



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:43 am GMT

PDB ID : 3ZK2  
Title : Crystal structure of the sodium binding rotor ring at pH 8.7.  
Authors : Schulz, S.; Meier, T.; Yildiz, O.  
Deposited on : 2013-01-21  
Resolution : 2.63 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

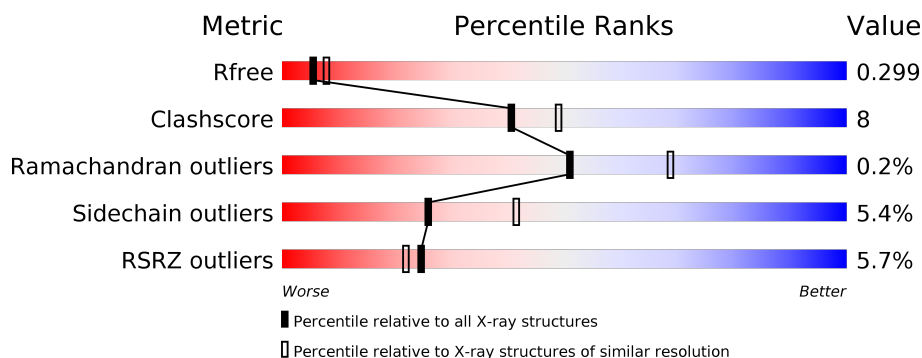
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.63 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 1044 (2.66-2.62)                                      |
| Clashscore            | 112137                      | 1092 (2.66-2.62)                                      |
| Ramachandran outliers | 110173                      | 1077 (2.66-2.62)                                      |
| Sidechain outliers    | 110143                      | 1077 (2.66-2.62)                                      |
| RSRZ outliers         | 101464                      | 1047 (2.66-2.62)                                      |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 89     | <div> <div>3%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div> |
| 1   | B     | 89     | <div> <div>%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>               |
| 1   | C     | 89     | <div> <div>%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>               |
| 1   | D     | 89     | <div> <div></div> <div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>  |
| 1   | E     | 89     | <div> <div>4%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>              |
| 1   | F     | 89     | <div> <div>%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>              |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | G     | 89     |                  |
| 1   | H     | 89     |                  |
| 1   | I     | 89     |                  |
| 1   | J     | 89     |                  |
| 1   | K     | 89     |                  |
| 1   | L     | 89     |                  |
| 1   | M     | 89     |                  |
| 1   | N     | 89     |                  |
| 1   | O     | 89     |                  |
| 1   | P     | 89     |                  |
| 1   | Q     | 89     |                  |
| 1   | R     | 89     |                  |
| 1   | S     | 89     |                  |
| 1   | T     | 89     |                  |
| 1   | U     | 89     |                  |
| 1   | V     | 89     |                  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | DMU  | A     | 92  | -         | -        | -       | X                |
| 3   | DMU  | A     | 93  | -         | -        | -       | X                |
| 3   | DMU  | B     | 92  | -         | -        | -       | X                |
| 3   | DMU  | C     | 92  | -         | -        | -       | X                |
| 3   | DMU  | D     | 92  | -         | -        | -       | X                |
| 3   | DMU  | E     | 92  | -         | -        | -       | X                |
| 3   | DMU  | F     | 92  | -         | -        | -       | X                |
| 3   | DMU  | G     | 92  | -         | -        | -       | X                |
| 3   | DMU  | H     | 92  | -         | -        | -       | X                |
| 3   | DMU  | I     | 92  | -         | -        | -       | X                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | DMU  | J     | 92  | X         | -        | -       | X                |
| 3   | DMU  | K     | 92  | -         | -        | -       | X                |
| 3   | DMU  | L     | 92  | -         | -        | -       | X                |
| 3   | DMU  | M     | 92  | -         | -        | -       | X                |
| 3   | DMU  | N     | 92  | -         | -        | -       | X                |
| 3   | DMU  | O     | 92  | -         | -        | -       | X                |
| 3   | DMU  | P     | 92  | -         | -        | -       | X                |
| 3   | DMU  | Q     | 92  | -         | -        | -       | X                |
| 3   | DMU  | S     | 92  | X         | -        | -       | X                |
| 3   | DMU  | T     | 92  | -         | -        | -       | X                |
| 3   | DMU  | U     | 92  | X         | -        | -       | X                |
| 3   | DMU  | V     | 92  | -         | -        | -       | X                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14537 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ATP SYNTHASE SUBUNIT C.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 89       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 620   | 398 | 101 | 117 | 4 |         |         |       |
| 1   | B     | 89       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 620   | 398 | 101 | 117 | 4 |         |         |       |
| 1   | C     | 89       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 620   | 398 | 101 | 117 | 4 |         |         |       |
| 1   | D     | 89       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 620   | 398 | 101 | 117 | 4 |         |         |       |
| 1   | E     | 89       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 620   | 398 | 101 | 117 | 4 |         |         |       |
| 1   | F     | 89       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 620   | 398 | 101 | 117 | 4 |         |         |       |
| 1   | G     | 89       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 620   | 398 | 101 | 117 | 4 |         |         |       |
| 1   | H     | 89       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 620   | 398 | 101 | 117 | 4 |         |         |       |
| 1   | I     | 89       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 620   | 398 | 101 | 117 | 4 |         |         |       |
| 1   | J     | 89       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 620   | 398 | 101 | 117 | 4 |         |         |       |
| 1   | K     | 89       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 619   | 398 | 101 | 116 | 4 |         |         |       |
| 1   | L     | 89       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 620   | 398 | 101 | 117 | 4 |         |         |       |
| 1   | M     | 89       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 620   | 398 | 101 | 117 | 4 |         |         |       |
| 1   | N     | 89       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 620   | 398 | 101 | 117 | 4 |         |         |       |
| 1   | O     | 89       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 620   | 398 | 101 | 117 | 4 |         |         |       |
| 1   | P     | 89       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 620   | 398 | 101 | 117 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms        |          |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| 1   | Q     | 89       | Total<br>620 | C<br>398 | N<br>101 | O<br>117 | S<br>4 | 0       | 0       | 0     |
| 1   | R     | 89       | Total<br>620 | C<br>398 | N<br>101 | O<br>117 | S<br>4 | 0       | 0       | 0     |
| 1   | S     | 89       | Total<br>620 | C<br>398 | N<br>101 | O<br>117 | S<br>4 | 0       | 0       | 0     |
| 1   | T     | 89       | Total<br>620 | C<br>398 | N<br>101 | O<br>117 | S<br>4 | 0       | 0       | 0     |
| 1   | U     | 89       | Total<br>620 | C<br>398 | N<br>101 | O<br>117 | S<br>4 | 0       | 0       | 0     |
| 1   | V     | 89       | Total<br>620 | C<br>398 | N<br>101 | O<br>117 | S<br>4 | 0       | 0       | 0     |

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

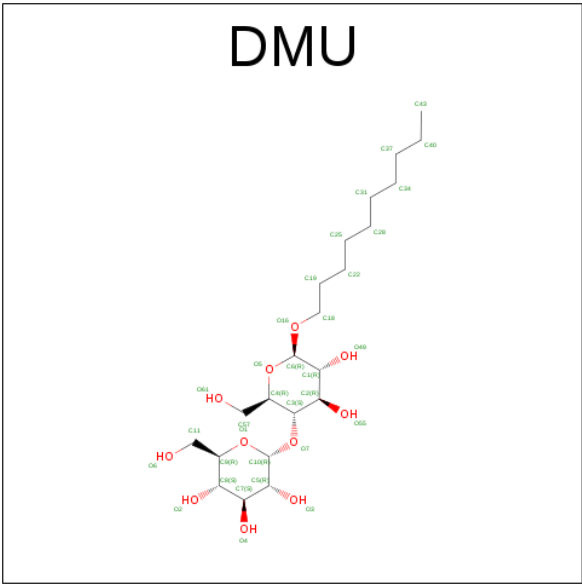
| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 2   | P     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 2   | K     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 2   | B     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 2   | N     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 2   | S     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 2   | J     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 2   | E     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 2   | V     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 2   | A     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 2   | R     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 2   | M     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 2   | D     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |
| 2   | I     | 1        | Total<br>1 | Na<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | U     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | L     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | G     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | Q     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | H     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | C     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | T     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | O     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | F     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 3 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 3   | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |

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| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 3   | B     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | D     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | E     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | F     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | G     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | H     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | I     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | J     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | K     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | L     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | M     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | N     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | O     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | P     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | Q     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | R     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | S     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | T     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | U     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |
| 3   | V     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 33    | 22 | 11 |         |         |



- Molecule 4 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 4   | A     | 15       | Total O<br>15 15 | 0       | 0       |
| 4   | B     | 4        | Total O<br>4 4   | 0       | 0       |
| 4   | C     | 2        | Total O<br>2 2   | 0       | 0       |
| 4   | D     | 3        | Total O<br>3 3   | 0       | 0       |
| 4   | E     | 4        | Total O<br>4 4   | 0       | 0       |
| 4   | F     | 4        | Total O<br>4 4   | 0       | 0       |
| 4   | G     | 5        | Total O<br>5 5   | 0       | 0       |
| 4   | H     | 5        | Total O<br>5 5   | 0       | 0       |
| 4   | I     | 3        | Total O<br>3 3   | 0       | 0       |
| 4   | J     | 8        | Total O<br>8 8   | 0       | 0       |
| 4   | K     | 7        | Total O<br>7 7   | 0       | 0       |
| 4   | L     | 8        | Total O<br>8 8   | 0       | 0       |
| 4   | M     | 5        | Total O<br>5 5   | 0       | 0       |
| 4   | N     | 3        | Total O<br>3 3   | 0       | 0       |
| 4   | O     | 2        | Total O<br>2 2   | 0       | 0       |
| 4   | P     | 6        | Total O<br>6 6   | 0       | 0       |
| 4   | Q     | 4        | Total O<br>4 4   | 0       | 0       |
| 4   | R     | 3        | Total O<br>3 3   | 0       | 0       |
| 4   | S     | 5        | Total O<br>5 5   | 0       | 0       |
| 4   | T     | 8        | Total O<br>8 8   | 0       | 0       |
| 4   | U     | 8        | Total O<br>8 8   | 0       | 0       |

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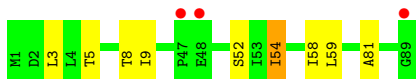
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| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 4   | V     | 5        | Total | O | 0       | 0       |
|     |       |          | 5     | 5 |         |         |

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

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

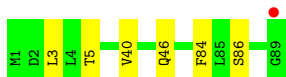
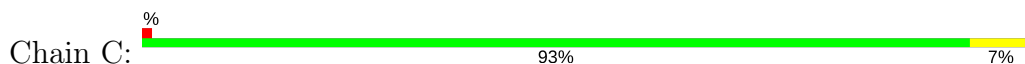
- Molecule 1: ATP SYNTHASE SUBUNIT C



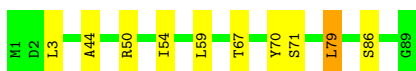
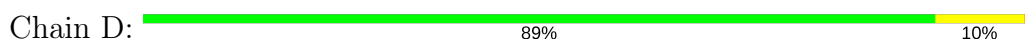
- Molecule 1: ATP SYNTHASE SUBUNIT C



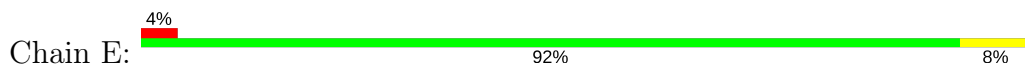
- Molecule 1: ATP SYNTHASE SUBUNIT C



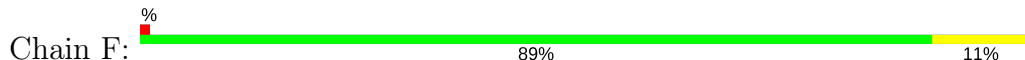
- Molecule 1: ATP SYNTHASE SUBUNIT C



- Molecule 1: ATP SYNTHASE SUBUNIT C

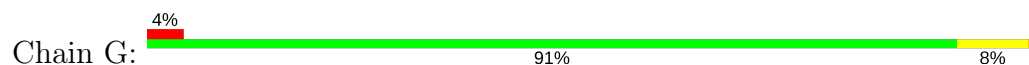


- Molecule 1: ATP SYNTHASE SUBUNIT C

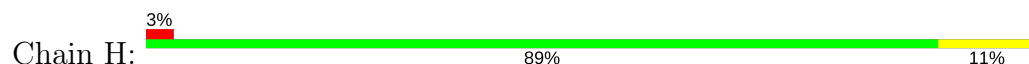




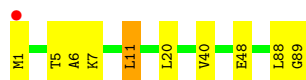
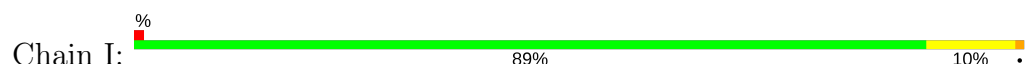
- Molecule 1: ATP SYNTHASE SUBUNIT C



- Molecule 1: ATP SYNTHASE SUBUNIT C



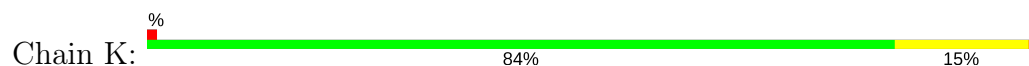
- Molecule 1: ATP SYNTHASE SUBUNIT C



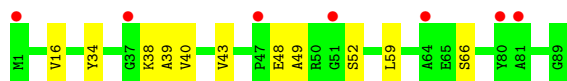
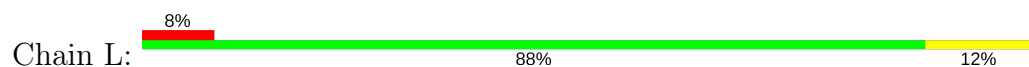
- Molecule 1: ATP SYNTHASE SUBUNIT C



- Molecule 1: ATP SYNTHASE SUBUNIT C

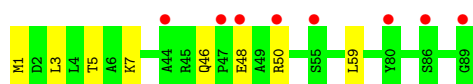


- Molecule 1: ATP SYNTHASE SUBUNIT C

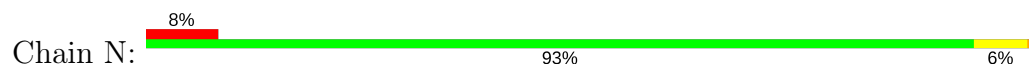


- Molecule 1: ATP SYNTHASE SUBUNIT C





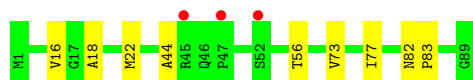
• Molecule 1: ATP SYNTHASE SUBUNIT C



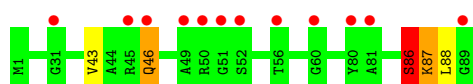
• Molecule 1: ATP SYNTHASE SUBUNIT C



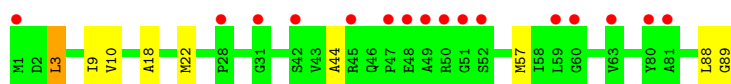
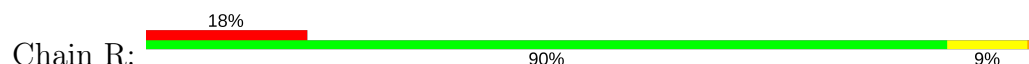
• Molecule 1: ATP SYNTHASE SUBUNIT C



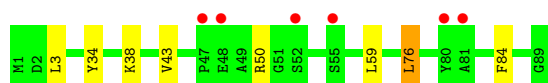
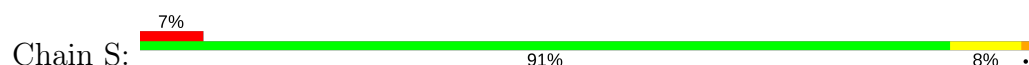
• Molecule 1: ATP SYNTHASE SUBUNIT C



