                     | 0.42              |
| 5:D:1261:SER:OG   | 3:F:302:GLY:O     | 2.29                     | 0.42              |
| 1:I:99:DA:H2''    | 1:I:100:DG:H5''   | 2.01                     | 0.42              |
| 8:I:2024:PYB:HD2  | 1:J:183:DT:H4'    | 2.01                     | 0.42              |
| 1:I:123:DT:H2''   | 1:I:124:DA:C8     | 2.55                     | 0.42              |
| 4:G:1102:ILE:HG23 | 5:H:1458:ILE:HD13 | 2.02                     | 0.42              |
| 1:I:99:DA:H1'     | 1:I:100:DG:H5''   | 2.02                     | 0.42              |
| 1:I:99:DA:C2'     | 1:I:100:DG:H5''   | 2.49                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:I:2024:PYB:O     | 1:J:183:DT:H4'    | 2.20                     | 0.41              |
| 4:C:881:ARG:HB2    | 2:E:658:THR:HG21  | 2.01                     | 0.41              |
| 1:I:36:DT:H4'      | 8:J:1904:PYB:C    | 2.49                     | 0.41              |
| 1:I:44:DC:H3'      | 12:I:2109:HOH:O   | 2.21                     | 0.41              |
| 1:I:45:DT:H5'      | 8:J:1928:PYB:O    | 2.19                     | 0.41              |
| 1:J:151:DA:H1'     | 1:J:152:DT:H5''   | 2.02                     | 0.41              |
| 1:J:259:DA:O4'     | 9:J:1905:ABU:CB   | 2.68                     | 0.41              |
| 4:G:1079:ILE:HB    | 4:G:1080:PRO:HD2  | 2.02                     | 0.41              |
| 1:I:133:DA:H1'     | 1:I:134:DG:H5''   | 2.03                     | 0.41              |
| 7:I:2021:IMT:O     | 8:I:2022:PYB:CB   | 2.66                     | 0.41              |
| 8:J:1906:PYB:O     | 8:J:1907:PYB:HB   | 2.20                     | 0.41              |
| 1:I:21:DT:C2       | 1:J:273:DA:H2     | 2.38                     | 0.41              |
| 1:I:106:DT:H4'     | 8:J:2003:PYB:CG1  | 2.51                     | 0.41              |
| 2:E:650:GLU:HB3    | 3:F:239:ARG:HG3   | 2.02                     | 0.41              |
| 1:I:40:DG:OP2      | 5:D:1283:ARG:NH2  | 2.53                     | 0.41              |
| 9:J:2005:ABU:OXT   | 8:J:2006:PYB:HB   | 2.20                     | 0.41              |
| 2:A:533:GLU:O      | 2:A:534:ARG:HB3   | 2.19                     | 0.41              |
| 1:I:91:DT:H5''     | 2:E:663:ARG:NH2   | 2.36                     | 0.41              |
| 2:A:468:GLN:OE1    | 2:A:472:ARG:NH2   | 2.53                     | 0.41              |
| 5:D:1267:PHE:CD1   | 5:D:1267:PHE:C    | 2.98                     | 0.41              |
| 1:I:36:DT:C2'      | 1:I:37:DT:H5''    | 2.50                     | 0.41              |
| 1:I:50:DC:H2''     | 1:I:51:DA:C8      | 2.55                     | 0.41              |
| 1:I:98:DG:H1'      | 1:I:99:DA:N7      | 2.36                     | 0.41              |
| 1:J:259:DA:OP1     | 4:C:842:ARG:HA    | 2.20                     | 0.41              |
| 1:J:262:DC:O4'     | 8:J:1908:PYB:CB1  | 2.69                     | 0.41              |
| 8:J:1926:PYB:O     | 8:J:1927:PYB:CB   | 2.67                     | 0.41              |
| 1:I:141:DA:C2      | 1:J:153:DA:C2     | 3.09                     | 0.40              |
| 11:I:2031:DIB:HE22 | 1:J:177:DG:O4'    | 2.21                     | 0.40              |
| 1:J:194:DT:H2''    | 1:J:195:DC:C6     | 2.56                     | 0.40              |
| 8:I:1967:PYB:O     | 8:I:1967:PYB:HD3  | 2.20                     | 0.40              |
| 1:J:187:DA:C6      | 1:J:188:DA:N6     | 2.89                     | 0.40              |
| 4:C:829:ARG:HG3    | 4:C:832:ARG:HH12  | 1.86                     | 0.40              |
| 4:C:879:ILE:HB     | 4:C:880:PRO:CD    | 2.52                     | 0.40              |
| 1:I:70:DG:H21      | 10:I:1970:BAL:HA2 | 1.86                     | 0.40              |
| 8:I:2026:PYB:O     | 8:I:2027:PYB:HB   | 2.20                     | 0.40              |
| 1:J:188:DA:C2'     | 1:J:189:DA:O5'    | 2.66                     | 0.40              |
| 8:J:1908:PYB:O     | 8:J:1909:PYB:CB   | 2.68                     | 0.40              |
| 4:C:871:ARG:NH2    | 12:C:638:HOH:O    | 2.53                     | 0.40              |
| 1:I:106:DT:H4'     | 8:J:2003:PYB:NG2  | 2.36                     | 0.40              |
| 1:I:138:DG:H4'     | 12:I:2105:HOH:O   | 2.21                     | 0.40              |
| 7:J:1921:IMT:O     | 8:J:1922:PYB:CB   | 2.68                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:J:184:DT:H2'' | 1:J:185:DG:C8   | 2.56                     | 0.40              |
| 1:J:262:DC:O4'  | 8:J:1908:PYB:CA | 2.69                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2   | A     | 98/135 (73%)  | 95 (97%)  | 1 (1%)  | 2 (2%)   | 6           | 5   |
| 2   | E     | 96/135 (71%)  | 96 (100%) | 0       | 0        | 100         | 100 |
| 3   | B     | 77/102 (76%)  | 76 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 3   | F     | 84/102 (82%)  | 82 (98%)  | 1 (1%)  | 1 (1%)   | 10          | 12  |
| 4   | C     | 105/129 (81%) | 103 (98%) | 1 (1%)  | 1 (1%)   | 12          | 15  |
| 4   | G     | 103/129 (80%) | 100 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 5   | D     | 92/125 (74%)  | 90 (98%)  | 1 (1%)  | 1 (1%)   | 11          | 13  |