• Molecule 1: ATP SYNTHASE SUBUNIT C

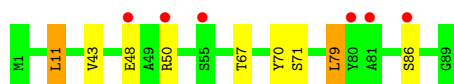


• Molecule 1: ATP SYNTHASE SUBUNIT C

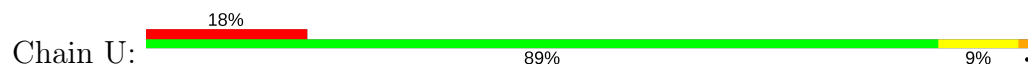


• Molecule 1: ATP SYNTHASE SUBUNIT C

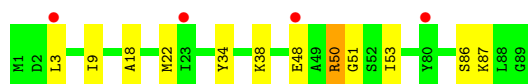
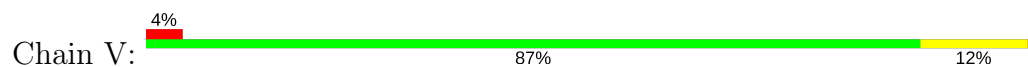




- Molecule 1: ATP SYNTHASE SUBUNIT C



- Molecule 1: ATP SYNTHASE SUBUNIT C



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 135.77Å 83.90Å 150.99Å<br>90.00° 112.85° 90.00°             | Depositor        |
| Resolution (Å)  | 47.00 – 2.63<br>47.00 – 2.63                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.7 (47.00-2.63)<br>98.9 (47.00-2.63)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.28  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.19 (at 2.61Å)   | Xtriage          |
| Refinement program  | PHENIX (PHENIX.REFINE)                                      | Depositor        |
| R, $R_{free}$   | 0.255 , 0.297<br>0.256 , 0.299                              | Depositor<br>DCC |
| $R_{free}$ test set   | 4609 reflections (5.00%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 36.9  | Xtriage          |
| Anisotropy  | 0.407   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 52.9   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.88  | EDS              |
| Total number of atoms   | 14537   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 47.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, DMU

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | A     | 0.24         | 0/626       | 0.45        | 0/846       |
| 1   | B     | 0.24         | 0/626       | 0.43        | 0/846       |
| 1   | C     | 0.23         | 0/626       | 0.43        | 0/846       |
| 1   | D     | 0.23         | 0/626       | 0.45        | 0/846       |
| 1   | E     | 0.23         | 0/626       | 0.43        | 0/846       |
| 1   | F     | 0.24         | 0/626       | 0.43        | 0/846       |
| 1   | G     | 0.24         | 0/626       | 0.43        | 0/846       |
| 1   | H     | 0.23         | 0/626       | 0.44        | 0/846       |
| 1   | I     | 0.23         | 0/626       | 0.43        | 0/846       |
| 1   | J     | 0.23         | 0/626       | 0.42        | 0/846       |
| 1   | K     | 0.24         | 0/625       | 0.43        | 0/846       |
| 1   | L     | 0.23         | 0/626       | 0.45        | 0/846       |
| 1   | M     | 0.23         | 0/626       | 0.45        | 0/846       |
| 1   | N     | 0.23         | 0/626       | 0.43        | 0/846       |
| 1   | O     | 0.21         | 0/626       | 0.43        | 0/846       |
| 1   | P     | 0.22         | 0/626       | 0.43        | 0/846       |
| 1   | Q     | 0.23         | 0/626       | 0.44        | 0/846       |
| 1   | R     | 0.22         | 0/626       | 0.41        | 0/846       |
| 1   | S     | 0.22         | 0/626       | 0.43        | 0/846       |
| 1   | T     | 0.23         | 0/626       | 0.42        | 0/846       |
| 1   | U     | 0.24         | 0/626       | 0.49        | 0/846       |
| 1   | V     | 0.22         | 0/626       | 0.42        | 0/846       |
| All | All   | 0.23         | 0/13771     | 0.44        | 0/18612     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 620   | 0        | 662      | 6       | 0            |
| 1   | B     | 620   | 0        | 662      | 4       | 1            |
| 1   | C     | 620   | 0        | 662      | 5       | 0            |
| 1   | D     | 620   | 0        | 662      | 5       | 0            |
| 1   | E     | 620   | 0        | 662      | 3       | 0            |
| 1   | F     | 620   | 0        | 662      | 3       | 0            |
| 1   | G     | 620   | 0        | 662      | 5       | 0            |
| 1   | H     | 620   | 0        | 662      | 3       | 1            |
| 1   | I     | 620   | 0        | 662      | 6       | 1            |
| 1   | J     | 620   | 0        | 662      | 4       | 0            |
| 1   | K     | 619   | 0        | 662      | 13      | 0            |
| 1   | L     | 620   | 0        | 662      | 6       | 0            |
| 1   | M     | 620   | 0        | 662      | 3       | 0            |
| 1   | N     | 620   | 0        | 662      | 2       | 0            |
| 1   | O     | 620   | 0        | 662      | 4       | 0            |
| 1   | P     | 620   | 0        | 662      | 6       | 0            |
| 1   | Q     | 620   | 0        | 662      | 3       | 0            |
| 1   | R     | 620   | 0        | 662      | 5       | 0            |
| 1   | S     | 620   | 0        | 662      | 4       | 0            |
| 1   | T     | 620   | 0        | 662      | 3       | 0            |
| 1   | U     | 620   | 0        | 662      | 6       | 0            |
| 1   | V     | 620   | 0        | 662      | 6       | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 2   | E     | 1     | 0        | 0        | 0       | 0            |
| 2   | F     | 1     | 0        | 0        | 0       | 0            |
| 2   | G     | 1     | 0        | 0        | 0       | 0            |
| 2   | H     | 1     | 0        | 0        | 0       | 0            |
| 2   | I     | 1     | 0        | 0        | 0       | 0            |
| 2   | J     | 1     | 0        | 0        | 0       | 0            |
| 2   | K     | 1     | 0        | 0        | 0       | 0            |
| 2   | L     | 1     | 0        | 0        | 0       | 0            |
| 2   | M     | 1     | 0        | 0        | 0       | 0            |
| 2   | N     | 1     | 0        | 0        | 0       | 0            |
| 2   | O     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | P     | 1     | 0        | 0        | 0       | 0            |
| 2   | Q     | 1     | 0        | 0        | 0       | 0            |
| 2   | R     | 1     | 0        | 0        | 0       | 0            |
| 2   | S     | 1     | 0        | 0        | 0       | 0            |
| 2   | T     | 1     | 0        | 0        | 0       | 0            |
| 2   | U     | 1     | 0        | 0        | 0       | 0            |
| 2   | V     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 66    | 0        | 84       | 7       | 0            |
| 3   | B     | 33    | 0        | 42       | 3       | 0            |
| 3   | C     | 33    | 0        | 42       | 6       | 0            |
| 3   | D     | 33    | 0        | 42       | 7       | 0            |
| 3   | E     | 33    | 0        | 42       | 9       | 0            |
| 3   | F     | 33    | 0        | 42       | 10      | 0            |
| 3   | G     | 33    | 0        | 42       | 9       | 0            |
| 3   | H     | 33    | 0        | 39       | 8       | 0            |
| 3   | I     | 33    | 0        | 42       | 4       | 0            |
| 3   | J     | 33    | 0        | 41       | 12      | 0            |
| 3   | K     | 33    | 0        | 42       | 11      | 0            |
| 3   | L     | 33    | 0        | 42       | 11      | 0            |
| 3   | M     | 33    | 0        | 40       | 12      | 0            |
| 3   | N     | 33    | 0        | 42       | 10      | 0            |
| 3   | O     | 33    | 0        | 42       | 6       | 0            |
| 3   | P     | 33    | 0        | 42       | 9       | 0            |
| 3   | Q     | 33    | 0        | 42       | 9       | 0            |
| 3   | R     | 33    | 0        | 42       | 10      | 0            |
| 3   | S     | 33    | 0        | 39       | 10      | 0            |
| 3   | T     | 33    | 0        | 42       | 12      | 0            |
| 3   | U     | 33    | 0        | 39       | 15      | 0            |
| 3   | V     | 33    | 0        | 42       | 12      | 0            |
| 4   | A     | 15    | 0        | 0        | 0       | 1            |
| 4   | B     | 4     | 0        | 0        | 0       | 0            |
| 4   | C     | 2     | 0        | 0        | 0       | 0            |
| 4   | D     | 3     | 0        | 0        | 0       | 0            |
| 4   | E     | 4     | 0        | 0        | 0       | 0            |
| 4   | F     | 4     | 0        | 0        | 0       | 0            |
| 4   | G     | 5     | 0        | 0        | 0       | 0            |
| 4   | H     | 5     | 0        | 0        | 0       | 0            |
| 4   | I     | 3     | 0        | 0        | 0       | 0            |
| 4   | J     | 8     | 0        | 0        | 0       | 0            |
| 4   | K     | 7     | 0        | 0        | 0       | 0            |
| 4   | L     | 8     | 0        | 0        | 0       | 0            |
| 4   | M     | 5     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | N     | 3     | 0        | 0        | 0       | 0            |
| 4   | O     | 2     | 0        | 0        | 0       | 0            |
| 4   | P     | 6     | 0        | 0        | 0       | 0            |
| 4   | Q     | 4     | 0        | 0        | 0       | 0            |
| 4   | R     | 3     | 0        | 0        | 0       | 0            |
| 4   | S     | 5     | 0        | 0        | 0       | 0            |
| 4   | T     | 8     | 0        | 0        | 0       | 0            |
| 4   | U     | 8     | 0        | 0        | 1       | 0            |
| 4   | V     | 5     | 0        | 0        | 0       | 0            |
| All | All   | 14537 | 0        | 15518    | 245     | 2            |

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 8.

All (245) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 3:J:92:DMU:C7  | 3:J:92:DMU:C5  | 1.78                     | 1.59              |
| 3:F:92:DMU:C7  | 3:F:92:DMU:C5  | 1.79                     | 1.58              |
| 3:I:92:DMU:C7  | 3:I:92:DMU:C5  | 1.75                     | 1.55              |
| 3:G:92:DMU:C9  | 3:G:92:DMU:C10 | 1.96                     | 1.44              |
| 3:A:92:DMU:C10 | 3:A:92:DMU:C9  | 1.95                     | 1.43              |
| 3:P:92:DMU:C10 | 3:P:92:DMU:C9  | 1.95                     | 1.42              |
| 3:T:92:DMU:C9  | 3:T:92:DMU:C10 | 1.96                     | 1.42              |
| 3:H:92:DMU:C9  | 3:H:92:DMU:C10 | 1.97                     | 1.42              |
| 3:N:92:DMU:C10 | 3:N:92:DMU:C9  | 1.96                     | 1.41              |
| 3:C:92:DMU:C9  | 3:C:92:DMU:C10 | 1.97                     | 1.41              |
| 3:E:92:DMU:C10 | 3:E:92:DMU:C9  | 1.97                     | 1.41              |
| 3:V:92:DMU:C10 | 3:V:92:DMU:C9  | 1.96                     | 1.41              |
| 3:M:92:DMU:C9  | 3:M:92:DMU:C10 | 1.98                     | 1.41              |
| 3:R:92:DMU:C9  | 3:R:92:DMU:C10 | 1.97                     | 1.41              |
| 3:S:92:DMU:C10 | 3:S:92:DMU:C7  | 1.99                     | 1.40              |
| 3:K:92:DMU:C9  | 3:K:92:DMU:C10 | 1.97                     | 1.39              |
| 3:U:92:DMU:C7  | 3:U:92:DMU:C10 | 1.99                     | 1.39              |
| 3:L:92:DMU:C9  | 3:L:92:DMU:C10 | 1.95                     | 1.39              |
| 3:D:92:DMU:C10 | 3:D:92:DMU:C9  | 1.95                     | 1.38              |
| 3:Q:92:DMU:C10 | 3:Q:92:DMU:C9  | 2.00                     | 1.37              |
| 3:U:92:DMU:C6  | 3:U:92:DMU:O5  | 1.71                     | 1.37              |
| 3:H:92:DMU:C10 | 3:H:92:DMU:O1  | 1.75                     | 1.33              |
| 3:C:92:DMU:C10 | 3:C:92:DMU:O1  | 1.78                     | 1.31              |
| 3:P:92:DMU:C10 | 3:P:92:DMU:O1  | 1.78                     | 1.31              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 3:R:92:DMU:O1  | 3:R:92:DMU:C10 | 1.79                     | 1.30              |
| 3:V:92:DMU:C10 | 3:V:92:DMU:O1  | 1.79                     | 1.30              |
| 3:D:92:DMU:C10 | 3:D:92:DMU:O1  | 1.76                     | 1.30              |
| 3:L:92:DMU:O1  | 3:L:92:DMU:C10 | 1.78                     | 1.30              |
| 3:G:92:DMU:O1  | 3:G:92:DMU:C10 | 1.78                     | 1.29              |
| 3:M:92:DMU:O1  | 3:M:92:DMU:C10 | 1.79                     | 1.27              |
| 3:K:92:DMU:C10 | 3:K:92:DMU:O1  | 1.79                     | 1.27              |
| 3:N:92:DMU:C10 | 3:N:92:DMU:O1  | 1.79                     | 1.27              |
| 3:E:92:DMU:O1  | 3:E:92:DMU:C10 | 1.77                     | 1.27              |
| 3:A:92:DMU:C10 | 3:A:92:DMU:O1  | 1.77                     | 1.27              |
| 3:U:92:DMU:C6  | 3:U:92:DMU:C4  | 2.08                     | 1.26              |
| 3:S:92:DMU:O4  | 3:S:92:DMU:C10 | 1.81                     | 1.26              |
| 3:T:92:DMU:O1  | 3:T:92:DMU:C10 | 1.80                     | 1.26              |
| 3:U:92:DMU:O4  | 3:U:92:DMU:C10 | 1.83                     | 1.25              |
| 3:Q:92:DMU:C10 | 3:Q:92:DMU:O1  | 1.80                     | 1.24              |
| 3:F:92:DMU:C5  | 3:F:92:DMU:C8  | 2.19                     | 1.19              |
| 3:I:92:DMU:C5  | 3:I:92:DMU:C8  | 2.13                     | 1.17              |
| 3:J:92:DMU:C8  | 3:J:92:DMU:C5  | 2.22                     | 1.11              |
| 3:G:92:DMU:H35 | 3:G:92:DMU:C10 | 1.94                     | 0.97              |
| 3:U:92:DMU:O5  | 3:U:92:DMU:H5  | 1.62                     | 0.97              |
| 3:L:92:DMU:C10 | 3:L:92:DMU:H35 | 1.96                     | 0.96              |
| 3:D:92:DMU:C10 | 3:D:92:DMU:H35 | 1.96                     | 0.94              |
| 3:U:92:DMU:H33 | 3:U:92:DMU:C10 | 1.95                     | 0.94              |
| 3:K:92:DMU:C10 | 3:K:92:DMU:H35 | 1.98                     | 0.93              |
| 3:V:92:DMU:H35 | 3:V:92:DMU:C10 | 1.96                     | 0.93              |
| 3:P:92:DMU:C10 | 3:P:92:DMU:H35 | 1.99                     | 0.92              |
| 3:A:92:DMU:C10 | 3:A:92:DMU:H35 | 2.01                     | 0.91              |
| 3:C:92:DMU:C10 | 3:C:92:DMU:H35 | 2.00                     | 0.88              |
| 3:D:92:DMU:H35 | 3:D:92:DMU:O7  | 1.73                     | 0.88              |
| 3:R:92:DMU:H35 | 3:R:92:DMU:C10 | 2.01                     | 0.88              |
| 3:P:92:DMU:H35 | 3:P:92:DMU:O7  | 1.74                     | 0.87              |
| 3:E:92:DMU:H35 | 3:E:92:DMU:C10 | 2.03                     | 0.87              |
| 3:H:92:DMU:H35 | 3:H:92:DMU:C10 | 2.02                     | 0.87              |
| 3:N:92:DMU:C10 | 3:N:92:DMU:H35 | 2.03                     | 0.86              |
| 3:T:92:DMU:C10 | 3:T:92:DMU:H35 | 2.04                     | 0.85              |
| 1:U:49:ALA:HA  | 1:U:50:ARG:HB3 | 1.59                     | 0.85              |
| 3:H:92:DMU:H35 | 3:H:92:DMU:O7  | 1.78                     | 0.84              |
| 3:L:92:DMU:O7  | 3:L:92:DMU:H35 | 1.77                     | 0.83              |
| 3:S:92:DMU:C10 | 3:S:92:DMU:H33 | 2.08                     | 0.83              |
| 3:J:92:DMU:O2  | 3:J:92:DMU:O3  | 1.97                     | 0.83              |
| 3:G:92:DMU:O7  | 3:G:92:DMU:H35 | 1.80                     | 0.82              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 3:N:92:DMU:O7   | 3:N:92:DMU:H35  | 1.78                     | 0.82              |
| 3:F:92:DMU:H37  | 3:F:92:DMU:H38  | 0.84                     | 0.81              |
| 3:Q:92:DMU:C10  | 3:Q:92:DMU:H35  | 2.08                     | 0.81              |
| 3:K:92:DMU:H35  | 3:K:92:DMU:O7   | 1.80                     | 0.81              |
| 3:V:92:DMU:H35  | 3:V:92:DMU:O7   | 1.81                     | 0.80              |
| 3:A:92:DMU:O7   | 3:A:92:DMU:H35  | 1.83                     | 0.79              |
| 3:F:92:DMU:C7   | 3:F:92:DMU:H32  | 2.07                     | 0.79              |
| 3:P:92:DMU:O3   | 3:Q:92:DMU:O1   | 2.00                     | 0.78              |
| 3:J:92:DMU:C7   | 3:J:92:DMU:H32  | 2.10                     | 0.77              |
| 3:E:92:DMU:O7   | 3:E:92:DMU:H35  | 1.86                     | 0.76              |
| 3:N:92:DMU:C9   | 3:N:92:DMU:O7   | 2.35                     | 0.75              |
| 3:C:92:DMU:O7   | 3:C:92:DMU:H35  | 1.85                     | 0.75              |
| 3:P:92:DMU:O3   | 3:P:92:DMU:O2   | 1.99                     | 0.74              |
| 3:R:92:DMU:H35  | 3:R:92:DMU:O7   | 1.86                     | 0.74              |
| 3:M:92:DMU:H35  | 3:M:92:DMU:C10  | 2.11                     | 0.74              |
| 3:N:92:DMU:H29  | 1:O:5:THR:HG21  | 1.71                     | 0.73              |
| 3:R:92:DMU:O2   | 3:R:92:DMU:O3   | 2.02                     | 0.70              |
| 3:T:92:DMU:O3   | 3:T:92:DMU:O2   | 2.07                     | 0.69              |
| 3:H:92:DMU:C9   | 3:H:92:DMU:O7   | 2.36                     | 0.69              |
| 3:G:92:DMU:O2   | 3:G:92:DMU:O3   | 2.02                     | 0.68              |
| 3:F:92:DMU:H37  | 3:F:92:DMU:C5   | 2.06                     | 0.68              |
| 3:O:92:DMU:H29  | 3:P:92:DMU:H6   | 1.75                     | 0.68              |
| 3:L:92:DMU:H2   | 3:M:92:DMU:H1   | 1.76                     | 0.67              |
| 3:Q:92:DMU:O7   | 3:Q:92:DMU:H35  | 1.94                     | 0.67              |
| 3:J:92:DMU:H38  | 3:J:92:DMU:H37  | 1.30                     | 0.66              |
| 3:U:92:DMU:C6   | 3:U:92:DMU:C57  | 2.73                     | 0.66              |
| 3:U:92:DMU:H33  | 3:U:92:DMU:O7   | 1.96                     | 0.66              |
| 3:E:92:DMU:O7   | 3:E:92:DMU:C9   | 2.43                     | 0.66              |
| 3:E:92:DMU:O3   | 3:E:92:DMU:O2   | 2.02                     | 0.66              |
| 1:G:41:GLU:HG3  | 1:G:45:ARG:HH21 | 1.59                     | 0.65              |
| 1:I:20:LEU:HD13 | 1:J:20:LEU:HD13 | 1.77                     | 0.65              |
| 3:A:92:DMU:O3   | 3:A:92:DMU:O2   | 2.06                     | 0.65              |
| 3:R:92:DMU:H36  | 3:S:92:DMU:H32  | 1.79                     | 0.65              |
| 1:R:3:LEU:HD21  | 1:R:89:GLY:HA3  | 1.77                     | 0.64              |
| 3:Q:92:DMU:H15  | 1:R:9:ILE:HG12  | 1.78                     | 0.64              |
| 3:Q:92:DMU:O2   | 3:Q:92:DMU:O3   | 2.05                     | 0.63              |
| 3:M:92:DMU:H35  | 3:M:92:DMU:O7   | 1.99                     | 0.63              |
| 3:T:92:DMU:O7   | 3:T:92:DMU:H35  | 1.98                     | 0.62              |
| 1:K:1:MET:HA    | 3:K:92:DMU:H41  | 1.81                     | 0.62              |
| 3:C:92:DMU:O3   | 3:C:92:DMU:O2   | 2.03                     | 0.62              |
| 3:J:92:DMU:H15  | 1:K:9:ILE:HG12  | 1.82                     | 0.61              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 3:J:92:DMU:H11  | 1:K:9:ILE:HD11  | 1.82                     | 0.61              |
| 3:F:92:DMU:C5   | 3:F:92:DMU:O2   | 2.47                     | 0.61              |
| 1:K:1:MET:SD    | 3:K:92:DMU:O61  | 2.60                     | 0.60              |
| 1:L:16:VAL:HG21 | 3:V:92:DMU:H26  | 1.83                     | 0.60              |
| 3:S:92:DMU:H33  | 3:S:92:DMU:O7   | 2.02                     | 0.59              |
| 3:M:92:DMU:C9   | 3:M:92:DMU:O7   | 2.49                     | 0.59              |
| 1:Q:86:SER:O    | 1:Q:88:LEU:N    | 2.36                     | 0.59              |
| 1:U:49:ALA:HB1  | 1:U:51:GLY:H    | 1.67                     | 0.58              |
| 3:Q:92:DMU:C9   | 3:Q:92:DMU:O7   | 2.48                     | 0.58              |
| 3:G:92:DMU:O61  | 3:G:92:DMU:H35  | 2.02                     | 0.58              |
| 3:I:92:DMU:C5   | 3:I:92:DMU:H34  | 2.29                     | 0.58              |
| 1:V:9:ILE:HD13  | 3:V:92:DMU:H9   | 1.84                     | 0.58              |
| 3:L:92:DMU:O3   | 3:M:92:DMU:O4   | 2.11                     | 0.57              |
| 3:T:92:DMU:H2   | 3:U:92:DMU:O3   | 2.05                     | 0.57              |
| 1:P:56:THR:HG21 | 1:Q:43:VAL:HG21 | 1.87                     | 0.57              |
| 1:A:8:THR:HG21  | 1:K:1:MET:HE1   | 1.87                     | 0.56              |
| 3:E:92:DMU:H23  | 3:F:92:DMU:H23  | 1.88                     | 0.55              |
| 1:K:3:LEU:HG    | 1:K:7:LYS:HD2   | 1.89                     | 0.55              |
| 3:S:92:DMU:O49  | 3:T:92:DMU:H29  | 2.07                     | 0.55              |
| 1:N:3:LEU:HD13  | 1:N:7:LYS:HD2   | 1.88                     | 0.55              |
| 3:J:92:DMU:C8   | 3:J:92:DMU:O3   | 2.54                     | 0.54              |
| 3:U:92:DMU:C3   | 3:U:92:DMU:H33  | 2.36                     | 0.54              |
| 3:L:92:DMU:O2   | 3:L:92:DMU:O3   | 2.01                     | 0.54              |
| 3:F:92:DMU:O3   | 3:F:92:DMU:O2   | 2.00                     | 0.54              |
| 1:A:52:SER:HB2  | 1:B:50:ARG:HH12 | 1.73                     | 0.54              |
| 3:O:92:DMU:H26  | 1:P:16:VAL:HG21 | 1.88                     | 0.53              |
| 3:V:92:DMU:H7   | 3:V:92:DMU:O49  | 2.07                     | 0.53              |
| 3:N:92:DMU:O3   | 3:N:92:DMU:O2   | 2.10                     | 0.53              |
| 3:M:92:DMU:O3   | 3:M:92:DMU:O2   | 2.04                     | 0.53              |
| 3:O:92:DMU:H35  | 3:O:92:DMU:O61  | 2.09                     | 0.53              |
| 3:D:92:DMU:C9   | 3:D:92:DMU:O7   | 2.36                     | 0.52              |
| 1:B:2:ASP:N     | 1:B:2:ASP:OD1   | 2.44                     | 0.51              |
| 3:V:92:DMU:H35  | 3:V:92:DMU:O61  | 2.11                     | 0.51              |
| 3:K:92:DMU:O2   | 3:K:92:DMU:O3   | 2.03                     | 0.51              |
| 1:M:3:LEU:HG    | 1:M:7:LYS:HE2   | 1.91                     | 0.51              |
| 3:V:92:DMU:C9   | 3:V:92:DMU:O7   | 2.45                     | 0.50              |
| 3:P:92:DMU:O7   | 3:P:92:DMU:C9   | 2.36                     | 0.50              |
| 1:L:52:SER:OG   | 1:M:50:ARG:NH1  | 2.44                     | 0.50              |
| 1:H:53:ILE:HG23 | 1:I:40:VAL:HG13 | 1.94                     | 0.50              |
| 1:F:67:THR:HA   | 1:F:70:TYR:CD2  | 2.47                     | 0.50              |
| 3:H:92:DMU:H35  | 3:H:92:DMU:O61  | 2.12                     | 0.50              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 3:F:92:DMU:H16  | 1:G:9:ILE:HG12  | 1.94                     | 0.49              |
| 1:M:1:MET:HG3   | 1:M:5:THR:HB    | 1.94                     | 0.49              |
| 1:C:84:PHE:CZ   | 1:D:79:LEU:HD22 | 2.48                     | 0.49              |
| 3:T:92:DMU:O7   | 3:T:92:DMU:C9   | 2.53                     | 0.49              |
| 3:U:92:DMU:C6   | 3:U:92:DMU:H29  | 2.43                     | 0.49              |
| 3:G:92:DMU:H31  | 3:G:92:DMU:H35  | 1.78                     | 0.49              |
| 3:D:92:DMU:O3   | 3:D:92:DMU:O2   | 2.04                     | 0.48              |
| 3:V:92:DMU:H35  | 3:V:92:DMU:H31  | 1.76                     | 0.48              |
| 3:J:92:DMU:O49  | 3:K:92:DMU:H3   | 2.13                     | 0.48              |
| 3:L:92:DMU:O61  | 3:L:92:DMU:H35  | 2.13                     | 0.48              |
| 1:U:47:PRO:O    | 1:U:49:ALA:N    | 2.46                     | 0.48              |
| 3:J:92:DMU:H40  | 3:K:92:DMU:O4   | 2.14                     | 0.48              |
| 3:R:92:DMU:O61  | 3:R:92:DMU:H35  | 2.13                     | 0.48              |
| 3:G:92:DMU:H30  | 1:H:5:THR:HG21  | 1.95                     | 0.47              |
| 3:C:92:DMU:H3   | 3:D:92:DMU:O49  | 2.14                     | 0.47              |
| 3:J:92:DMU:O2   | 3:J:92:DMU:C5   | 2.52                     | 0.47              |
| 3:J:92:DMU:H36  | 3:J:92:DMU:H4   | 1.49                     | 0.47              |
| 1:D:50:ARG:O    | 1:D:54:ILE:HG12 | 2.15                     | 0.47              |
| 1:D:67:THR:HA   | 1:D:70:TYR:CD2  | 2.50                     | 0.47              |
| 3:L:92:DMU:H2   | 3:M:92:DMU:C1   | 2.44                     | 0.47              |
| 3:N:92:DMU:H31  | 3:N:92:DMU:H35  | 1.78                     | 0.47              |
| 3:U:92:DMU:O16  | 3:U:92:DMU:H29  | 2.15                     | 0.47              |
| 1:E:89:GLY:HA3  | 1:F:4:LEU:HD13  | 1.96                     | 0.46              |
| 3:I:92:DMU:H41  | 3:I:92:DMU:H36  | 1.62                     | 0.46              |
| 1:V:50:ARG:HG3  | 1:V:51:GLY:N    | 2.29                     | 0.46              |
| 3:U:92:DMU:O6   | 3:U:92:DMU:O2   | 2.13                     | 0.46              |
| 1:U:50:ARG:N    | 4:U:2002:HOH:O  | 2.48                     | 0.46              |
| 1:O:46:GLN:NE2  | 1:P:44:ALA:O    | 2.43                     | 0.46              |
| 3:E:92:DMU:H23  | 3:F:92:DMU:C40  | 2.45                     | 0.46              |
| 1:L:48:GLU:HG2  | 1:L:49:ALA:N    | 2.31                     | 0.46              |
| 1:V:34:TYR:O    | 1:V:38:LYS:HG2  | 2.15                     | 0.46              |
| 3:K:92:DMU:C9   | 3:K:92:DMU:O7   | 2.42                     | 0.46              |
| 1:E:67:THR:HA   | 1:E:70:TYR:CD2  | 2.51                     | 0.45              |
| 1:B:1:MET:N     | 3:B:92:DMU:O6   | 2.46                     | 0.45              |
| 1:S:84:PHE:CZ   | 1:T:79:LEU:HD22 | 2.51                     | 0.45              |
| 3:T:92:DMU:H36  | 3:T:92:DMU:O1   | 2.01                     | 0.45              |
| 3:N:92:DMU:H4   | 3:O:92:DMU:O55  | 2.17                     | 0.44              |
| 3:U:92:DMU:H7   | 3:V:92:DMU:O49  | 2.17                     | 0.44              |
| 3:L:92:DMU:O3   | 3:M:92:DMU:H36  | 2.17                     | 0.44              |
| 1:H:84:PHE:CD1  | 1:I:11:LEU:HG   | 2.53                     | 0.44              |
| 1:Q:46:GLN:HE22 | 1:R:44:ALA:HB1  | 1.82                     | 0.44              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:U:65:GLU:HG3  | 1:U:69:ILE:HD13 | 2.00                     | 0.44              |
| 1:J:67:THR:HA   | 1:J:70:TYR:CD2  | 2.52                     | 0.44              |
| 3:V:92:DMU:O2   | 3:V:92:DMU:O3   | 2.02                     | 0.44              |
| 1:A:5:THR:HA    | 1:K:1:MET:SD    | 2.57                     | 0.44              |
| 3:R:92:DMU:O4   | 3:S:92:DMU:H32  | 2.18                     | 0.44              |
| 1:T:67:THR:HA   | 1:T:70:TYR:CD2  | 2.52                     | 0.44              |
| 1:K:67:THR:HA   | 1:K:70:TYR:CD2  | 2.53                     | 0.44              |
| 3:E:92:DMU:O49  | 3:E:92:DMU:H7   | 2.17                     | 0.44              |
| 1:G:82:ASN:HA   | 1:G:83:PRO:HD3  | 1.84                     | 0.44              |
| 3:O:92:DMU:H29  | 3:P:92:DMU:C18  | 2.44                     | 0.44              |
| 3:H:92:DMU:O3   | 3:H:92:DMU:O2   | 2.02                     | 0.43              |
| 3:A:92:DMU:O55  | 3:B:92:DMU:H1   | 2.18                     | 0.43              |
| 3:N:92:DMU:H14  | 1:O:9:ILE:HG12  | 1.99                     | 0.43              |
| 3:T:92:DMU:O49  | 3:U:92:DMU:H30  | 2.19                     | 0.43              |
| 1:B:53:ILE:HG23 | 1:C:40:VAL:HG13 | 2.01                     | 0.43              |
| 3:L:92:DMU:H38  | 3:M:92:DMU:H36  | 1.82                     | 0.43              |
| 3:R:92:DMU:H1   | 3:S:92:DMU:H30  | 2.00                     | 0.43              |
| 3:T:92:DMU:H6   | 3:T:92:DMU:H1   | 1.66                     | 0.42              |
| 1:K:34:TYR:O    | 1:K:38:LYS:HG2  | 2.20                     | 0.42              |
| 3:O:92:DMU:H6   | 3:O:92:DMU:H1   | 1.44                     | 0.42              |
| 1:A:81:ALA:HB1  | 3:A:93:DMU:H14  | 2.02                     | 0.42              |
| 1:E:66:SER:OG   | 1:F:65:GLU:OE2  | 2.37                     | 0.42              |
| 1:C:84:PHE:HZ   | 1:D:79:LEU:HD22 | 1.84                     | 0.42              |
| 1:J:76:LEU:HD12 | 1:J:76:LEU:HA   | 1.92                     | 0.42              |
| 1:V:18:ALA:O    | 1:V:22:MET:HG2  | 2.20                     | 0.42              |
| 1:S:76:LEU:HA   | 1:S:76:LEU:HD12 | 1.82                     | 0.42              |
| 1:L:40:VAL:HG13 | 1:V:53:ILE:HG23 | 2.00                     | 0.42              |
| 3:B:92:DMU:H41  | 1:C:5:THR:OG1   | 2.20                     | 0.42              |
| 1:G:67:THR:HA   | 1:G:70:TYR:CD2  | 2.54                     | 0.42              |
| 1:C:46:GLN:HG2  | 1:D:44:ALA:O    | 2.20                     | 0.42              |
| 1:P:82:ASN:HA   | 1:P:83:PRO:HD3  | 1.73                     | 0.41              |
| 1:U:47:PRO:HB2  | 1:U:48:GLU:H    | 1.62                     | 0.41              |
| 1:L:39:ALA:O    | 1:L:43:VAL:HG13 | 2.20                     | 0.41              |
| 3:M:92:DMU:H35  | 3:M:92:DMU:H30  | 2.01                     | 0.41              |
| 1:R:10:VAL:HG21 | 1:R:88:LEU:HD11 | 2.02                     | 0.41              |
| 1:J:53:ILE:HG23 | 1:K:40:VAL:HG13 | 2.03                     | 0.41              |
| 1:P:73:VAL:O    | 1:P:77:ILE:HG13 | 2.21                     | 0.41              |
| 1:A:54:ILE:O    | 1:A:58:ILE:HG12 | 2.21                     | 0.41              |
| 1:K:82:ASN:HA   | 1:K:83:PRO:HD3  | 1.77                     | 0.41              |
| 1:G:9:ILE:HD13  | 3:G:92:DMU:H9   | 2.03                     | 0.41              |
| 1:I:6:ALA:HB1   | 1:I:88:LEU:HD13 | 2.03                     | 0.41              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:O:10:VAL:HG21 | 1:O:88:LEU:HD11 | 2.01                     | 0.41              |
| 1:V:48:GLU:CD   | 1:V:48:GLU:H    | 2.24                     | 0.41              |
| 1:I:7:LYS:HE3   | 1:I:7:LYS:HB2   | 1.87                     | 0.41              |
| 1:K:1:MET:HE3   | 1:K:9:ILE:HD12  | 2.03                     | 0.41              |
| 1:S:34:TYR:O    | 1:S:38:LYS:HG2  | 2.21                     | 0.41              |
| 3:Q:92:DMU:H38  | 3:Q:92:DMU:H37  | 1.58                     | 0.41              |
| 3:S:92:DMU:O55  | 3:T:92:DMU:H29  | 2.21                     | 0.41              |
| 1:L:34:TYR:O    | 1:L:38:LYS:HG2  | 2.21                     | 0.40              |
| 1:S:84:PHE:CD1  | 1:T:11:LEU:HG   | 2.56                     | 0.40              |
| 1:K:87:LYS:N    | 1:K:87:LYS:HD2  | 2.36                     | 0.40              |
| 1:P:18:ALA:O    | 1:P:22:MET:HG2  | 2.21                     | 0.40              |
| 1:R:18:ALA:O    | 1:R:22:MET:HG2  | 2.22                     | 0.40              |
| 3:R:92:DMU:O55  | 3:S:92:DMU:O3   | 2.33                     | 0.40              |
| 1:A:9:ILE:HG12  | 3:K:92:DMU:H11  | 2.04                     | 0.40              |
| 3:H:92:DMU:H30  | 1:I:5:THR:HG21  | 2.03                     | 0.40              |
| 1:N:6:ALA:HB1   | 1:N:88:LEU:HD13 | 2.03                     | 0.40              |