| 5   | H     | 92/125 (74%)  | 90 (98%)  | 1 (1%)  | 1 (1%)   | 11          | 13  |
| All | All   | 747/982 (76%) | 732 (98%) | 9 (1%)  | 6 (1%)   | 16          | 20  |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | A     | 438  | PRO  |
| 2   | A     | 439  | HIS  |
| 5   | H     | 1501 | GLY  |
| 4   | C     | 919  | LYS  |
| 5   | D     | 1301 | GLY  |
| 3   | F     | 218  | HIS  |

### 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 |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2   | A     | 87/111 (78%)  | 77 (88%)  | 10 (12%) | 5           | 6  |
| 2   | E     | 85/111 (77%)  | 79 (93%)  | 6 (7%)   | 13          | 19 |
| 3   | B     | 64/78 (82%)   | 60 (94%)  | 4 (6%)   | 16          | 23 |
| 3   | F     | 71/78 (91%)   | 66 (93%)  | 5 (7%)   | 14          | 19 |
| 4   | C     | 85/100 (85%)  | 79 (93%)  | 6 (7%)   | 13          | 19 |
| 4   | G     | 84/100 (84%)  | 80 (95%)  | 4 (5%)   | 23          | 35 |
| 5   | D     | 80/105 (76%)  | 76 (95%)  | 4 (5%)   | 22          | 33 |
| 5   | H     | 80/105 (76%)  | 74 (92%)  | 6 (8%)   | 12          | 17 |
| All | All   | 636/788 (81%) | 591 (93%) | 45 (7%)  | 13          | 19 |

All (45) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 437 | LYS  |
| 2   | A     | 442 | ARG  |
| 2   | A     | 452 | ARG  |
| 2   | A     | 453 | ARG  |
| 2   | A     | 459 | GLU  |
| 2   | A     | 468 | GLN  |
| 2   | A     | 472 | ARG  |
| 2   | A     | 528 | ARG  |
| 2   | A     | 529 | ARG  |
| 2   | A     | 534 | ARG  |
| 3   | B     | 45  | ARG  |
| 3   | B     | 47  | SER  |
| 3   | B     | 92  | ARG  |
| 3   | B     | 95  | ARG  |
| 4   | C     | 829 | ARG  |
| 4   | C     | 832 | ARG  |
| 4   | C     | 859 | THR  |
| 4   | C     | 873 | ASN  |
| 4   | C     | 881 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | C     | 918  | LYS  |
| 5   | D     | 1254 | LYS  |
| 5   | D     | 1277 | LEU  |
| 5   | D     | 1283 | ARG  |
| 5   | D     | 1289 | ARG  |
| 2   | E     | 642  | ARG  |
| 2   | E     | 653  | ARG  |
| 2   | E     | 659  | GLU  |
| 2   | E     | 683  | ARG  |
| 2   | E     | 726  | LEU  |
| 2   | E     | 729  | ARG  |
| 3   | F     | 217  | ARG  |
| 3   | F     | 219  | ARG  |
| 3   | F     | 235  | ARG  |
| 3   | F     | 245  | ARG  |
| 3   | F     | 292  | ARG  |
| 4   | G     | 1016 | THR  |
| 4   | G     | 1020 | ARG  |
| 4   | G     | 1042 | ARG  |
| 4   | G     | 1071 | ARG  |
| 5   | H     | 1433 | SER  |
| 5   | H     | 1483 | ARG  |
| 5   | H     | 1484 | SER  |
| 5   | H     | 1489 | ARG  |
| 5   | H     | 1496 | ARG  |
| 5   | H     | 1503 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | C     | 838  | ASN  |
| 5   | D     | 1264 | ASN  |
| 5   | D     | 1292 | GLN  |
| 4   | G     | 1031 | HIS  |
| 4   | G     | 1073 | ASN  |
| 5   | H     | 1506 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 66 ligands modelled in this entry, 11 are monoatomic - leaving 55 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$ |
| 9   | ABU  | J     | 2005 | 8    | 5,5,6        | 1.64 | 1 (20%)     | 4,4,6       | 0.46 | 0           |
| 8   | PYB  | J     | 2006 | 8,9  | 8,9,10       | 1.84 | 3 (37%)     | 6,12,14     | 2.83 | 3 (50%)     |
| 8   | PYB  | J     | 2008 | 8    | 8,9,10       | 1.67 | 2 (25%)     | 6,12,14     | 2.89 | 2 (33%)     |
| 8   | PYB  | I     | 1966 | 8,9  | 8,9,10       | 1.93 | 3 (37%)     | 6,12,14     | 2.92 | 3 (50%)     |
| 8   | PYB  | J     | 1929 | 8,10 | 8,9,10       | 1.69 | 2 (25%)     | 6,12,14     | 2.79 | 3 (50%)     |
| 8   | PYB  | I     | 1964 | 8,9  | 8,9,10       | 1.92 | 3 (37%)     | 6,12,14     | 2.75 | 3 (50%)     |
| 8   | PYB  | J     | 1907 | 8    | 8,9,10       | 1.81 | 3 (37%)     | 6,12,14     | 2.92 | 2 (33%)     |
| 11  | DIB  | J     | 1931 | 10   | 6,6,6        | 0.74 | 0           | 6,6,6       | 0.42 | 0           |
| 8   | PYB  | J     | 1904 | 8,9  | 8,9,10       | 1.95 | 3 (37%)     | 6,12,14     | 2.73 | 4 (66%)     |
| 8   | PYB  | J     | 1903 | 8    | 8,9,10       | 1.73 | 3 (37%)     | 6,12,14     | 2.98 | 2 (33%)     |
| 8   | PYB  | J     | 1922 | 8,7  | 8,9,10       | 1.59 | 2 (25%)     | 6,12,14     | 2.93 | 3 (50%)     |
| 8   | PYB  | J     | 1928 | 8    | 8,9,10       | 1.46 | 2 (25%)     | 6,12,14     | 2.99 | 3 (50%)     |
| 8   | PYB  | J     | 2003 | 8    | 8,9,10       | 1.64 | 3 (37%)     | 6,12,14     | 2.90 | 2 (33%)     |
| 8   | PYB  | I     | 2023 | 8    | 8,9,10       | 1.55 | 2 (25%)     | 6,12,14     | 2.83 | 3 (50%)     |
| 9   | ABU  | I     | 1965 | 8    | 5,5,6        | 1.62 | 1 (20%)     | 4,4,6       | 0.44 | 0           |
| 8   | PYB  | J     | 1926 | 8,9  | 8,9,10       | 1.91 | 3 (37%)     | 6,12,14     | 2.84 | 3 (50%)     |
| 8   | PYB  | J     | 2004 | 8,9  | 8,9,10       | 1.77 | 2 (25%)     | 6,12,14     | 2.69 | 3 (50%)     |
| 7   | IMT  | J     | 2001 | 8    | 7,8,10       | 1.93 | 4 (57%)     | 9,10,14     | 2.23 | 5 (55%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 8   | PYB  | J     | 2009 | 8,10 | 8,9,10       | 1.79 | 3 (37%)  | 6,12,14     | 2.90 | 3 (50%)  |