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

| Atom-1       | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|--------------|-----------------------|--------------------------|-------------------|
| 1:H:88:LEU:O | 4:A:2003:HOH:O[2_645] | 2.17                     | 0.03              |
| 1:B:7:LYS:NZ | 1:I:89:GLY:O[2_655]   | 2.18                     | 0.02              |

## 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 |     |
|-----|-------|-------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 87/89 (98%) | 87 (100%) | 0       | 0        | 100         | 100 |
| 1   | B     | 87/89 (98%) | 86 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | C     | 87/89 (98%) | 86 (99%)  | 1 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | D     | 87/89 (98%)     | 85 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 1   | E     | 87/89 (98%)     | 85 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 1   | F     | 87/89 (98%)     | 86 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 1   | G     | 87/89 (98%)     | 86 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 1   | H     | 87/89 (98%)     | 86 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 1   | I     | 87/89 (98%)     | 86 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 1   | J     | 87/89 (98%)     | 87 (100%)  | 0       | 0        | 100         | 100 |
| 1   | K     | 87/89 (98%)     | 86 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 1   | L     | 87/89 (98%)     | 85 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 1   | M     | 87/89 (98%)     | 85 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 1   | N     | 87/89 (98%)     | 83 (95%)   | 4 (5%)  | 0        | 100         | 100 |
| 1   | O     | 87/89 (98%)     | 86 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 1   | P     | 87/89 (98%)     | 86 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 1   | Q     | 87/89 (98%)     | 84 (97%)   | 1 (1%)  | 2 (2%)   | 7           | 10  |
| 1   | R     | 87/89 (98%)     | 86 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 1   | S     | 87/89 (98%)     | 84 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 1   | T     | 87/89 (98%)     | 83 (95%)   | 4 (5%)  | 0        | 100         | 100 |
| 1   | U     | 87/89 (98%)     | 82 (94%)   | 3 (3%)  | 2 (2%)   | 7           | 10  |
| 1   | V     | 87/89 (98%)     | 86 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| All | All   | 1914/1958 (98%) | 1876 (98%) | 34 (2%) | 4 (0%)   | 51          | 69  |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Q     | 87  | LYS  |
| 1   | U     | 47  | PRO  |
| 1   | Q     | 86  | SER  |
| 1   | U     | 48  | GLU  |

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 1   | A     | 62/62 (100%)     | 59 (95%)   | 3 (5%)   | 30          | 47  |
| 1   | B     | 62/62 (100%)     | 60 (97%)   | 2 (3%)   | 44          | 65  |
| 1   | C     | 62/62 (100%)     | 60 (97%)   | 2 (3%)   | 44          | 65  |
| 1   | D     | 62/62 (100%)     | 57 (92%)   | 5 (8%)   | 14          | 21  |
| 1   | E     | 62/62 (100%)     | 59 (95%)   | 3 (5%)   | 30          | 47  |
| 1   | F     | 62/62 (100%)     | 56 (90%)   | 6 (10%)  | 9           | 14  |
| 1   | G     | 62/62 (100%)     | 60 (97%)   | 2 (3%)   | 44          | 65  |
| 1   | H     | 62/62 (100%)     | 56 (90%)   | 6 (10%)  | 9           | 14  |
| 1   | I     | 62/62 (100%)     | 59 (95%)   | 3 (5%)   | 30          | 47  |
| 1   | J     | 62/62 (100%)     | 58 (94%)   | 4 (6%)   | 20          | 32  |
| 1   | K     | 62/62 (100%)     | 59 (95%)   | 3 (5%)   | 30          | 47  |
| 1   | L     | 62/62 (100%)     | 60 (97%)   | 2 (3%)   | 44          | 65  |
| 1   | M     | 62/62 (100%)     | 59 (95%)   | 3 (5%)   | 30          | 47  |
| 1   | N     | 62/62 (100%)     | 59 (95%)   | 3 (5%)   | 30          | 47  |
| 1   | O     | 62/62 (100%)     | 59 (95%)   | 3 (5%)   | 30          | 47  |
| 1   | P     | 62/62 (100%)     | 62 (100%)  | 0        | 100         | 100 |
| 1   | Q     | 62/62 (100%)     | 59 (95%)   | 3 (5%)   | 30          | 47  |
| 1   | R     | 62/62 (100%)     | 60 (97%)   | 2 (3%)   | 44          | 65  |
| 1   | S     | 62/62 (100%)     | 57 (92%)   | 5 (8%)   | 14          | 21  |
| 1   | T     | 62/62 (100%)     | 55 (89%)   | 7 (11%)  | 7           | 9   |
| 1   | U     | 62/62 (100%)     | 59 (95%)   | 3 (5%)   | 30          | 47  |
| 1   | V     | 62/62 (100%)     | 58 (94%)   | 4 (6%)   | 20          | 32  |
| All | All   | 1364/1364 (100%) | 1290 (95%) | 74 (5%)  | 26          | 41  |

All (74) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | LEU  |
| 1   | A     | 54  | ILE  |
| 1   | A     | 59  | LEU  |
| 1   | B     | 48  | GLU  |
| 1   | B     | 59  | LEU  |
| 1   | C     | 3   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 86  | SER  |
| 1   | D     | 3   | LEU  |
| 1   | D     | 59  | LEU  |
| 1   | D     | 71  | SER  |
| 1   | D     | 79  | LEU  |
| 1   | D     | 86  | SER  |
| 1   | E     | 46  | GLN  |
| 1   | E     | 48  | GLU  |
| 1   | E     | 50  | ARG  |
| 1   | F     | 48  | GLU  |
| 1   | F     | 50  | ARG  |
| 1   | F     | 59  | LEU  |
| 1   | F     | 71  | SER  |
| 1   | F     | 86  | SER  |
| 1   | F     | 87  | LYS  |
| 1   | G     | 3   | LEU  |
| 1   | G     | 45  | ARG  |
| 1   | H     | 10  | VAL  |
| 1   | H     | 45  | ARG  |
| 1   | H     | 55  | SER  |
| 1   | H     | 59  | LEU  |
| 1   | H     | 76  | LEU  |
| 1   | H     | 87  | LYS  |
| 1   | I     | 1   | MET  |
| 1   | I     | 11  | LEU  |
| 1   | I     | 48  | GLU  |
| 1   | J     | 20  | LEU  |
| 1   | J     | 41  | GLU  |
| 1   | J     | 46  | GLN  |
| 1   | J     | 76  | LEU  |
| 1   | K     | 2   | ASP  |
| 1   | K     | 10  | VAL  |
| 1   | K     | 87  | LYS  |
| 1   | L     | 59  | LEU  |
| 1   | L     | 66  | SER  |
| 1   | M     | 46  | GLN  |
| 1   | M     | 48  | GLU  |
| 1   | M     | 59  | LEU  |
| 1   | N     | 3   | LEU  |
| 1   | N     | 46  | GLN  |
| 1   | N     | 48  | GLU  |
| 1   | O     | 3   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 48  | GLU  |
| 1   | O     | 59  | LEU  |
| 1   | Q     | 46  | GLN  |
| 1   | Q     | 86  | SER  |
| 1   | Q     | 87  | LYS  |
| 1   | R     | 3   | LEU  |
| 1   | R     | 57  | MET  |
| 1   | S     | 3   | LEU  |
| 1   | S     | 43  | VAL  |
| 1   | S     | 50  | ARG  |
| 1   | S     | 59  | LEU  |
| 1   | S     | 76  | LEU  |
| 1   | T     | 11  | LEU  |
| 1   | T     | 43  | VAL  |
| 1   | T     | 48  | GLU  |
| 1   | T     | 50  | ARG  |
| 1   | T     | 71  | SER  |
| 1   | T     | 79  | LEU  |
| 1   | T     | 86  | SER  |
| 1   | U     | 3   | LEU  |
| 1   | U     | 76  | LEU  |
| 1   | U     | 86  | SER  |
| 1   | V     | 3   | LEU  |
| 1   | V     | 50  | ARG  |
| 1   | V     | 86  | SER  |
| 1   | V     | 87  | LYS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 45 ligands modelled in this entry, 22 are monoatomic - leaving 23 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 |
| 3   | DMU  | A     | 92  | -    | 34,34,34     | 3.76  | 8 (23%)  | 45,45,45    | 4.65  | 15 (33%) |
| 3   | DMU  | A     | 93  | -    | 34,34,34     | 0.83  | 2 (5%)   | 45,45,45    | 1.16  | 5 (11%)  |
| 3   | DMU  | B     | 92  | -    | 34,34,34     | 3.38  | 8 (23%)  | 45,45,45    | 4.75  | 15 (33%) |
| 3   | DMU  | C     | 92  | -    | 34,34,34     | 3.76  | 8 (23%)  | 45,45,45    | 4.59  | 13 (28%) |
| 3   | DMU  | D     | 92  | -    | 34,34,34     | 3.73  | 7 (20%)  | 45,45,45    | 4.63  | 14 (31%) |
| 3   | DMU  | E     | 92  | -    | 34,34,34     | 3.84  | 9 (26%)  | 45,45,45    | 4.76  | 16 (35%) |
| 3   | DMU  | F     | 92  | -    | 34,34,34     | 3.31  | 5 (14%)  | 45,45,45    | 4.70  | 17 (37%) |
| 3   | DMU  | G     | 92  | -    | 34,34,34     | 3.74  | 6 (17%)  | 45,45,45    | 4.61  | 13 (28%) |
| 3   | DMU  | H     | 92  | -    | 34,34,34     | 68.43 | 12 (35%) | 45,45,45    | 8.02  | 22 (48%) |
| 3   | DMU  | I     | 92  | -    | 34,34,34     | 3.29  | 7 (20%)  | 45,45,45    | 4.41  | 13 (28%) |
| 3   | DMU  | J     | 92  | -    | 34,34,34     | 4.29  | 11 (32%) | 45,45,45    | 8.22  | 30 (66%) |
| 3   | DMU  | K     | 92  | -    | 34,34,34     | 3.77  | 6 (17%)  | 45,45,45    | 4.64  | 15 (33%) |
| 3   | DMU  | L     | 92  | -    | 34,34,34     | 3.82  | 8 (23%)  | 45,45,45    | 4.69  | 14 (31%) |
| 3   | DMU  | M     | 92  | -    | 34,34,34     | 4.58  | 12 (35%) | 45,45,45    | 6.49  | 21 (46%) |
| 3   | DMU  | N     | 92  | -    | 34,34,34     | 3.82  | 9 (26%)  | 45,45,45    | 4.74  | 16 (35%) |
| 3   | DMU  | O     | 92  | -    | 34,34,34     | 0.93  | 1 (2%)   | 45,45,45    | 1.40  | 6 (13%)  |
| 3   | DMU  | P     | 92  | -    | 34,34,34     | 3.81  | 6 (17%)  | 45,45,45    | 4.73  | 19 (42%) |
| 3   | DMU  | Q     | 92  | -    | 34,34,34     | 3.84  | 7 (20%)  | 45,45,45    | 4.55  | 14 (31%) |
| 3   | DMU  | R     | 92  | -    | 34,34,34     | 3.79  | 7 (20%)  | 45,45,45    | 4.57  | 13 (28%) |
| 3   | DMU  | S     | 92  | -    | 34,34,34     | 12.85 | 8 (23%)  | 45,45,45    | 9.78  | 18 (40%) |
| 3   | DMU  | T     | 92  | -    | 34,34,34     | 3.89  | 9 (26%)  | 45,45,45    | 4.66  | 14 (31%) |
| 3   | DMU  | U     | 92  | -    | 34,34,34     | 14.01 | 14 (41%) | 45,45,45    | 11.09 | 22 (48%) |
| 3   | DMU  | V     | 92  | -    | 34,34,34     | 3.80  | 8 (23%)  | 45,45,45    | 4.63  | 13 (28%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals   | Torsions   | Rings   |
|-----|------|-------|-----|------|-----------|------------|---------|
| 3   | DMU  | A     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | A     | 93  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | B     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | C     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | D     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | E     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | F     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | G     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | H     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | I     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | J     | 92  | -    | 1/1/10/10 | 0/19/59/59 | 1/2/2/2 |
| 3   | DMU  | K     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | L     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | M     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | N     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | O     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | P     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | Q     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | R     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | S     | 92  | -    | 3/3/10/10 | 1/19/59/59 | 0/2/2/2 |
| 3   | DMU  | T     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | U     | 92  | -    | 3/3/10/10 | 0/19/59/59 | 0/2/2/2 |
| 3   | DMU  | V     | 92  | -    | -         | 0/19/59/59 | 0/2/2/2 |

All (178) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 3   | F     | 92  | DMU  | O1-C10 | -11.01 | 1.14        | 1.41     |
| 3   | I     | 92  | DMU  | O1-C10 | -10.64 | 1.15        | 1.41     |
| 3   | B     | 92  | DMU  | O5-C4  | -10.53 | 1.18        | 1.44     |
| 3   | J     | 92  | DMU  | C2-C1  | -10.40 | 1.25        | 1.52     |
| 3   | J     | 92  | DMU  | O1-C10 | -10.20 | 1.16        | 1.41     |
| 3   | P     | 92  | DMU  | C5-C7  | -10.06 | 1.26        | 1.52     |
| 3   | U     | 92  | DMU  | C2-C1  | -10.02 | 1.26        | 1.52     |
| 3   | T     | 92  | DMU  | O1-C9  | -9.97  | 1.20        | 1.44     |
| 3   | D     | 92  | DMU  | C5-C7  | -9.92  | 1.27        | 1.52     |
| 3   | U     | 92  | DMU  | O5-C4  | -9.84  | 1.20        | 1.44     |
| 3   | Q     | 92  | DMU  | O1-C9  | -9.71  | 1.20        | 1.44     |
| 3   | S     | 92  | DMU  | O4-C7  | -9.68  | 1.20        | 1.43     |
| 3   | E     | 92  | DMU  | C5-C7  | -9.65  | 1.27        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | Q     | 92  | DMU  | C5-C7  | -9.64 | 1.27        | 1.52     |
| 3   | C     | 92  | DMU  | C5-C7  | -9.62 | 1.27        | 1.52     |
| 3   | A     | 92  | DMU  | C5-C7  | -9.61 | 1.27        | 1.52     |
| 3   | M     | 92  | DMU  | C5-C7  | -9.54 | 1.28        | 1.52     |
| 3   | H     | 92  | DMU  | C5-C7  | -9.46 | 1.28        | 1.52     |
| 3   | G     | 92  | DMU  | C5-C7  | -9.46 | 1.28        | 1.52     |
| 3   | A     | 92  | DMU  | O1-C9  | -9.43 | 1.21        | 1.44     |
| 3   | R     | 92  | DMU  | C5-C7  | -9.41 | 1.28        | 1.52     |
| 3   | K     | 92  | DMU  | C5-C7  | -9.40 | 1.28        | 1.52     |
| 3   | V     | 92  | DMU  | C5-C7  | -9.38 | 1.28        | 1.52     |
| 3   | T     | 92  | DMU  | C5-C7  | -9.38 | 1.28        | 1.52     |
| 3   | L     | 92  | DMU  | C5-C7  | -9.35 | 1.28        | 1.52     |
| 3   | N     | 92  | DMU  | O1-C9  | -9.25 | 1.21        | 1.44     |
| 3   | L     | 92  | DMU  | O1-C9  | -9.21 | 1.22        | 1.44     |
| 3   | M     | 92  | DMU  | C2-C1  | -9.20 | 1.28        | 1.52     |
| 3   | B     | 92  | DMU  | C2-C1  | -9.20 | 1.28        | 1.52     |
| 3   | K     | 92  | DMU  | O1-C9  | -9.19 | 1.22        | 1.44     |
| 3   | E     | 92  | DMU  | O1-C9  | -9.18 | 1.22        | 1.44     |
| 3   | G     | 92  | DMU  | O1-C9  | -9.13 | 1.22        | 1.44     |
| 3   | R     | 92  | DMU  | O1-C9  | -9.10 | 1.22        | 1.44     |
| 3   | C     | 92  | DMU  | O1-C9  | -9.07 | 1.22        | 1.44     |
| 3   | P     | 92  | DMU  | O1-C9  | -9.06 | 1.22        | 1.44     |
| 3   | M     | 92  | DMU  | O1-C9  | -9.03 | 1.22        | 1.44     |
| 3   | V     | 92  | DMU  | O1-C9  | -9.01 | 1.22        | 1.44     |
| 3   | N     | 92  | DMU  | C5-C7  | -8.94 | 1.29        | 1.52     |
| 3   | U     | 92  | DMU  | O4-C7  | -8.83 | 1.22        | 1.43     |
| 3   | D     | 92  | DMU  | O1-C9  | -8.57 | 1.23        | 1.44     |
| 3   | H     | 92  | DMU  | O1-C9  | -8.22 | 1.24        | 1.44     |
| 3   | J     | 92  | DMU  | C2-C3  | -7.67 | 1.31        | 1.52     |
| 3   | I     | 92  | DMU  | C8-C7  | -7.47 | 1.33        | 1.52     |
| 3   | U     | 92  | DMU  | C11-C9 | -7.41 | 1.26        | 1.51     |
| 3   | S     | 92  | DMU  | C11-C9 | -7.00 | 1.28        | 1.51     |
| 3   | H     | 92  | DMU  | C2-C1  | -6.57 | 1.35        | 1.52     |
| 3   | F     | 92  | DMU  | C8-C7  | -6.38 | 1.36        | 1.52     |
| 3   | J     | 92  | DMU  | C8-C7  | -5.58 | 1.38        | 1.52     |
| 3   | M     | 92  | DMU  | O5-C4  | -5.51 | 1.31        | 1.44     |
| 3   | H     | 92  | DMU  | O5-C4  | -4.28 | 1.33        | 1.44     |
| 3   | A     | 92  | DMU  | O4-C7  | 2.00  | 1.47        | 1.43     |
| 3   | K     | 92  | DMU  | O7-C3  | 2.06  | 1.48        | 1.43     |
| 3   | L     | 92  | DMU  | O4-C7  | 2.08  | 1.47        | 1.43     |
| 3   | E     | 92  | DMU  | O7-C3  | 2.09  | 1.48        | 1.43     |
| 3   | G     | 92  | DMU  | O4-C7  | 2.11  | 1.47        | 1.43     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 3   | V     | 92  | DMU  | O7-C3  | 2.12 | 1.49        | 1.43     |
| 3   | Q     | 92  | DMU  | O7-C3  | 2.13 | 1.49        | 1.43     |
| 3   | D     | 92  | DMU  | O4-C7  | 2.14 | 1.47        | 1.43     |
| 3   | T     | 92  | DMU  | O4-C7  | 2.16 | 1.47        | 1.43     |
| 3   | C     | 92  | DMU  | O16-C6 | 2.16 | 1.44        | 1.40     |
| 3   | R     | 92  | DMU  | O16-C6 | 2.17 | 1.44        | 1.40     |
| 3   | A     | 93  | DMU  | O16-C6 | 2.17 | 1.44        | 1.40     |
| 3   | V     | 92  | DMU  | O4-C7  | 2.18 | 1.48        | 1.43     |
| 3   | E     | 92  | DMU  | O4-C7  | 2.20 | 1.48        | 1.43     |
| 3   | N     | 92  | DMU  | O4-C7  | 2.20 | 1.48        | 1.43     |
| 3   | R     | 92  | DMU  | O4-C7  | 2.21 | 1.48        | 1.43     |
| 3   | S     | 92  | DMU  | O7-C3  | 2.22 | 1.49        | 1.43     |
| 3   | C     | 92  | DMU  | O4-C7  | 2.24 | 1.48        | 1.43     |
| 3   | Q     | 92  | DMU  | O4-C7  | 2.27 | 1.48        | 1.43     |
| 3   | E     | 92  | DMU  | O5-C6  | 2.27 | 1.47        | 1.41     |
| 3   | A     | 93  | DMU  | O5-C6  | 2.29 | 1.47        | 1.41     |
| 3   | M     | 92  | DMU  | O7-C10 | 2.32 | 1.47        | 1.41     |
| 3   | A     | 92  | DMU  | O5-C6  | 2.33 | 1.47        | 1.41     |
| 3   | C     | 92  | DMU  | O5-C6  | 2.36 | 1.47        | 1.41     |
| 3   | L     | 92  | DMU  | O7-C3  | 2.43 | 1.49        | 1.43     |
| 3   | I     | 92  | DMU  | O16-C6 | 2.47 | 1.44        | 1.40     |
| 3   | N     | 92  | DMU  | O7-C10 | 2.47 | 1.48        | 1.41     |
| 3   | M     | 92  | DMU  | O4-C7  | 2.49 | 1.48        | 1.43     |
| 3   | N     | 92  | DMU  | O7-C3  | 2.56 | 1.50        | 1.43     |
| 3   | T     | 92  | DMU  | O7-C10 | 2.62 | 1.48        | 1.41     |
| 3   | T     | 92  | DMU  | O16-C6 | 2.66 | 1.44        | 1.40     |
| 3   | H     | 92  | DMU  | O4-C7  | 2.72 | 1.49        | 1.43     |
| 3   | U     | 92  | DMU  | O7-C3  | 2.73 | 1.50        | 1.43     |
| 3   | T     | 92  | DMU  | O7-C3  | 2.78 | 1.50        | 1.43     |
| 3   | A     | 92  | DMU  | O16-C6 | 2.78 | 1.45        | 1.40     |
| 3   | N     | 92  | DMU  | O16-C6 | 2.96 | 1.45        | 1.40     |
| 3   | I     | 92  | DMU  | C3-C4  | 3.17 | 1.61        | 1.52     |
| 3   | S     | 92  | DMU  | C8-C7  | 3.21 | 1.60        | 1.52     |
| 3   | S     | 92  | DMU  | O7-C10 | 3.31 | 1.50        | 1.41     |
| 3   | O     | 92  | DMU  | O16-C6 | 3.32 | 1.46        | 1.40     |
| 3   | H     | 92  | DMU  | O16-C6 | 3.33 | 1.46        | 1.40     |
| 3   | V     | 92  | DMU  | O16-C6 | 3.33 | 1.46        | 1.40     |
| 3   | U     | 92  | DMU  | C3-C4  | 3.47 | 1.62        | 1.52     |
| 3   | J     | 92  | DMU  | C6-C1  | 3.55 | 1.62        | 1.52     |
| 3   | U     | 92  | DMU  | C8-C7  | 3.56 | 1.61        | 1.52     |
| 3   | M     | 92  | DMU  | O16-C6 | 3.57 | 1.46        | 1.40     |
| 3   | P     | 92  | DMU  | O16-C6 | 3.63 | 1.46        | 1.40     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 3   | B     | 92  | DMU  | O7-C10 | 3.66 | 1.51        | 1.41     |
| 3   | H     | 92  | DMU  | C3-C4  | 3.84 | 1.63        | 1.52     |
| 3   | T     | 92  | DMU  | C8-C9  | 3.95 | 1.61        | 1.53     |
| 3   | D     | 92  | DMU  | O16-C6 | 3.96 | 1.47        | 1.40     |
| 3   | U     | 92  | DMU  | O7-C10 | 4.00 | 1.52        | 1.41     |
| 3   | L     | 92  | DMU  | O16-C6 | 4.00 | 1.47        | 1.40     |
| 3   | K     | 92  | DMU  | C8-C9  | 4.00 | 1.61        | 1.53     |
| 3   | P     | 92  | DMU  | C8-C9  | 4.03 | 1.61        | 1.53     |
| 3   | J     | 92  | DMU  | C3-C4  | 4.10 | 1.64        | 1.52     |
| 3   | C     | 92  | DMU  | C8-C9  | 4.19 | 1.61        | 1.53     |
| 3   | L     | 92  | DMU  | C8-C9  | 4.19 | 1.61        | 1.53     |
| 3   | G     | 92  | DMU  | C8-C9  | 4.20 | 1.62        | 1.53     |
| 3   | B     | 92  | DMU  | O16-C6 | 4.20 | 1.47        | 1.40     |
| 3   | R     | 92  | DMU  | C8-C9  | 4.25 | 1.62        | 1.53     |
| 3   | V     | 92  | DMU  | C8-C9  | 4.27 | 1.62        | 1.53     |
| 3   | Q     | 92  | DMU  | C8-C9  | 4.34 | 1.62        | 1.53     |
| 3   | E     | 92  | DMU  | O16-C6 | 4.36 | 1.47        | 1.40     |
| 3   | B     | 92  | DMU  | C3-C4  | 4.40 | 1.64        | 1.52     |
| 3   | E     | 92  | DMU  | C8-C9  | 4.46 | 1.62        | 1.53     |
| 3   | A     | 92  | DMU  | C8-C9  | 4.53 | 1.62        | 1.53     |
| 3   | D     | 92  | DMU  | C8-C9  | 4.68 | 1.63        | 1.53     |
| 3   | M     | 92  | DMU  | C3-C4  | 4.78 | 1.65        | 1.52     |
| 3   | B     | 92  | DMU  | C6-C1  | 5.12 | 1.67        | 1.52     |
| 3   | U     | 92  | DMU  | C6-C1  | 5.12 | 1.67        | 1.52     |
| 3   | S     | 92  | DMU  | O16-C6 | 5.13 | 1.49        | 1.40     |
| 3   | M     | 92  | DMU  | C8-C9  | 5.21 | 1.64        | 1.53     |
| 3   | J     | 92  | DMU  | O5-C4  | 5.47 | 1.57        | 1.44     |
| 3   | N     | 92  | DMU  | C8-C9  | 5.48 | 1.64        | 1.53     |
| 3   | J     | 92  | DMU  | C8-C9  | 5.64 | 1.65        | 1.53     |
| 3   | N     | 92  | DMU  | C10-C5 | 5.78 | 1.69        | 1.52     |
| 3   | M     | 92  | DMU  | C10-C5 | 5.88 | 1.69        | 1.52     |
| 3   | H     | 92  | DMU  | O5-C6  | 6.16 | 1.57        | 1.41     |
| 3   | I     | 92  | DMU  | C8-C9  | 6.18 | 1.66        | 1.53     |
| 3   | Q     | 92  | DMU  | C10-C5 | 6.22 | 1.70        | 1.52     |
| 3   | H     | 92  | DMU  | C8-C9  | 6.24 | 1.66        | 1.53     |
| 3   | T     | 92  | DMU  | C10-C5 | 6.29 | 1.70        | 1.52     |
| 3   | F     | 92  | DMU  | C8-C9  | 6.31 | 1.66        | 1.53     |
| 3   | P     | 92  | DMU  | C10-C5 | 6.36 | 1.70        | 1.52     |
| 3   | R     | 92  | DMU  | C10-C5 | 6.39 | 1.70        | 1.52     |
| 3   | U     | 92  | DMU  | C2-C3  | 6.39 | 1.69        | 1.52     |
| 3   | H     | 92  | DMU  | C10-C5 | 6.44 | 1.71        | 1.52     |
| 3   | L     | 92  | DMU  | C10-C5 | 6.60 | 1.71        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 3   | B     | 92  | DMU  | C2-C3   | 6.70   | 1.70        | 1.52     |
| 3   | C     | 92  | DMU  | C10-C5  | 6.72   | 1.71        | 1.52     |
| 3   | G     | 92  | DMU  | C10-C5  | 6.73   | 1.71        | 1.52     |
| 3   | I     | 92  | DMU  | C10-C5  | 6.74   | 1.71        | 1.52     |
| 3   | U     | 92  | DMU  | O16-C6  | 6.81   | 1.52        | 1.40     |
| 3   | E     | 92  | DMU  | C10-C5  | 6.85   | 1.72        | 1.52     |
| 3   | V     | 92  | DMU  | C10-C5  | 6.86   | 1.72        | 1.52     |
| 3   | D     | 92  | DMU  | C10-C5  | 6.88   | 1.72        | 1.52     |
| 3   | J     | 92  | DMU  | C10-C5  | 6.89   | 1.72        | 1.52     |
| 3   | F     | 92  | DMU  | C10-C5  | 6.93   | 1.72        | 1.52     |
| 3   | A     | 92  | DMU  | C10-C5  | 7.16   | 1.73        | 1.52     |
| 3   | K     | 92  | DMU  | C10-C5  | 7.30   | 1.73        | 1.52     |
| 3   | B     | 92  | DMU  | O5-C6   | 7.47   | 1.60        | 1.41     |
| 3   | J     | 92  | DMU  | O5-C6   | 8.22   | 1.62        | 1.41     |
| 3   | M     | 92  | DMU  | O5-C6   | 8.59   | 1.63        | 1.41     |
| 3   | I     | 92  | DMU  | C5-C7   | 9.06   | 1.75        | 1.52     |
| 3   | J     | 92  | DMU  | C5-C7   | 10.39  | 1.78        | 1.52     |
| 3   | F     | 92  | DMU  | C5-C7   | 10.50  | 1.79        | 1.52     |
| 3   | U     | 92  | DMU  | O5-C6   | 11.96  | 1.71        | 1.41     |
| 3   | H     | 92  | DMU  | O1-C10  | 13.51  | 1.75        | 1.41     |
| 3   | D     | 92  | DMU  | O1-C10  | 14.07  | 1.76        | 1.41     |
| 3   | A     | 92  | DMU  | O1-C10  | 14.13  | 1.77        | 1.41     |
| 3   | E     | 92  | DMU  | O1-C10  | 14.52  | 1.77        | 1.41     |
| 3   | P     | 92  | DMU  | O1-C10  | 14.80  | 1.78        | 1.41     |
| 3   | C     | 92  | DMU  | O1-C10  | 14.84  | 1.78        | 1.41     |
| 3   | G     | 92  | DMU  | O1-C10  | 14.85  | 1.78        | 1.41     |
| 3   | L     | 92  | DMU  | O1-C10  | 14.92  | 1.78        | 1.41     |
| 3   | K     | 92  | DMU  | O1-C10  | 14.95  | 1.79        | 1.41     |
| 3   | M     | 92  | DMU  | O1-C10  | 14.96  | 1.79        | 1.41     |
| 3   | V     | 92  | DMU  | O1-C10  | 15.02  | 1.79        | 1.41     |
| 3   | N     | 92  | DMU  | O1-C10  | 15.20  | 1.79        | 1.41     |
| 3   | R     | 92  | DMU  | O1-C10  | 15.29  | 1.79        | 1.41     |
| 3   | Q     | 92  | DMU  | O1-C10  | 15.46  | 1.80        | 1.41     |
| 3   | T     | 92  | DMU  | O1-C10  | 15.48  | 1.80        | 1.41     |
| 3   | S     | 92  | DMU  | O1-C10  | 31.43  | 2.20        | 1.41     |
| 3   | U     | 92  | DMU  | O1-C10  | 32.67  | 2.23        | 1.41     |
| 3   | S     | 92  | DMU  | C10-C5  | 66.46  | 3.43        | 1.52     |
| 3   | U     | 92  | DMU  | C10-C5  | 70.41  | 3.54        | 1.52     |
| 3   | H     | 92  | DMU  | O16-C18 | 398.32 | 12.14       | 1.43     |