| 7   | IMT  | J     | 1921 | 8    | 7,8,10       | 2.23 | 4 (57%)  | 9,10,14     | 2.28 | 5 (55%)  |
| 8   | PYB  | I     | 1962 | 8,7  | 8,9,10       | 1.68 | 3 (37%)  | 6,12,14     | 3.05 | 2 (33%)  |
| 9   | ABU  | J     | 1905 | 8    | 5,5,6        | 1.68 | 1 (20%)  | 4,4,6       | 0.45 | 0        |
| 8   | PYB  | I     | 2022 | 8,7  | 8,9,10       | 1.56 | 2 (25%)  | 6,12,14     | 2.97 | 2 (33%)  |
| 9   | ABU  | J     | 1925 | 8    | 5,5,6        | 1.63 | 1 (20%)  | 4,4,6       | 0.51 | 0        |
| 8   | PYB  | I     | 1968 | 8    | 8,9,10       | 1.65 | 3 (37%)  | 6,12,14     | 2.97 | 2 (33%)  |
| 7   | IMT  | J     | 1901 | 8    | 7,8,10       | 2.00 | 3 (42%)  | 9,10,14     | 2.32 | 5 (55%)  |
| 8   | PYB  | I     | 1969 | 8,10 | 8,9,10       | 1.94 | 3 (37%)  | 6,12,14     | 2.76 | 3 (50%)  |
| 8   | PYB  | J     | 1906 | 8,9  | 8,9,10       | 1.64 | 3 (37%)  | 6,12,14     | 2.99 | 2 (33%)  |
| 8   | PYB  | J     | 1923 | 8    | 8,9,10       | 1.67 | 3 (37%)  | 6,12,14     | 2.91 | 3 (50%)  |
| 11  | DIB  | I     | 1971 | 10   | 6,6,6        | 0.73 | 0        | 6,6,6       | 0.46 | 0        |
| 11  | DIB  | I     | 2031 | 10   | 6,6,6        | 0.71 | 0        | 6,6,6       | 0.47 | 0        |
| 10  | BAL  | I     | 1970 | 8,11 | 3,4,5        | 0.44 | 0        | 3,3,5       | 1.09 | 0        |
| 8   | PYB  | I     | 1963 | 8    | 8,9,10       | 1.50 | 2 (25%)  | 6,12,14     | 3.00 | 2 (33%)  |
| 8   | PYB  | I     | 2027 | 8    | 8,9,10       | 1.81 | 3 (37%)  | 6,12,14     | 2.94 | 3 (50%)  |
| 8   | PYB  | J     | 2002 | 8,7  | 8,9,10       | 1.60 | 3 (37%)  | 6,12,14     | 2.92 | 3 (50%)  |
| 7   | IMT  | I     | 2021 | 8    | 7,8,10       | 1.84 | 3 (42%)  | 9,10,14     | 2.22 | 4 (44%)  |
| 10  | BAL  | I     | 2030 | 8,11 | 3,4,5        | 0.48 | 0        | 3,3,5       | 1.08 | 0        |
| 8   | PYB  | I     | 2024 | 8,9  | 8,9,10       | 1.81 | 3 (37%)  | 6,12,14     | 2.72 | 3 (50%)  |
| 10  | BAL  | J     | 1910 | 8,11 | 3,4,5        | 0.46 | 0        | 3,3,5       | 1.00 | 0        |
| 8   | PYB  | J     | 1909 | 8,10 | 8,9,10       | 2.01 | 3 (37%)  | 6,12,14     | 2.83 | 4 (66%)  |
| 10  | BAL  | J     | 1930 | 8,11 | 3,4,5        | 0.46 | 0        | 3,3,5       | 0.98 | 0        |
| 10  | BAL  | J     | 2010 | 8,11 | 3,4,5        | 0.63 | 0        | 3,3,5       | 1.32 | 0        |
| 8   | PYB  | J     | 1908 | 8    | 8,9,10       | 1.66 | 2 (25%)  | 6,12,14     | 2.86 | 2 (33%)  |
| 8   | PYB  | J     | 1924 | 8,9  | 8,9,10       | 1.71 | 3 (37%)  | 6,12,14     | 2.81 | 3 (50%)  |
| 8   | PYB  | I     | 1967 | 8    | 8,9,10       | 1.54 | 2 (25%)  | 6,12,14     | 2.89 | 2 (33%)  |
| 8   | PYB  | I     | 2029 | 8,10 | 8,9,10       | 1.82 | 3 (37%)  | 6,12,14     | 2.77 | 4 (66%)  |
| 8   | PYB  | I     | 2028 | 8    | 8,9,10       | 1.67 | 3 (37%)  | 6,12,14     | 2.86 | 2 (33%)  |
| 7   | IMT  | I     | 1961 | 8    | 7,8,10       | 2.04 | 4 (57%)  | 9,10,14     | 2.24 | 4 (44%)  |
| 11  | DIB  | J     | 2011 | 10   | 6,6,6        | 0.70 | 0        | 6,6,6       | 0.57 | 0        |
| 8   | PYB  | J     | 2007 | 8    | 8,9,10       | 1.77 | 3 (37%)  | 6,12,14     | 2.82 | 2 (33%)  |
| 8   | PYB  | J     | 1902 | 8,7  | 8,9,10       | 1.62 | 2 (25%)  | 6,12,14     | 2.97 | 3 (50%)  |
| 11  | DIB  | J     | 1911 | 10   | 6,6,6        | 0.64 | 0        | 6,6,6       | 0.36 | 0        |
| 8   | PYB  | I     | 2026 | 8,9  | 8,9,10       | 1.73 | 3 (37%)  | 6,12,14     | 2.86 | 3 (50%)  |
| 9   | ABU  | I     | 2025 | 8    | 5,5,6        | 1.63 | 1 (20%)  | 4,4,6       | 0.45 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 8   | PYB  | J     | 1927 | 8    | 8,9,10       | 1.67 | 2 (25%)  | 6,12,14     | 2.90 | 3 (50%)  |

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   |
|-----|------|-------|------|------|---------|----------|---------|
| 9   | ABU  | J     | 2005 | 8    | -       | 3/3/3/4  | -       |
| 8   | PYB  | J     | 2006 | 8,9  | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | J     | 2008 | 8    | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | I     | 1966 | 8,9  | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | J     | 1929 | 8,10 | -       | 2/2/2/4  | 0/1/1/1 |
| 8   | PYB  | I     | 1964 | 8,9  | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | J     | 1907 | 8    | -       | 0/2/2/4  | 0/1/1/1 |
| 11  | DIB  | J     | 1931 | 10   | -       | 1/4/4/4  | -       |
| 8   | PYB  | J     | 1904 | 8,9  | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | J     | 1903 | 8    | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | J     | 1922 | 8,7  | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | J     | 1928 | 8    | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | J     | 2003 | 8    | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | I     | 2023 | 8    | -       | 0/2/2/4  | 0/1/1/1 |
| 9   | ABU  | I     | 1965 | 8    | -       | 3/3/3/4  | -       |
| 8   | PYB  | J     | 1926 | 8,9  | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | J     | 2004 | 8,9  | -       | 0/2/2/4  | 0/1/1/1 |
| 7   | IMT  | J     | 2001 | 8    | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | J     | 2009 | 8,10 | -       | 0/2/2/4  | 0/1/1/1 |
| 7   | IMT  | J     | 1921 | 8    | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | I     | 1962 | 8,7  | -       | 1/2/2/4  | 0/1/1/1 |
| 9   | ABU  | J     | 1905 | 8    | -       | 2/3/3/4  | -       |
| 8   | PYB  | I     | 2022 | 8,7  | -       | 0/2/2/4  | 0/1/1/1 |
| 9   | ABU  | J     | 1925 | 8    | -       | 3/3/3/4  | -       |
| 8   | PYB  | I     | 1968 | 8    | -       | 0/2/2/4  | 0/1/1/1 |
| 7   | IMT  | J     | 1901 | 8    | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | I     | 1969 | 8,10 | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | J     | 1906 | 8,9  | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | J     | 1923 | 8    | -       | 0/2/2/4  | 0/1/1/1 |
| 11  | DIB  | I     | 1971 | 10   | -       | 0/4/4/4  | -       |
| 11  | DIB  | I     | 2031 | 10   | -       | 1/4/4/4  | -       |
| 10  | BAL  | I     | 1970 | 8,11 | -       | 0/1/2/3  | -       |
| 8   | PYB  | I     | 1963 | 8    | -       | 0/2/2/4  | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 8   | PYB  | I     | 2027 | 8    | -       | 1/2/2/4  | 0/1/1/1 |
| 8   | PYB  | J     | 2002 | 8,7  | -       | 0/2/2/4  | 0/1/1/1 |
| 7   | IMT  | I     | 2021 | 8    | -       | 0/2/2/4  | 0/1/1/1 |
| 10  | BAL  | I     | 2030 | 8,11 | -       | 0/1/2/3  | -       |
| 8   | PYB  | I     | 2024 | 8,9  | -       | 0/2/2/4  | 0/1/1/1 |
| 10  | BAL  | J     | 1910 | 8,11 | -       | 0/1/2/3  | -       |
| 8   | PYB  | J     | 1909 | 8,10 | -       | 0/2/2/4  | 0/1/1/1 |
| 10  | BAL  | J     | 1930 | 8,11 | -       | 0/1/2/3  | -       |
| 10  | BAL  | J     | 2010 | 8,11 | -       | 0/1/2/3  | -       |
| 8   | PYB  | J     | 1908 | 8    | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | J     | 1924 | 8,9  | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | I     | 1967 | 8    | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | I     | 2029 | 8,10 | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | I     | 2028 | 8    | -       | 0/2/2/4  | 0/1/1/1 |
| 7   | IMT  | I     | 1961 | 8    | -       | 0/2/2/4  | 0/1/1/1 |
| 11  | DIB  | J     | 2011 | 10   | -       | 4/4/4/4  | -       |
| 8   | PYB  | J     | 2007 | 8    | -       | 0/2/2/4  | 0/1/1/1 |
| 8   | PYB  | J     | 1902 | 8,7  | -       | 1/2/2/4  | 0/1/1/1 |
| 11  | DIB  | J     | 1911 | 10   | -       | 3/4/4/4  | -       |
| 8   | PYB  | I     | 2026 | 8,9  | -       | 0/2/2/4  | 0/1/1/1 |
| 9   | ABU  | I     | 2025 | 8    | -       | 3/3/3/4  | -       |
| 8   | PYB  | J     | 1927 | 8    | -       | 0/2/2/4  | 0/1/1/1 |

All (116) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9   | J     | 1905 | ABU  | OXT-C | -3.73 | 1.23        | 1.42     |
| 9   | I     | 2025 | ABU  | OXT-C | -3.61 | 1.23        | 1.42     |
| 8   | J     | 1904 | PYB  | CB-CA | 3.61  | 1.41        | 1.35     |
| 9   | J     | 1925 | ABU  | OXT-C | -3.61 | 1.23        | 1.42     |
| 9   | J     | 2005 | ABU  | OXT-C | -3.60 | 1.23        | 1.42     |
| 8   | J     | 1926 | PYB  | CB-CA | 3.56  | 1.41        | 1.35     |
| 8   | I     | 1964 | PYB  | CB-CA | 3.55  | 1.41        | 1.35     |
| 9   | I     | 1965 | ABU  | OXT-C | -3.49 | 1.24        | 1.42     |
| 8   | I     | 1969 | PYB  | CB-CA | 3.48  | 1.41        | 1.35     |
| 8   | I     | 2024 | PYB  | CB-CA | 3.33  | 1.41        | 1.35     |
| 8   | J     | 1909 | PYB  | CB-CA | 3.19  | 1.40        | 1.35     |
| 8   | I     | 2029 | PYB  | CB-CA | 3.17  | 1.40        | 1.35     |
| 8   | J     | 1929 | PYB  | CB-CA | 3.16  | 1.40        | 1.35     |
| 8   | J     | 2004 | PYB  | CB-CA | 3.16  | 1.40        | 1.35     |
| 8   | I     | 1962 | PYB  | CB-CA | 3.15  | 1.40        | 1.35     |
| 8   | I     | 2027 | PYB  | CB-CA | 3.13  | 1.40        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 8   | J     | 1903 | PYB  | CB-CA   | 3.11 | 1.40        | 1.35     |
| 8   | J     | 2009 | PYB  | CB-CA   | 3.10 | 1.40        | 1.35     |
| 8   | J     | 1923 | PYB  | CB-CA   | 3.08 | 1.40        | 1.35     |
| 8   | I     | 1966 | PYB  | CB-CA   | 3.08 | 1.40        | 1.35     |
| 8   | I     | 2029 | PYB  | CB-NG2  | 3.07 | 1.43        | 1.37     |
| 7   | J     | 1921 | IMT  | CG1-NB1 | 3.06 | 1.37        | 1.33     |
| 7   | J     | 1921 | IMT  | CG1-NG2 | 3.06 | 1.44        | 1.36     |
| 8   | J     | 2007 | PYB  | CB-CA   | 3.06 | 1.40        | 1.35     |
| 8   | I     | 2023 | PYB  | CB-CA   | 3.06 | 1.40        | 1.35     |
| 8   | J     | 1924 | PYB  | CB-CA   | 3.06 | 1.40        | 1.35     |
| 7   | J     | 1901 | IMT  | CG1-NG2 | 3.05 | 1.44        | 1.36     |
| 8   | I     | 2026 | PYB  | CB-CA   | 3.05 | 1.40        | 1.35     |
| 8   | J     | 2006 | PYB  | CB-CA   | 3.05 | 1.40        | 1.35     |
| 7   | I     | 1961 | IMT  | CG1-NG2 | 3.04 | 1.44        | 1.36     |
| 8   | J     | 1904 | PYB  | CB-NG2  | 3.04 | 1.43        | 1.37     |
| 8   | J     | 1927 | PYB  | CB-CA   | 3.04 | 1.40        | 1.35     |