All (358) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 3   | U     | 92  | DMU  | C10-C5-C7   | -56.79 | 4.41        | 109.98   |
| 3   | S     | 92  | DMU  | C10-C5-C7   | -51.31 | 14.60       | 109.98   |
| 3   | S     | 92  | DMU  | C10-O1-C9   | -28.05 | 60.88       | 113.72   |
| 3   | U     | 92  | DMU  | C10-O1-C9   | -27.71 | 61.52       | 113.72   |
| 3   | H     | 92  | DMU  | O16-C18-C19 | -22.77 | 28.45       | 109.68   |
| 3   | N     | 92  | DMU  | C10-O1-C9   | -18.64 | 78.60       | 113.72   |
| 3   | P     | 92  | DMU  | C10-O1-C9   | -18.57 | 78.73       | 113.72   |
| 3   | L     | 92  | DMU  | C10-O1-C9   | -18.56 | 78.74       | 113.72   |
| 3   | V     | 92  | DMU  | C10-O1-C9   | -18.42 | 79.01       | 113.72   |
| 3   | G     | 92  | DMU  | C10-O1-C9   | -18.42 | 79.02       | 113.72   |
| 3   | D     | 92  | DMU  | C10-O1-C9   | -18.41 | 79.03       | 113.72   |
| 3   | T     | 92  | DMU  | C10-O1-C9   | -18.40 | 79.05       | 113.72   |
| 3   | A     | 92  | DMU  | C10-O1-C9   | -18.23 | 79.38       | 113.72   |
| 3   | R     | 92  | DMU  | C10-O1-C9   | -18.19 | 79.44       | 113.72   |
| 3   | C     | 92  | DMU  | C10-O1-C9   | -18.16 | 79.50       | 113.72   |
| 3   | K     | 92  | DMU  | C10-O1-C9   | -18.12 | 79.59       | 113.72   |
| 3   | H     | 92  | DMU  | O5-C6-O16   | -18.09 | 67.06       | 110.02   |
| 3   | M     | 92  | DMU  | C10-O1-C9   | -17.98 | 79.85       | 113.72   |
| 3   | E     | 92  | DMU  | C10-O1-C9   | -17.94 | 79.91       | 113.72   |
| 3   | H     | 92  | DMU  | C10-O1-C9   | -17.70 | 80.38       | 113.72   |
| 3   | Q     | 92  | DMU  | C10-O1-C9   | -17.52 | 80.71       | 113.72   |
| 3   | M     | 92  | DMU  | O5-C6-O16   | -17.07 | 69.50       | 110.02   |
| 3   | J     | 92  | DMU  | O1-C10-C5   | -16.22 | 79.00       | 110.30   |
| 3   | N     | 92  | DMU  | C10-C5-C7   | -16.11 | 80.03       | 109.98   |
| 3   | I     | 92  | DMU  | O1-C10-C5   | -16.04 | 79.35       | 110.30   |
| 3   | B     | 92  | DMU  | O16-C6-C1   | -15.99 | 82.14       | 108.23   |
| 3   | A     | 92  | DMU  | C10-C5-C7   | -15.60 | 80.98       | 109.98   |
| 3   | K     | 92  | DMU  | C10-C5-C7   | -15.55 | 81.07       | 109.98   |
| 3   | E     | 92  | DMU  | C10-C5-C7   | -15.46 | 81.25       | 109.98   |
| 3   | T     | 92  | DMU  | C10-C5-C7   | -15.44 | 81.29       | 109.98   |
| 3   | R     | 92  | DMU  | C10-C5-C7   | -15.43 | 81.29       | 109.98   |
| 3   | D     | 92  | DMU  | C10-C5-C7   | -15.41 | 81.34       | 109.98   |
| 3   | V     | 92  | DMU  | C10-C5-C7   | -15.37 | 81.40       | 109.98   |
| 3   | C     | 92  | DMU  | C10-C5-C7   | -15.36 | 81.43       | 109.98   |
| 3   | U     | 92  | DMU  | O16-C6-C1   | -15.35 | 83.18       | 108.23   |
| 3   | L     | 92  | DMU  | C10-C5-C7   | -15.33 | 81.48       | 109.98   |
| 3   | H     | 92  | DMU  | C10-C5-C7   | -15.32 | 81.49       | 109.98   |
| 3   | Q     | 92  | DMU  | C10-C5-C7   | -15.29 | 81.55       | 109.98   |
| 3   | F     | 92  | DMU  | O1-C10-C5   | -15.28 | 80.82       | 110.30   |
| 3   | P     | 92  | DMU  | C10-C5-C7   | -15.26 | 81.62       | 109.98   |
| 3   | G     | 92  | DMU  | C10-C5-C7   | -15.24 | 81.65       | 109.98   |
| 3   | J     | 92  | DMU  | C6-C1-C2    | -15.11 | 81.89       | 109.98   |
| 3   | M     | 92  | DMU  | C10-C5-C7   | -14.87 | 82.34       | 109.98   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 3   | J     | 92  | DMU  | C2-C3-C4   | -14.12 | 80.92       | 110.88   |
| 3   | I     | 92  | DMU  | C8-C7-C5   | -13.83 | 86.44       | 110.84   |
| 3   | F     | 92  | DMU  | C8-C7-C5   | -13.46 | 87.10       | 110.84   |
| 3   | J     | 92  | DMU  | C18-O16-C6 | -13.22 | 91.17       | 113.87   |
| 3   | J     | 92  | DMU  | C8-C7-C5   | -12.88 | 88.11       | 110.84   |
| 3   | U     | 92  | DMU  | C6-O5-C4   | -12.74 | 89.72       | 113.72   |
| 3   | M     | 92  | DMU  | O7-C3-C4   | -12.09 | 79.61       | 109.34   |
| 3   | B     | 92  | DMU  | O7-C3-C2   | -11.55 | 79.41       | 107.19   |
| 3   | I     | 92  | DMU  | C10-O1-C9  | -11.43 | 92.19       | 113.72   |
| 3   | H     | 92  | DMU  | O7-C3-C4   | -10.80 | 82.78       | 109.34   |
| 3   | J     | 92  | DMU  | O3-C5-C10  | -10.77 | 87.51       | 110.03   |
| 3   | J     | 92  | DMU  | O55-C2-C1  | -10.33 | 87.88       | 110.36   |
| 3   | F     | 92  | DMU  | O3-C5-C10  | -10.26 | 88.58       | 110.03   |
| 3   | U     | 92  | DMU  | O7-C3-C2   | -9.87  | 83.44       | 107.19   |
| 3   | J     | 92  | DMU  | O16-C6-C1  | -9.35  | 92.98       | 108.23   |
| 3   | S     | 92  | DMU  | O4-C7-C5   | -9.09  | 90.58       | 110.36   |
| 3   | M     | 92  | DMU  | O1-C9-C8   | -8.54  | 93.92       | 109.66   |
| 3   | J     | 92  | DMU  | O55-C2-C3  | -8.47  | 90.59       | 109.87   |
| 3   | S     | 92  | DMU  | O1-C10-C5  | -8.40  | 94.08       | 110.30   |
| 3   | N     | 92  | DMU  | O1-C9-C8   | -8.10  | 94.75       | 109.66   |
| 3   | B     | 92  | DMU  | C6-O5-C4   | -8.02  | 98.61       | 113.72   |
| 3   | M     | 92  | DMU  | C6-O5-C4   | -7.81  | 99.00       | 113.72   |
| 3   | I     | 92  | DMU  | C7-C8-C9   | -7.78  | 96.52       | 110.22   |
| 3   | F     | 92  | DMU  | C7-C8-C9   | -7.69  | 96.66       | 110.22   |
| 3   | U     | 92  | DMU  | C1-C2-C3   | -7.66  | 93.72       | 109.61   |
| 3   | H     | 92  | DMU  | O1-C9-C8   | -7.53  | 95.79       | 109.66   |
| 3   | U     | 92  | DMU  | C6-C1-C2   | -7.41  | 96.21       | 109.98   |
| 3   | E     | 92  | DMU  | C18-O16-C6 | -7.39  | 101.18      | 113.87   |
| 3   | Q     | 92  | DMU  | O1-C9-C8   | -7.27  | 96.28       | 109.66   |
| 3   | J     | 92  | DMU  | C10-O7-C3  | -7.23  | 100.37      | 118.00   |
| 3   | F     | 92  | DMU  | C18-O16-C6 | -7.18  | 101.54      | 113.87   |
| 3   | J     | 92  | DMU  | O7-C10-O1  | -7.11  | 93.43       | 110.70   |
| 3   | B     | 92  | DMU  | C10-O7-C3  | -7.11  | 100.67      | 118.00   |
| 3   | J     | 92  | DMU  | C6-O5-C4   | -7.10  | 100.34      | 113.72   |
| 3   | G     | 92  | DMU  | O7-C10-C5  | -7.08  | 92.15       | 108.11   |
| 3   | B     | 92  | DMU  | C18-O16-C6 | -7.04  | 101.79      | 113.87   |
| 3   | M     | 92  | DMU  | O1-C9-C11  | -6.80  | 90.13       | 106.41   |
| 3   | T     | 92  | DMU  | O1-C9-C11  | -6.74  | 90.26       | 106.41   |
| 3   | K     | 92  | DMU  | O7-C10-C5  | -6.67  | 93.09       | 108.11   |
| 3   | V     | 92  | DMU  | O7-C10-C5  | -6.66  | 93.11       | 108.11   |
| 3   | C     | 92  | DMU  | O7-C10-C5  | -6.63  | 93.17       | 108.11   |
| 3   | T     | 92  | DMU  | O7-C10-C5  | -6.58  | 93.29       | 108.11   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | A     | 92  | DMU  | O7-C10-C5  | -6.55 | 93.36       | 108.11   |
| 3   | G     | 92  | DMU  | C8-C7-C5   | -6.48 | 99.41       | 110.84   |
| 3   | D     | 92  | DMU  | C8-C7-C5   | -6.37 | 99.61       | 110.84   |
| 3   | B     | 92  | DMU  | C6-C1-C2   | -6.35 | 98.18       | 109.98   |
| 3   | B     | 92  | DMU  | C1-C2-C3   | -6.34 | 96.47       | 109.61   |
| 3   | C     | 92  | DMU  | C8-C7-C5   | -6.33 | 99.67       | 110.84   |
| 3   | L     | 92  | DMU  | C8-C7-C5   | -6.30 | 99.72       | 110.84   |
| 3   | E     | 92  | DMU  | C8-C7-C5   | -6.25 | 99.81       | 110.84   |
| 3   | K     | 92  | DMU  | C8-C7-C5   | -6.24 | 99.82       | 110.84   |
| 3   | E     | 92  | DMU  | O7-C10-C5  | -6.20 | 94.15       | 108.11   |
| 3   | E     | 92  | DMU  | O1-C9-C8   | -6.20 | 98.25       | 109.66   |
| 3   | L     | 92  | DMU  | O7-C10-C5  | -6.18 | 94.18       | 108.11   |
| 3   | J     | 92  | DMU  | C7-C8-C9   | -6.18 | 99.33       | 110.22   |
| 3   | V     | 92  | DMU  | C8-C7-C5   | -6.17 | 99.95       | 110.84   |
| 3   | Q     | 92  | DMU  | C8-C7-C5   | -6.15 | 99.99       | 110.84   |
| 3   | S     | 92  | DMU  | O4-C7-C8   | -6.14 | 96.99       | 110.36   |
| 3   | U     | 92  | DMU  | O7-C10-C5  | -6.08 | 94.40       | 108.11   |
| 3   | U     | 92  | DMU  | O4-C7-C8   | -6.07 | 97.14       | 110.36   |
| 3   | T     | 92  | DMU  | O1-C9-C8   | -6.05 | 98.52       | 109.66   |
| 3   | C     | 92  | DMU  | O1-C9-C8   | -6.02 | 98.57       | 109.66   |
| 3   | M     | 92  | DMU  | C8-C7-C5   | -6.01 | 100.24      | 110.84   |
| 3   | R     | 92  | DMU  | O7-C10-C5  | -6.00 | 94.60       | 108.11   |
| 3   | R     | 92  | DMU  | O1-C9-C8   | -5.98 | 98.65       | 109.66   |
| 3   | P     | 92  | DMU  | C8-C7-C5   | -5.76 | 100.67      | 110.84   |
| 3   | P     | 92  | DMU  | O1-C9-C8   | -5.75 | 99.07       | 109.66   |
| 3   | D     | 92  | DMU  | O7-C10-C5  | -5.71 | 95.24       | 108.11   |
| 3   | D     | 92  | DMU  | O1-C9-C8   | -5.69 | 99.18       | 109.66   |
| 3   | V     | 92  | DMU  | O1-C9-C8   | -5.66 | 99.24       | 109.66   |
| 3   | A     | 92  | DMU  | C8-C7-C5   | -5.64 | 100.89      | 110.84   |
| 3   | Q     | 92  | DMU  | O7-C10-C5  | -5.61 | 95.48       | 108.11   |
| 3   | A     | 92  | DMU  | O1-C9-C8   | -5.53 | 99.47       | 109.66   |
| 3   | R     | 92  | DMU  | C8-C7-C5   | -5.48 | 101.17      | 110.84   |
| 3   | G     | 92  | DMU  | O1-C9-C8   | -5.45 | 99.63       | 109.66   |
| 3   | H     | 92  | DMU  | C8-C7-C5   | -5.41 | 101.29      | 110.84   |
| 3   | H     | 92  | DMU  | O5-C4-C57  | -5.36 | 93.58       | 106.41   |
| 3   | L     | 92  | DMU  | O1-C9-C8   | -5.35 | 99.81       | 109.66   |
| 3   | U     | 92  | DMU  | C11-C9-C8  | -5.18 | 100.88      | 113.00   |
| 3   | K     | 92  | DMU  | O1-C9-C8   | -5.14 | 100.20      | 109.66   |
| 3   | F     | 92  | DMU  | O7-C10-O1  | -5.13 | 98.24       | 110.70   |
| 3   | U     | 92  | DMU  | O5-C4-C3   | -5.11 | 99.30       | 109.75   |
| 3   | L     | 92  | DMU  | C18-O16-C6 | -5.01 | 105.27      | 113.87   |
| 3   | P     | 92  | DMU  | O7-C10-C5  | -4.95 | 96.96       | 108.11   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | T     | 92  | DMU  | C8-C7-C5    | -4.72 | 102.50      | 110.84   |
| 3   | S     | 92  | DMU  | C11-C9-C8   | -4.59 | 102.27      | 113.00   |
| 3   | B     | 92  | DMU  | O5-C4-C3    | -4.53 | 100.48      | 109.75   |
| 3   | N     | 92  | DMU  | O1-C9-C11   | -4.49 | 95.66       | 106.41   |
| 3   | H     | 92  | DMU  | C10-O7-C3   | -4.46 | 107.13      | 118.00   |
| 3   | N     | 92  | DMU  | C8-C7-C5    | -4.42 | 103.03      | 110.84   |
| 3   | M     | 92  | DMU  | O7-C10-C5   | -4.33 | 98.36       | 108.11   |
| 3   | H     | 92  | DMU  | O7-C10-C5   | -4.19 | 98.67       | 108.11   |
| 3   | H     | 92  | DMU  | C6-O5-C4    | -4.11 | 105.97      | 113.72   |
| 3   | Q     | 92  | DMU  | O1-C9-C11   | -4.07 | 96.66       | 106.41   |
| 3   | O     | 92  | DMU  | C18-O16-C6  | -4.02 | 106.96      | 113.87   |
| 3   | N     | 92  | DMU  | O3-C5-C7    | -3.98 | 101.69      | 110.36   |
| 3   | P     | 92  | DMU  | O3-C5-C7    | -3.95 | 101.76      | 110.36   |
| 3   | H     | 92  | DMU  | O3-C5-C7    | -3.72 | 102.26      | 110.36   |
| 3   | A     | 92  | DMU  | O1-C9-C11   | -3.67 | 97.62       | 106.41   |
| 3   | O     | 92  | DMU  | C10-O7-C3   | -3.59 | 109.25      | 118.00   |
| 3   | U     | 92  | DMU  | O1-C10-C5   | -3.46 | 103.62      | 110.30   |
| 3   | P     | 92  | DMU  | C22-C19-C18 | -3.38 | 98.29       | 113.48   |
| 3   | A     | 92  | DMU  | C2-C3-C4    | -3.27 | 103.93      | 110.88   |
| 3   | E     | 92  | DMU  | O1-C9-C11   | -3.27 | 98.58       | 106.41   |
| 3   | S     | 92  | DMU  | O7-C10-C5   | -3.12 | 101.08      | 108.11   |
| 3   | A     | 92  | DMU  | C11-C9-C8   | -3.05 | 105.86      | 113.00   |
| 3   | L     | 92  | DMU  | O3-C5-C7    | -3.03 | 103.75      | 110.36   |
| 3   | D     | 92  | DMU  | O3-C5-C7    | -3.03 | 103.77      | 110.36   |
| 3   | H     | 92  | DMU  | C2-C3-C4    | -2.97 | 104.56      | 110.88   |
| 3   | R     | 92  | DMU  | O3-C5-C7    | -2.91 | 104.03      | 110.36   |
| 3   | A     | 92  | DMU  | O3-C5-C7    | -2.90 | 104.05      | 110.36   |
| 3   | V     | 92  | DMU  | C18-O16-C6  | -2.87 | 108.94      | 113.87   |
| 3   | N     | 92  | DMU  | O7-C10-O1   | -2.85 | 103.78      | 110.70   |
| 3   | P     | 92  | DMU  | C25-C28-C31 | -2.84 | 99.81       | 114.45   |
| 3   | K     | 92  | DMU  | O3-C5-C7    | -2.83 | 104.19      | 110.36   |
| 3   | M     | 92  | DMU  | C10-O7-C3   | -2.82 | 111.13      | 118.00   |
| 3   | R     | 92  | DMU  | O1-C9-C11   | -2.81 | 99.67       | 106.41   |
| 3   | S     | 92  | DMU  | C8-C7-C5    | -2.80 | 105.89      | 110.84   |
| 3   | K     | 92  | DMU  | O5-C4-C57   | -2.78 | 99.76       | 106.41   |
| 3   | U     | 92  | DMU  | O3-C5-C10   | -2.76 | 104.25      | 110.03   |
| 3   | Q     | 92  | DMU  | C11-C9-C8   | -2.75 | 106.57      | 113.00   |
| 3   | T     | 92  | DMU  | C18-O16-C6  | -2.70 | 109.23      | 113.87   |
| 3   | V     | 92  | DMU  | O3-C5-C7    | -2.66 | 104.57      | 110.36   |
| 3   | A     | 93  | DMU  | C11-C9-C8   | -2.65 | 106.80      | 113.00   |
| 3   | B     | 92  | DMU  | C8-C7-C5    | -2.60 | 106.26      | 110.84   |
| 3   | K     | 92  | DMU  | C18-O16-C6  | -2.60 | 109.41      | 113.87   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | N     | 92  | DMU  | C18-O16-C6  | -2.56 | 109.47      | 113.87   |
| 3   | M     | 92  | DMU  | C11-C9-C8   | -2.54 | 107.06      | 113.00   |
| 3   | T     | 92  | DMU  | O3-C5-C7    | -2.53 | 104.85      | 110.36   |
| 3   | E     | 92  | DMU  | O3-C5-C7    | -2.52 | 104.87      | 110.36   |
| 3   | E     | 92  | DMU  | C11-C9-C8   | -2.50 | 107.14      | 113.00   |
| 3   | A     | 93  | DMU  | C8-C7-C5    | -2.50 | 106.43      | 110.84   |
| 3   | S     | 92  | DMU  | C2-C3-C4    | -2.48 | 105.62      | 110.88   |
| 3   | P     | 92  | DMU  | C11-C9-C8   | -2.47 | 107.22      | 113.00   |
| 3   | P     | 92  | DMU  | O1-C9-C11   | -2.44 | 100.56      | 106.41   |
| 3   | G     | 92  | DMU  | O3-C5-C7    | -2.40 | 105.12      | 110.36   |
| 3   | M     | 92  | DMU  | O3-C5-C7    | -2.38 | 105.18      | 110.36   |
| 3   | N     | 92  | DMU  | O7-C10-C5   | -2.37 | 102.76      | 108.11   |
| 3   | O     | 92  | DMU  | O7-C10-O1   | -2.32 | 105.06      | 110.70   |
| 3   | C     | 92  | DMU  | O3-C5-C7    | -2.32 | 105.31      | 110.36   |
| 3   | M     | 92  | DMU  | C57-C4-C3   | -2.29 | 106.98      | 113.24   |
| 3   | A     | 93  | DMU  | C6-O5-C4    | -2.29 | 109.41      | 113.72   |
| 3   | R     | 92  | DMU  | C2-C3-C4    | -2.28 | 106.04      | 110.88   |
| 3   | O     | 92  | DMU  | O3-C5-C7    | -2.28 | 105.40      | 110.36   |
| 3   | G     | 92  | DMU  | C57-C4-C3   | -2.27 | 107.03      | 113.24   |
| 3   | H     | 92  | DMU  | O7-C10-O1   | -2.26 | 105.20      | 110.70   |
| 3   | E     | 92  | DMU  | O5-C6-C1    | -2.25 | 105.96      | 110.30   |
| 3   | J     | 92  | DMU  | O3-C5-C7    | -2.23 | 105.51      | 110.36   |
| 3   | I     | 92  | DMU  | C6-O5-C4    | -2.22 | 109.53      | 113.72   |
| 3   | C     | 92  | DMU  | C57-C4-C3   | -2.19 | 107.25      | 113.24   |
| 3   | Q     | 92  | DMU  | O3-C5-C7    | -2.18 | 105.61      | 110.36   |
| 3   | Q     | 92  | DMU  | C18-O16-C6  | -2.18 | 110.13      | 113.87   |
| 3   | K     | 92  | DMU  | C11-C9-C8   | -2.18 | 107.91      | 113.00   |
| 3   | A     | 92  | DMU  | O5-C4-C57   | -2.16 | 101.24      | 106.41   |
| 3   | D     | 92  | DMU  | C57-C4-C3   | -2.11 | 107.48      | 113.24   |
| 3   | F     | 92  | DMU  | O55-C2-C1   | -2.10 | 105.79      | 110.36   |
| 3   | A     | 93  | DMU  | C25-C28-C31 | -2.09 | 103.69      | 114.45   |
| 3   | L     | 92  | DMU  | C11-C9-C8   | -2.09 | 108.11      | 113.00   |
| 3   | A     | 93  | DMU  | C2-C3-C4    | -2.08 | 106.47      | 110.88   |
| 3   | J     | 92  | DMU  | C19-C22-C25 | -2.05 | 103.88      | 114.45   |
| 3   | O     | 92  | DMU  | C7-C8-C9    | -2.05 | 106.61      | 110.22   |
| 3   | D     | 92  | DMU  | C2-C3-C4    | -2.03 | 106.57      | 110.88   |
| 3   | T     | 92  | DMU  | C57-C4-C3   | -2.03 | 107.71      | 113.24   |
| 3   | P     | 92  | DMU  | O7-C10-O1   | -2.02 | 105.79      | 110.70   |
| 3   | C     | 92  | DMU  | O1-C9-C11   | -2.02 | 101.57      | 106.41   |
| 3   | I     | 92  | DMU  | O5-C4-C57   | -2.01 | 101.58      | 106.41   |
| 3   | V     | 92  | DMU  | O7-C3-C2    | 2.01  | 112.04      | 107.19   |
| 3   | A     | 92  | DMU  | C18-O16-C6  | 2.07  | 117.43      | 113.87   |