| 8   | J     | 1909 | PYB  | CB-NG2  | 3.02 | 1.43        | 1.37     |
| 8   | J     | 1902 | PYB  | CB-CA   | 2.98 | 1.40        | 1.35     |
| 8   | J     | 1907 | PYB  | CB-CA   | 2.97 | 1.40        | 1.35     |
| 8   | I     | 1964 | PYB  | CB-NG2  | 2.93 | 1.43        | 1.37     |
| 8   | J     | 2003 | PYB  | CB-CA   | 2.91 | 1.40        | 1.35     |
| 8   | J     | 1922 | PYB  | CB-CA   | 2.91 | 1.40        | 1.35     |
| 8   | J     | 1926 | PYB  | CB-NG2  | 2.90 | 1.43        | 1.37     |
| 7   | J     | 1921 | IMT  | CB-NG2  | 2.90 | 1.43        | 1.37     |
| 8   | J     | 2006 | PYB  | CB-NG2  | 2.89 | 1.42        | 1.37     |
| 8   | J     | 2008 | PYB  | CB-CA   | 2.87 | 1.40        | 1.35     |
| 8   | I     | 1969 | PYB  | CB-NG2  | 2.86 | 1.42        | 1.37     |
| 8   | I     | 1963 | PYB  | CB-CA   | 2.86 | 1.40        | 1.35     |
| 8   | J     | 2004 | PYB  | CB-NG2  | 2.86 | 1.42        | 1.37     |
| 8   | J     | 2007 | PYB  | CB-NG2  | 2.84 | 1.42        | 1.37     |
| 8   | I     | 1966 | PYB  | CB-NG2  | 2.84 | 1.42        | 1.37     |
| 8   | J     | 1908 | PYB  | CB-CA   | 2.84 | 1.40        | 1.35     |
| 8   | I     | 2028 | PYB  | CB-CA   | 2.82 | 1.40        | 1.35     |
| 7   | I     | 2021 | IMT  | CG1-NG2 | 2.80 | 1.43        | 1.36     |
| 8   | I     | 2024 | PYB  | CB-NG2  | 2.79 | 1.42        | 1.37     |
| 8   | I     | 1968 | PYB  | CB-CA   | 2.79 | 1.40        | 1.35     |
| 8   | I     | 2027 | PYB  | CB-NG2  | 2.75 | 1.42        | 1.37     |
| 8   | I     | 1967 | PYB  | CB-CA   | 2.66 | 1.40        | 1.35     |
| 8   | J     | 1907 | PYB  | CB-NG2  | 2.66 | 1.42        | 1.37     |
| 8   | J     | 1928 | PYB  | CB-CA   | 2.65 | 1.40        | 1.35     |
| 8   | J     | 1909 | PYB  | CG1-NG2 | 2.65 | 1.43        | 1.38     |
| 7   | J     | 2001 | IMT  | CG1-NG2 | 2.64 | 1.43        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 8   | J     | 1924 | PYB  | CB-NG2  | 2.64 | 1.42        | 1.37     |
| 7   | J     | 1901 | IMT  | CG1-NB1 | 2.63 | 1.37        | 1.33     |
| 8   | J     | 1906 | PYB  | CB-CA   | 2.62 | 1.40        | 1.35     |
| 8   | I     | 2028 | PYB  | CB-NG2  | 2.62 | 1.42        | 1.37     |
| 8   | J     | 2002 | PYB  | CB-CA   | 2.62 | 1.40        | 1.35     |
| 8   | I     | 2026 | PYB  | CB-NG2  | 2.61 | 1.42        | 1.37     |
| 8   | J     | 2009 | PYB  | CB-NG2  | 2.61 | 1.42        | 1.37     |
| 8   | J     | 2008 | PYB  | CB-NG2  | 2.61 | 1.42        | 1.37     |
| 7   | I     | 1961 | IMT  | CG1-NB1 | 2.60 | 1.37        | 1.33     |
| 8   | I     | 2022 | PYB  | CB-CA   | 2.59 | 1.39        | 1.35     |
| 7   | J     | 2001 | IMT  | CG1-NB1 | 2.56 | 1.37        | 1.33     |
| 7   | J     | 2001 | IMT  | CB-NG2  | 2.54 | 1.42        | 1.37     |
| 8   | J     | 2002 | PYB  | CB-NG2  | 2.51 | 1.42        | 1.37     |
| 8   | J     | 1929 | PYB  | CB-NG2  | 2.51 | 1.42        | 1.37     |
| 7   | I     | 1961 | IMT  | CB-NG2  | 2.48 | 1.42        | 1.37     |
| 7   | J     | 1901 | IMT  | CB-NG2  | 2.48 | 1.42        | 1.37     |
| 8   | I     | 1966 | PYB  | CG1-NG2 | 2.48 | 1.43        | 1.38     |
| 8   | J     | 1908 | PYB  | CB-NG2  | 2.47 | 1.42        | 1.37     |
| 8   | I     | 1968 | PYB  | CB-NG2  | 2.45 | 1.42        | 1.37     |
| 8   | I     | 2027 | PYB  | CG1-NG2 | 2.44 | 1.43        | 1.38     |
| 8   | J     | 1927 | PYB  | CB-NG2  | 2.43 | 1.42        | 1.37     |
| 8   | J     | 1902 | PYB  | CB-NG2  | 2.43 | 1.42        | 1.37     |
| 7   | I     | 2021 | IMT  | CB-NG2  | 2.42 | 1.42        | 1.37     |
| 8   | I     | 2022 | PYB  | CB-NG2  | 2.41 | 1.42        | 1.37     |
| 8   | J     | 2006 | PYB  | CG1-NG2 | 2.40 | 1.43        | 1.38     |
| 8   | I     | 1967 | PYB  | CB-NG2  | 2.39 | 1.41        | 1.37     |
| 8   | J     | 2003 | PYB  | CB-NG2  | 2.38 | 1.41        | 1.37     |
| 8   | J     | 1923 | PYB  | CB-NG2  | 2.38 | 1.41        | 1.37     |
| 8   | J     | 1903 | PYB  | CB-NG2  | 2.37 | 1.41        | 1.37     |
| 8   | J     | 1922 | PYB  | CB-NG2  | 2.36 | 1.41        | 1.37     |
| 8   | J     | 2009 | PYB  | CG1-NG2 | 2.34 | 1.43        | 1.38     |
| 8   | I     | 1962 | PYB  | CB-NG2  | 2.34 | 1.41        | 1.37     |
| 8   | J     | 1907 | PYB  | CG1-NG2 | 2.32 | 1.43        | 1.38     |
| 7   | I     | 2021 | IMT  | CG1-NB1 | 2.30 | 1.36        | 1.33     |
| 8   | I     | 2026 | PYB  | CG1-NG2 | 2.24 | 1.42        | 1.38     |
| 8   | J     | 1926 | PYB  | CG1-NG2 | 2.23 | 1.42        | 1.38     |
| 8   | J     | 1906 | PYB  | CG1-NG2 | 2.22 | 1.42        | 1.38     |
| 8   | J     | 1903 | PYB  | CG1-NG2 | 2.21 | 1.42        | 1.38     |
| 8   | J     | 2007 | PYB  | CG1-NG2 | 2.21 | 1.42        | 1.38     |
| 8   | J     | 1906 | PYB  | CB-NG2  | 2.19 | 1.41        | 1.37     |
| 8   | I     | 2024 | PYB  | CG1-NG2 | 2.15 | 1.42        | 1.38     |
| 8   | J     | 1904 | PYB  | CG1-NG2 | 2.15 | 1.42        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 7   | J     | 1921 | IMT  | CB-CA   | 2.13 | 1.40        | 1.35     |
| 7   | I     | 1961 | IMT  | CB-CA   | 2.12 | 1.40        | 1.35     |
| 8   | I     | 1968 | PYB  | CG1-NG2 | 2.11 | 1.42        | 1.38     |
| 7   | J     | 2001 | IMT  | CB-CA   | 2.10 | 1.40        | 1.35     |
| 8   | I     | 1962 | PYB  | CG1-NG2 | 2.10 | 1.42        | 1.38     |
| 8   | J     | 1923 | PYB  | CG1-NG2 | 2.09 | 1.42        | 1.38     |
| 8   | J     | 2002 | PYB  | CG1-NG2 | 2.09 | 1.42        | 1.38     |
| 8   | J     | 1924 | PYB  | CG1-NG2 | 2.09 | 1.42        | 1.38     |
| 8   | I     | 2029 | PYB  | CG1-NG2 | 2.09 | 1.42        | 1.38     |
| 8   | I     | 1963 | PYB  | CB-NG2  | 2.08 | 1.41        | 1.37     |
| 8   | I     | 1964 | PYB  | CG1-NG2 | 2.07 | 1.42        | 1.38     |
| 8   | I     | 1969 | PYB  | CG1-NG2 | 2.04 | 1.42        | 1.38     |
| 8   | J     | 1928 | PYB  | CG1-NG2 | 2.04 | 1.42        | 1.38     |
| 8   | I     | 2023 | PYB  | CB-NG2  | 2.04 | 1.41        | 1.37     |
| 8   | I     | 2028 | PYB  | CG1-NG2 | 2.03 | 1.42        | 1.38     |
| 8   | J     | 2003 | PYB  | CG1-NG2 | 2.01 | 1.42        | 1.38     |

All (118) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 8   | I     | 1962 | PYB  | O-C-CG1    | -5.00 | 115.09      | 126.63   |
| 8   | J     | 1926 | PYB  | CD-NG2-CG1 | 4.99  | 131.43      | 126.62   |
| 8   | I     | 2022 | PYB  | O-C-CG1    | -4.91 | 115.31      | 126.63   |
| 8   | J     | 1928 | PYB  | CD-NG2-CG1 | 4.89  | 131.34      | 126.62   |
| 8   | J     | 1902 | PYB  | O-C-CG1    | -4.88 | 115.36      | 126.63   |
| 8   | J     | 1927 | PYB  | CD-NG2-CG1 | 4.88  | 131.32      | 126.62   |
| 8   | J     | 2009 | PYB  | CD-NG2-CG1 | 4.88  | 131.32      | 126.62   |
| 8   | I     | 1963 | PYB  | O-C-CG1    | -4.87 | 115.40      | 126.63   |
| 8   | I     | 2026 | PYB  | CD-NG2-CG1 | 4.83  | 131.28      | 126.62   |
| 8   | I     | 1968 | PYB  | O-C-CG1    | -4.82 | 115.50      | 126.63   |
| 8   | J     | 1909 | PYB  | CD-NG2-CG1 | 4.82  | 131.26      | 126.62   |
| 8   | I     | 2027 | PYB  | CD-NG2-CG1 | 4.78  | 131.22      | 126.62   |
| 8   | J     | 1906 | PYB  | O-C-CG1    | -4.76 | 115.64      | 126.63   |
| 8   | J     | 1924 | PYB  | CD-NG2-CG1 | 4.74  | 131.19      | 126.62   |
| 8   | J     | 1903 | PYB  | CD-NG2-CG1 | 4.74  | 131.19      | 126.62   |
| 8   | J     | 1923 | PYB  | CD-NG2-CG1 | 4.74  | 131.19      | 126.62   |
| 8   | I     | 2024 | PYB  | CD-NG2-CG1 | 4.73  | 131.18      | 126.62   |
| 8   | J     | 1928 | PYB  | O-C-CG1    | -4.69 | 115.82      | 126.63   |
| 8   | J     | 2002 | PYB  | CD-NG2-CG1 | 4.68  | 131.13      | 126.62   |
| 8   | J     | 2008 | PYB  | O-C-CG1    | -4.68 | 115.84      | 126.63   |
| 8   | J     | 2003 | PYB  | CD-NG2-CG1 | 4.67  | 131.12      | 126.62   |
| 8   | I     | 2029 | PYB  | CD-NG2-CG1 | 4.67  | 131.12      | 126.62   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 8   | I     | 1966 | PYB  | CD-NG2-CG1 | 4.67  | 131.12      | 126.62   |
| 8   | J     | 1906 | PYB  | CD-NG2-CG1 | 4.66  | 131.11      | 126.62   |
| 8   | J     | 1922 | PYB  | CD-NG2-CG1 | 4.66  | 131.11      | 126.62   |
| 8   | J     | 2006 | PYB  | CD-NG2-CG1 | 4.66  | 131.11      | 126.62   |
| 8   | J     | 1922 | PYB  | O-C-CG1    | -4.64 | 115.93      | 126.63   |
| 8   | I     | 2028 | PYB  | CD-NG2-CG1 | 4.62  | 131.07      | 126.62   |
| 8   | J     | 1903 | PYB  | O-C-CG1    | -4.60 | 116.02      | 126.63   |
| 8   | I     | 1962 | PYB  | CD-NG2-CG1 | 4.59  | 131.05      | 126.62   |
| 8   | I     | 2023 | PYB  | CD-NG2-CG1 | 4.59  | 131.05      | 126.62   |
| 8   | J     | 1908 | PYB  | CD-NG2-CG1 | 4.59  | 131.04      | 126.62   |
| 8   | J     | 2004 | PYB  | CD-NG2-CG1 | 4.59  | 131.04      | 126.62   |
| 8   | I     | 1967 | PYB  | CD-NG2-CG1 | 4.58  | 131.03      | 126.62   |
| 8   | J     | 1904 | PYB  | CD-NG2-CG1 | 4.57  | 131.02      | 126.62   |
| 8   | J     | 2002 | PYB  | O-C-CG1    | -4.56 | 116.10      | 126.63   |
| 8   | I     | 1969 | PYB  | CD-NG2-CG1 | 4.55  | 131.01      | 126.62   |
| 8   | J     | 1907 | PYB  | O-C-CG1    | -4.54 | 116.14      | 126.63   |
| 8   | J     | 1907 | PYB  | CD-NG2-CG1 | 4.54  | 131.00      | 126.62   |
| 8   | J     | 2007 | PYB  | CD-NG2-CG1 | 4.53  | 130.98      | 126.62   |
| 8   | I     | 1963 | PYB  | CD-NG2-CG1 | 4.51  | 130.96      | 126.62   |
| 8   | I     | 1967 | PYB  | O-C-CG1    | -4.49 | 116.26      | 126.63   |
| 8   | I     | 2027 | PYB  | O-C-CG1    | -4.48 | 116.29      | 126.63   |
| 8   | I     | 1964 | PYB  | CD-NG2-CG1 | 4.45  | 130.90      | 126.62   |
| 8   | J     | 1923 | PYB  | O-C-CG1    | -4.44 | 116.38      | 126.63   |
| 8   | J     | 1929 | PYB  | CD-NG2-CG1 | 4.44  | 130.90      | 126.62   |
| 8   | J     | 2003 | PYB  | O-C-CG1    | -4.43 | 116.41      | 126.63   |
| 8   | I     | 1968 | PYB  | CD-NG2-CG1 | 4.43  | 130.89      | 126.62   |
| 8   | I     | 2022 | PYB  | CD-NG2-CG1 | 4.39  | 130.85      | 126.62   |
| 8   | J     | 2008 | PYB  | CD-NG2-CG1 | 4.39  | 130.85      | 126.62   |
| 8   | J     | 1908 | PYB  | O-C-CG1    | -4.37 | 116.54      | 126.63   |
| 8   | I     | 1966 | PYB  | O-C-CG1    | -4.37 | 116.54      | 126.63   |
| 8   | J     | 1927 | PYB  | O-C-CG1    | -4.36 | 116.57      | 126.63   |