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| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3   | B     | 92  | DMU  | O3-C5-C7    | 2.11 | 114.95      | 110.36   |
| 3   | I     | 92  | DMU  | O7-C3-C4    | 2.16 | 114.66      | 109.34   |
| 3   | J     | 92  | DMU  | O2-C8-C9    | 2.19 | 114.80      | 109.28   |
| 3   | G     | 92  | DMU  | O7-C3-C2    | 2.19 | 112.47      | 107.19   |
| 3   | L     | 92  | DMU  | O7-C3-C2    | 2.23 | 112.55      | 107.19   |
| 3   | F     | 92  | DMU  | O7-C3-C2    | 2.25 | 112.60      | 107.19   |
| 3   | P     | 92  | DMU  | C19-C22-C25 | 2.28 | 126.19      | 114.45   |
| 3   | N     | 92  | DMU  | C10-O7-C3   | 2.28 | 123.56      | 118.00   |
| 3   | G     | 92  | DMU  | C10-O7-C3   | 2.32 | 123.66      | 118.00   |
| 3   | F     | 92  | DMU  | C10-O7-C3   | 2.34 | 123.70      | 118.00   |
| 3   | P     | 92  | DMU  | O7-C3-C2    | 2.34 | 112.83      | 107.19   |
| 3   | H     | 92  | DMU  | O4-C7-C5    | 2.34 | 115.45      | 110.36   |
| 3   | J     | 92  | DMU  | O5-C4-C57   | 2.41 | 112.18      | 106.41   |
| 3   | I     | 92  | DMU  | O1-C9-C11   | 2.42 | 112.21      | 106.41   |
| 3   | J     | 92  | DMU  | O5-C4-C3    | 2.44 | 114.73      | 109.75   |
| 3   | F     | 92  | DMU  | O2-C8-C9    | 2.44 | 115.43      | 109.28   |
| 3   | F     | 92  | DMU  | O2-C8-C7    | 2.45 | 115.70      | 110.36   |
| 3   | Q     | 92  | DMU  | O7-C3-C2    | 2.48 | 113.15      | 107.19   |
| 3   | K     | 92  | DMU  | O7-C3-C2    | 2.48 | 113.16      | 107.19   |
| 3   | J     | 92  | DMU  | O2-C8-C7    | 2.49 | 115.78      | 110.36   |
| 3   | R     | 92  | DMU  | O55-C2-C3   | 2.51 | 115.58      | 109.87   |
| 3   | T     | 92  | DMU  | O7-C3-C2    | 2.53 | 113.28      | 107.19   |
| 3   | V     | 92  | DMU  | C10-O7-C3   | 2.54 | 124.18      | 118.00   |
| 3   | S     | 92  | DMU  | O55-C2-C3   | 2.61 | 115.80      | 109.87   |
| 3   | S     | 92  | DMU  | O49-C1-C6   | 2.63 | 115.53      | 110.03   |
| 3   | N     | 92  | DMU  | O4-C7-C5    | 2.77 | 116.38      | 110.36   |
| 3   | J     | 92  | DMU  | O7-C3-C4    | 2.77 | 116.15      | 109.34   |
| 3   | I     | 92  | DMU  | C57-C4-C3   | 2.81 | 120.89      | 113.24   |
| 3   | M     | 92  | DMU  | O4-C7-C5    | 2.81 | 116.48      | 110.36   |
| 3   | A     | 92  | DMU  | O4-C7-C5    | 2.82 | 116.49      | 110.36   |
| 3   | S     | 92  | DMU  | O55-C2-C1   | 2.84 | 116.54      | 110.36   |
| 3   | J     | 92  | DMU  | O1-C9-C8    | 2.85 | 114.91      | 109.66   |
| 3   | D     | 92  | DMU  | O5-C4-C57   | 2.88 | 113.31      | 106.41   |
| 3   | S     | 92  | DMU  | O5-C4-C57   | 2.91 | 113.38      | 106.41   |
| 3   | C     | 92  | DMU  | C10-O7-C3   | 2.93 | 125.12      | 118.00   |
| 3   | K     | 92  | DMU  | C10-O7-C3   | 2.95 | 125.17      | 118.00   |
| 3   | G     | 92  | DMU  | O4-C7-C5    | 3.00 | 116.89      | 110.36   |
| 3   | T     | 92  | DMU  | O4-C7-C5    | 3.02 | 116.92      | 110.36   |
| 3   | P     | 92  | DMU  | O4-C7-C5    | 3.04 | 116.98      | 110.36   |
| 3   | N     | 92  | DMU  | O5-C4-C57   | 3.09 | 113.80      | 106.41   |
| 3   | C     | 92  | DMU  | O4-C7-C5    | 3.11 | 117.13      | 110.36   |
| 3   | K     | 92  | DMU  | O4-C7-C5    | 3.12 | 117.15      | 110.36   |