| 8   | I     | 2023 | PYB  | O-C-CG1    | -4.31 | 116.68      | 126.63   |
| 8   | J     | 1902 | PYB  | CD-NG2-CG1 | 4.29  | 130.76      | 126.62   |
| 8   | I     | 2028 | PYB  | O-C-CG1    | -4.28 | 116.75      | 126.63   |
| 8   | J     | 2007 | PYB  | O-C-CG1    | -4.27 | 116.78      | 126.63   |
| 8   | J     | 1929 | PYB  | O-C-CG1    | -4.25 | 116.83      | 126.63   |
| 8   | I     | 2026 | PYB  | O-C-CG1    | -4.16 | 117.03      | 126.63   |
| 8   | J     | 2009 | PYB  | O-C-CG1    | -4.15 | 117.06      | 126.63   |
| 8   | J     | 2006 | PYB  | O-C-CG1    | -4.11 | 117.15      | 126.63   |
| 7   | J     | 2001 | IMT  | CD-NG2-CG1 | 4.08  | 131.54      | 127.84   |
| 8   | J     | 1924 | PYB  | O-C-CG1    | -4.04 | 117.30      | 126.63   |
| 8   | I     | 1964 | PYB  | O-C-CG1    | -4.02 | 117.35      | 126.63   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 7   | J     | 1901 | IMT  | CD-NG2-CG1 | 3.95  | 131.42      | 127.84   |
| 7   | I     | 1961 | IMT  | CD-NG2-CG1 | 3.93  | 131.41      | 127.84   |
| 7   | I     | 2021 | IMT  | CD-NG2-CG1 | 3.90  | 131.38      | 127.84   |
| 7   | J     | 1921 | IMT  | CD-NG2-CG1 | 3.89  | 131.37      | 127.84   |
| 8   | I     | 1969 | PYB  | O-C-CG1    | -3.87 | 117.70      | 126.63   |
| 8   | I     | 2029 | PYB  | O-C-CG1    | -3.78 | 117.92      | 126.63   |
| 8   | J     | 1904 | PYB  | O-C-CG1    | -3.77 | 117.93      | 126.63   |
| 8   | J     | 1909 | PYB  | O-C-CG1    | -3.76 | 117.95      | 126.63   |
| 8   | J     | 1926 | PYB  | O-C-CG1    | -3.76 | 117.95      | 126.63   |
| 8   | J     | 2004 | PYB  | O-C-CG1    | -3.70 | 118.09      | 126.63   |
| 8   | I     | 2024 | PYB  | O-C-CG1    | -3.59 | 118.36      | 126.63   |
| 7   | J     | 1921 | IMT  | CA-NB1-CG1 | 2.91  | 109.42      | 104.75   |
| 7   | J     | 1901 | IMT  | C-CG1-NB1  | 2.86  | 127.56      | 122.28   |
| 7   | J     | 1901 | IMT  | CA-NB1-CG1 | 2.82  | 109.28      | 104.75   |
| 7   | I     | 2021 | IMT  | CA-NB1-CG1 | 2.81  | 109.26      | 104.75   |
| 7   | J     | 2001 | IMT  | CA-NB1-CG1 | 2.77  | 109.20      | 104.75   |
| 7   | I     | 1961 | IMT  | C-CG1-NB1  | 2.72  | 127.31      | 122.28   |
| 7   | I     | 1961 | IMT  | CA-NB1-CG1 | 2.67  | 109.03      | 104.75   |
| 7   | J     | 1921 | IMT  | C-CG1-NB1  | 2.61  | 127.10      | 122.28   |
| 7   | I     | 2021 | IMT  | C-CG1-NB1  | 2.52  | 126.93      | 122.28   |
| 8   | J     | 1926 | PYB  | CB-NG2-CG1 | -2.50 | 105.60      | 108.85   |
| 8   | J     | 1927 | PYB  | CB-NG2-CG1 | -2.45 | 105.67      | 108.85   |
| 8   | I     | 2024 | PYB  | CB-NG2-CG1 | -2.26 | 105.91      | 108.85   |
| 7   | J     | 2001 | IMT  | C-CG1-NB1  | 2.26  | 126.46      | 122.28   |
| 8   | J     | 1909 | PYB  | CG1-CB1-CA | 2.24  | 108.82      | 106.11   |
| 7   | J     | 2001 | IMT  | CA-CB-NG2  | 2.23  | 108.49      | 106.46   |
| 8   | I     | 2029 | PYB  | CG1-CB1-CA | 2.22  | 108.79      | 106.11   |
| 8   | I     | 1969 | PYB  | CB-NG2-CG1 | -2.21 | 105.99      | 108.85   |
| 8   | J     | 1924 | PYB  | CB-NG2-CG1 | -2.19 | 106.01      | 108.85   |
| 7   | J     | 1921 | IMT  | CA-CB-NG2  | 2.19  | 108.45      | 106.46   |
| 8   | J     | 1904 | PYB  | CB-NG2-CG1 | -2.18 | 106.01      | 108.85   |
| 8   | I     | 2027 | PYB  | CB-NG2-CG1 | -2.15 | 106.05      | 108.85   |
| 8   | I     | 1964 | PYB  | CB-NG2-CG1 | -2.15 | 106.06      | 108.85   |
| 8   | J     | 2004 | PYB  | CB-NG2-CG1 | -2.13 | 106.08      | 108.85   |
| 7   | J     | 2001 | IMT  | CB-CA-NB1  | -2.12 | 107.96      | 110.74   |
| 8   | I     | 2026 | PYB  | CB-NG2-CG1 | -2.12 | 106.10      | 108.85   |
| 8   | J     | 1909 | PYB  | CB-NG2-CG1 | -2.11 | 106.11      | 108.85   |
| 8   | J     | 1929 | PYB  | CB-NG2-CG1 | -2.10 | 106.12      | 108.85   |
| 8   | J     | 1923 | PYB  | CB-NG2-CG1 | -2.10 | 106.12      | 108.85   |
| 8   | J     | 1928 | PYB  | CB-NG2-CG1 | -2.10 | 106.13      | 108.85   |
| 8   | J     | 2006 | PYB  | CG1-CB1-CA | 2.10  | 108.64      | 106.11   |
| 8   | I     | 2029 | PYB  | CB-NG2-CG1 | -2.09 | 106.13      | 108.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 7   | J     | 1901 | IMT  | NG2-CG1-NB1 | -2.08 | 108.30      | 111.26   |
| 8   | J     | 2009 | PYB  | CB-NG2-CG1  | -2.08 | 106.15      | 108.85   |
| 7   | J     | 1901 | IMT  | CA-CB-NG2   | 2.07  | 108.34      | 106.46   |
| 7   | I     | 1961 | IMT  | CA-CB-NG2   | 2.06  | 108.33      | 106.46   |
| 7   | J     | 1921 | IMT  | CB-CA-NB1   | -2.05 | 108.05      | 110.74   |
| 8   | I     | 1966 | PYB  | CG1-CB1-CA  | 2.04  | 108.58      | 106.11   |
| 8   | J     | 2002 | PYB  | CB-NG2-CG1  | -2.04 | 106.20      | 108.85   |
| 8   | J     | 1904 | PYB  | CG1-CB1-CA  | 2.02  | 108.55      | 106.11   |
| 8   | J     | 1922 | PYB  | CB-NG2-CG1  | -2.02 | 106.23      | 108.85   |
| 8   | J     | 1902 | PYB  | CB1-CG1-C   | 2.02  | 129.90      | 126.34   |
| 8   | I     | 2023 | PYB  | CB-NG2-CG1  | -2.01 | 106.23      | 108.85   |
| 7   | I     | 2021 | IMT  | CA-CB-NG2   | 2.01  | 108.29      | 106.46   |

There are no chirality outliers.

All (28) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 8   | J     | 1929 | PYB  | O-C-CG1-NG2  |
| 11  | J     | 2011 | DIB  | CB-CG-ND-CE1 |
| 11  | J     | 2011 | DIB  | CB-CG-ND-CE2 |
| 11  | J     | 1931 | DIB  | CA-CB-CG-ND  |
| 11  | J     | 2011 | DIB  | CA-CB-CG-ND  |
| 11  | J     | 1911 | DIB  | CB-CG-ND-CE1 |
| 9   | J     | 1925 | ABU  | CD-CB-CG-C   |
| 9   | J     | 2005 | ABU  | CD-CB-CG-C   |
| 11  | J     | 1911 | DIB  | CA-CB-CG-ND  |
| 9   | J     | 1905 | ABU  | OXT-C-CG-CB  |
| 9   | J     | 1925 | ABU  | OXT-C-CG-CB  |
| 9   | I     | 1965 | ABU  | CD-CB-CG-C   |
| 9   | I     | 2025 | ABU  | CD-CB-CG-C   |
| 11  | J     | 1911 | DIB  | CB-CG-ND-CE2 |
| 9   | I     | 1965 | ABU  | OXT-C-CG-CB  |
| 9   | I     | 2025 | ABU  | OXT-C-CG-CB  |
| 9   | J     | 2005 | ABU  | OXT-C-CG-CB  |
| 11  | I     | 2031 | DIB  | CA-CB-CG-ND  |
| 11  | J     | 2011 | DIB  | N-CA-CB-CG   |
| 9   | I     | 1965 | ABU  | CG-CB-CD-N   |
| 9   | J     | 1925 | ABU  | CG-CB-CD-N   |
| 9   | J     | 2005 | ABU  | CG-CB-CD-N   |
| 8   | J     | 1929 | PYB  | O-C-CG1-CB1  |
| 9   | J     | 1905 | ABU  | CG-CB-CD-N   |
| 8   | I     | 2027 | PYB  | O-C-CG1-NG2  |

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| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 9   | I     | 2025 | ABU  | CG-CB-CD-N  |
| 8   | I     | 1962 | PYB  | O-C-CG1-NG2 |
| 8   | J     | 1902 | PYB  | O-C-CG1-NG2 |

There are no ring outliers.

52 monomers are involved in 126 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 9   | J     | 2005 | ABU  | 1       | 0            |
| 8   | J     | 2006 | PYB  | 3       | 0            |
| 8   | J     | 2008 | PYB  | 5       | 0            |
| 8   | I     | 1966 | PYB  | 2       | 0            |
| 8   | J     | 1929 | PYB  | 7       | 0            |
| 8   | I     | 1964 | PYB  | 3       | 0            |
| 8   | J     | 1907 | PYB  | 4       | 0            |
| 11  | J     | 1931 | DIB  | 3       | 0            |
| 8   | J     | 1904 | PYB  | 3       | 0            |
| 8   | J     | 1903 | PYB  | 5       | 0            |
| 8   | J     | 1922 | PYB  | 3       | 0            |
| 8   | J     | 1928 | PYB  | 7       | 0            |
| 8   | J     | 2003 | PYB  | 6       | 0            |
| 8   | I     | 2023 | PYB  | 4       | 0            |
| 8   | J     | 1926 | PYB  | 2       | 0            |
| 8   | J     | 2004 | PYB  | 2       | 0            |
| 7   | J     | 2001 | IMT  | 1       | 0            |
| 8   | J     | 2009 | PYB  | 5       | 0            |
| 7   | J     | 1921 | IMT  | 2       | 0            |
| 8   | I     | 1962 | PYB  | 4       | 0            |
| 9   | J     | 1905 | ABU  | 6       | 0            |
| 8   | I     | 2022 | PYB  | 4       | 0            |
| 8   | I     | 1968 | PYB  | 5       | 0            |
| 7   | J     | 1901 | IMT  | 4       | 0            |
| 8   | I     | 1969 | PYB  | 4       | 0            |
| 8   | J     | 1906 | PYB  | 5       | 0            |
| 8   | J     | 1923 | PYB  | 3       | 0            |
| 11  | I     | 1971 | DIB  | 2       | 0            |
| 11  | I     | 2031 | DIB  | 3       | 0            |
| 10  | I     | 1970 | BAL  | 1       | 0            |
| 8   | I     | 1963 | PYB  | 4       | 0            |
| 8   | I     | 2027 | PYB  | 3       | 0            |
| 8   | J     | 2002 | PYB  | 3       | 0            |
| 7   | I     | 2021 | IMT  | 3       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 10  | I     | 2030 | BAL  | 2       | 0            |
| 8   | I     | 2024 | PYB  | 5       | 0            |
| 8   | J     | 1909 | PYB  | 2       | 0            |
| 10  | J     | 1930 | BAL  | 1       | 0            |
| 10  | J     | 2010 | BAL  | 1       | 0            |
| 8   | J     | 1908 | PYB  | 6       | 0            |
| 8   | J     | 1924 | PYB  | 3       | 0            |
| 8   | I     | 1967 | PYB  | 5       | 0            |
| 8   | I     | 2029 | PYB  | 9       | 0            |
| 8   | I     | 2028 | PYB  | 5       | 0            |
| 7   | I     | 1961 | IMT  | 4       | 0            |
| 11  | J     | 2011 | DIB  | 2       | 0            |
| 8   | J     | 2007 | PYB  | 3       | 0            |
| 8   | J     | 1902 | PYB  | 4       | 0            |
| 11  | J     | 1911 | DIB  | 3       | 0            |
| 8   | I     | 2026 | PYB  | 2       | 0            |
| 9   | I     | 2025 | ABU  | 2       | 0            |
| 8   | J     | 1927 | PYB  | 4       | 0            |

## 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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.