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| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3   | P     | 92  | DMU  | C10-O7-C3   | 3.13 | 125.61      | 118.00   |
| 3   | E     | 92  | DMU  | O16-C18-C19 | 3.17 | 120.98      | 109.68   |
| 3   | U     | 92  | DMU  | C18-O16-C6  | 3.21 | 119.38      | 113.87   |
| 3   | V     | 92  | DMU  | O4-C7-C5    | 3.28 | 117.49      | 110.36   |
| 3   | E     | 92  | DMU  | O4-C7-C5    | 3.29 | 117.52      | 110.36   |
| 3   | Q     | 92  | DMU  | O4-C7-C5    | 3.30 | 117.55      | 110.36   |
| 3   | O     | 92  | DMU  | O1-C9-C11   | 3.32 | 114.36      | 106.41   |
| 3   | E     | 92  | DMU  | C10-O7-C3   | 3.34 | 126.13      | 118.00   |
| 3   | D     | 92  | DMU  | O4-C7-C5    | 3.34 | 117.63      | 110.36   |
| 3   | H     | 92  | DMU  | C1-C2-C3    | 3.36 | 116.58      | 109.61   |
| 3   | R     | 92  | DMU  | O4-C7-C5    | 3.43 | 117.83      | 110.36   |
| 3   | D     | 92  | DMU  | C10-O7-C3   | 3.46 | 126.42      | 118.00   |
| 3   | S     | 92  | DMU  | O16-C6-C1   | 3.53 | 114.00      | 108.23   |
| 3   | F     | 92  | DMU  | O4-C7-C8    | 3.54 | 118.05      | 110.36   |
| 3   | L     | 92  | DMU  | O4-C7-C5    | 3.57 | 118.13      | 110.36   |
| 3   | N     | 92  | DMU  | O7-C3-C2    | 3.65 | 115.97      | 107.19   |
| 3   | L     | 92  | DMU  | C10-O7-C3   | 3.74 | 127.10      | 118.00   |
| 3   | J     | 92  | DMU  | C57-C4-C3   | 3.97 | 124.06      | 113.24   |
| 3   | U     | 92  | DMU  | O7-C3-C4    | 4.01 | 119.20      | 109.34   |
| 3   | F     | 92  | DMU  | O1-C9-C11   | 4.05 | 116.11      | 106.41   |
| 3   | B     | 92  | DMU  | C2-C3-C4    | 4.10 | 119.58      | 110.88   |
| 3   | J     | 92  | DMU  | C10-O1-C9   | 4.21 | 121.65      | 113.72   |
| 3   | M     | 92  | DMU  | O5-C6-C1    | 4.23 | 118.44      | 110.30   |
| 3   | U     | 92  | DMU  | O1-C9-C11   | 4.33 | 116.77      | 106.41   |
| 3   | L     | 92  | DMU  | C7-C8-C9    | 4.38 | 117.93      | 110.22   |
| 3   | J     | 92  | DMU  | O4-C7-C8    | 4.41 | 119.95      | 110.36   |
| 3   | D     | 92  | DMU  | C7-C8-C9    | 4.48 | 118.12      | 110.22   |
| 3   | T     | 92  | DMU  | C7-C8-C9    | 4.53 | 118.19      | 110.22   |
| 3   | G     | 92  | DMU  | C7-C8-C9    | 4.61 | 118.33      | 110.22   |
| 3   | R     | 92  | DMU  | C7-C8-C9    | 4.63 | 118.38      | 110.22   |
| 3   | A     | 92  | DMU  | C7-C8-C9    | 4.64 | 118.40      | 110.22   |
| 3   | V     | 92  | DMU  | C7-C8-C9    | 4.67 | 118.44      | 110.22   |
| 3   | P     | 92  | DMU  | C7-C8-C9    | 4.68 | 118.47      | 110.22   |
| 3   | K     | 92  | DMU  | C7-C8-C9    | 4.68 | 118.47      | 110.22   |
| 3   | S     | 92  | DMU  | O1-C9-C11   | 4.70 | 117.67      | 106.41   |
| 3   | N     | 92  | DMU  | C7-C8-C9    | 4.72 | 118.54      | 110.22   |
| 3   | E     | 92  | DMU  | C7-C8-C9    | 4.84 | 118.75      | 110.22   |
| 3   | C     | 92  | DMU  | C7-C8-C9    | 4.84 | 118.75      | 110.22   |
| 3   | H     | 92  | DMU  | C7-C8-C9    | 4.94 | 118.92      | 110.22   |
| 3   | I     | 92  | DMU  | O1-C9-C8    | 5.08 | 119.03      | 109.66   |
| 3   | F     | 92  | DMU  | O1-C9-C8    | 5.19 | 119.22      | 109.66   |
| 3   | S     | 92  | DMU  | C7-C8-C9    | 5.20 | 119.38      | 110.22   |

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| Mol | Chain | Res | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3   | M     | 92  | DMU  | C18-O16-C6 | 5.28 | 122.93      | 113.87   |
| 3   | U     | 92  | DMU  | C7-C8-C9   | 5.38 | 119.70      | 110.22   |
| 3   | Q     | 92  | DMU  | C7-C8-C9   | 5.41 | 119.76      | 110.22   |
| 3   | I     | 92  | DMU  | O3-C5-C10  | 5.51 | 121.56      | 110.03   |
| 3   | U     | 92  | DMU  | C2-C3-C4   | 5.53 | 122.62      | 110.88   |
| 3   | I     | 92  | DMU  | C10-C5-C7  | 5.57 | 120.34      | 109.98   |
| 3   | F     | 92  | DMU  | O5-C4-C57  | 5.59 | 119.81      | 106.41   |
| 3   | M     | 92  | DMU  | C7-C8-C9   | 5.92 | 120.64      | 110.22   |
| 3   | J     | 92  | DMU  | O1-C9-C11  | 5.93 | 120.61      | 106.41   |
| 3   | P     | 92  | DMU  | O5-C4-C57  | 5.99 | 120.76      | 106.41   |
| 3   | B     | 92  | DMU  | O5-C6-C1   | 6.31 | 122.47      | 110.30   |
| 3   | B     | 92  | DMU  | O7-C3-C4   | 6.84 | 126.17      | 109.34   |
| 3   | U     | 92  | DMU  | O5-C6-C1   | 7.06 | 123.91      | 110.30   |
| 3   | S     | 92  | DMU  | O3-C5-C10  | 7.69 | 126.11      | 110.03   |
| 3   | N     | 92  | DMU  | O3-C5-C10  | 8.04 | 126.84      | 110.03   |
| 3   | M     | 92  | DMU  | O3-C5-C10  | 8.21 | 127.19      | 110.03   |
| 3   | H     | 92  | DMU  | O3-C5-C10  | 8.27 | 127.32      | 110.03   |
| 3   | U     | 92  | DMU  | O5-C4-C57  | 8.75 | 127.38      | 106.41   |
| 3   | Q     | 92  | DMU  | O1-C10-C5  | 8.89 | 127.44      | 110.30   |
| 3   | P     | 92  | DMU  | O3-C5-C10  | 8.93 | 128.71      | 110.03   |
| 3   | A     | 92  | DMU  | O3-C5-C10  | 8.95 | 128.75      | 110.03   |
| 3   | T     | 92  | DMU  | O3-C5-C10  | 8.95 | 128.75      | 110.03   |
| 3   | M     | 92  | DMU  | O1-C10-C5  | 9.26 | 128.15      | 110.30   |
| 3   | Q     | 92  | DMU  | O3-C5-C10  | 9.37 | 129.62      | 110.03   |
| 3   | D     | 92  | DMU  | O3-C5-C10  | 9.39 | 129.68      | 110.03   |
| 3   | E     | 92  | DMU  | O1-C10-C5  | 9.42 | 128.46      | 110.30   |
| 3   | R     | 92  | DMU  | O3-C5-C10  | 9.42 | 129.74      | 110.03   |
| 3   | C     | 92  | DMU  | O1-C10-C5  | 9.50 | 128.61      | 110.30   |
| 3   | C     | 92  | DMU  | O3-C5-C10  | 9.53 | 129.97      | 110.03   |
| 3   | V     | 92  | DMU  | O3-C5-C10  | 9.56 | 130.02      | 110.03   |
| 3   | G     | 92  | DMU  | O1-C10-C5  | 9.59 | 128.78      | 110.30   |
| 3   | E     | 92  | DMU  | O3-C5-C10  | 9.62 | 130.15      | 110.03   |
| 3   | L     | 92  | DMU  | O1-C10-C5  | 9.63 | 128.88      | 110.30   |
| 3   | I     | 92  | DMU  | O7-C10-O1  | 9.64 | 134.10      | 110.70   |
| 3   | G     | 92  | DMU  | O3-C5-C10  | 9.64 | 130.19      | 110.03   |
| 3   | V     | 92  | DMU  | O1-C10-C5  | 9.64 | 128.90      | 110.30   |
| 3   | K     | 92  | DMU  | O1-C10-C5  | 9.66 | 128.93      | 110.30   |
| 3   | R     | 92  | DMU  | O1-C10-C5  | 9.68 | 128.97      | 110.30   |
| 3   | K     | 92  | DMU  | O3-C5-C10  | 9.76 | 130.43      | 110.03   |
| 3   | L     | 92  | DMU  | O3-C5-C10  | 9.78 | 130.49      | 110.03   |
| 3   | F     | 92  | DMU  | O7-C10-C5  | 9.79 | 130.18      | 108.11   |
| 3   | T     | 92  | DMU  | O1-C10-C5  | 9.84 | 129.28      | 110.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | B     | 92  | DMU  | O5-C4-C57  | 9.96  | 130.26      | 106.41   |
| 3   | F     | 92  | DMU  | C10-C5-C7  | 9.98  | 128.53      | 109.98   |
| 3   | D     | 92  | DMU  | O1-C10-C5  | 10.12 | 129.82      | 110.30   |
| 3   | P     | 92  | DMU  | O1-C10-C5  | 10.15 | 129.88      | 110.30   |
| 3   | A     | 92  | DMU  | O1-C10-C5  | 10.38 | 130.31      | 110.30   |
| 3   | H     | 92  | DMU  | O1-C10-C5  | 10.46 | 130.47      | 110.30   |
| 3   | J     | 92  | DMU  | C10-C5-C7  | 10.50 | 129.50      | 109.98   |
| 3   | J     | 92  | DMU  | O5-C6-O16  | 10.79 | 135.64      | 110.02   |
| 3   | J     | 92  | DMU  | O7-C10-C5  | 10.95 | 132.79      | 108.11   |
| 3   | B     | 92  | DMU  | O5-C6-O16  | 11.05 | 136.26      | 110.02   |
| 3   | N     | 92  | DMU  | O1-C10-C5  | 11.07 | 131.64      | 110.30   |
| 3   | U     | 92  | DMU  | O5-C6-O16  | 11.66 | 137.71      | 110.02   |
| 3   | M     | 92  | DMU  | O7-C3-C2   | 12.78 | 137.94      | 107.19   |
| 3   | J     | 92  | DMU  | O7-C3-C2   | 13.91 | 140.67      | 107.19   |
| 3   | M     | 92  | DMU  | O16-C6-C1  | 15.12 | 132.90      | 108.23   |
| 3   | H     | 92  | DMU  | O7-C3-C2   | 15.20 | 143.76      | 107.19   |
| 3   | H     | 92  | DMU  | O16-C6-C1  | 18.85 | 138.98      | 108.23   |
| 3   | H     | 92  | DMU  | C18-O16-C6 | 19.05 | 146.56      | 113.87   |
| 3   | U     | 92  | DMU  | O7-C10-O1  | 19.94 | 159.11      | 110.70   |
| 3   | S     | 92  | DMU  | O7-C10-O1  | 21.70 | 163.39      | 110.70   |
| 3   | J     | 92  | DMU  | C1-C2-C3   | 27.33 | 166.28      | 109.61   |

All (7) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 3   | U     | 92  | DMU  | C8   |
| 3   | U     | 92  | DMU  | C5   |
| 3   | U     | 92  | DMU  | C10  |
| 3   | S     | 92  | DMU  | C8   |
| 3   | S     | 92  | DMU  | C5   |
| 3   | S     | 92  | DMU  | C10  |
| 3   | J     | 92  | DMU  | C2   |

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 3   | S     | 92  | DMU  | C18-O16-C6-O5 |

All (1) ring outliers are listed below:

| Mol | Chain | Res | Type | Atoms             |
|-----|-------|-----|------|-------------------|
| 3   | J     | 92  | DMU  | C1-C2-C3-C4-C6-O5 |

23 monomers are involved in 178 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 92  | DMU  | 6       | 0            |
| 3   | A     | 93  | DMU  | 1       | 0            |
| 3   | B     | 92  | DMU  | 3       | 0            |
| 3   | C     | 92  | DMU  | 6       | 0            |
| 3   | D     | 92  | DMU  | 7       | 0            |
| 3   | E     | 92  | DMU  | 9       | 0            |
| 3   | F     | 92  | DMU  | 10      | 0            |
| 3   | G     | 92  | DMU  | 9       | 0            |
| 3   | H     | 92  | DMU  | 8       | 0            |
| 3   | I     | 92  | DMU  | 4       | 0            |
| 3   | J     | 92  | DMU  | 12      | 0            |
| 3   | K     | 92  | DMU  | 11      | 0            |
| 3   | L     | 92  | DMU  | 11      | 0            |
| 3   | M     | 92  | DMU  | 12      | 0            |
| 3   | N     | 92  | DMU  | 10      | 0            |
| 3   | O     | 92  | DMU  | 6       | 0            |
| 3   | P     | 92  | DMU  | 9       | 0            |
| 3   | Q     | 92  | DMU  | 9       | 0            |
| 3   | R     | 92  | DMU  | 10      | 0            |
| 3   | S     | 92  | DMU  | 10      | 0            |
| 3   | T     | 92  | DMU  | 12      | 0            |
| 3   | U     | 92  | DMU  | 15      | 0            |
| 3   | V     | 92  | DMU  | 12      | 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 ⓘ

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

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|----------------|-----------------------|-------|
| 1   | A     | 89/89 (100%)     | 0.20   | 3 (3%) 46 42   | 21, 32, 54, 74        | 0     |
| 1   | B     | 89/89 (100%)     | 0.07   | 1 (1%) 80 78   | 22, 33, 60, 74        | 0     |
| 1   | C     | 89/89 (100%)     | -0.09  | 1 (1%) 80 78   | 22, 33, 56, 86        | 0     |
| 1   | D     | 89/89 (100%)     | -0.17  | 0 100 100      | 22, 33, 57, 74        | 0     |
| 1   | E     | 89/89 (100%)     | 0.07   | 4 (4%) 34 30   | 21, 33, 62, 107       | 0     |
| 1   | F     | 89/89 (100%)     | -0.13  | 1 (1%) 80 78   | 22, 33, 62, 106       | 0     |
| 1   | G     | 89/89 (100%)     | 0.07   | 4 (4%) 34 30   | 22, 35, 54, 83        | 0     |
| 1   | H     | 89/89 (100%)     | 0.13   | 3 (3%) 46 42   | 23, 34, 56, 76        | 0     |
| 1   | I     | 89/89 (100%)     | 0.09   | 1 (1%) 80 78   | 22, 33, 60, 88        | 0     |
| 1   | J     | 89/89 (100%)     | 0.25   | 0 100 100      | 21, 31, 62, 95        | 0     |
| 1   | K     | 89/89 (100%)     | 0.20   | 1 (1%) 80 78   | 23, 31, 58, 74        | 0     |
| 1   | L     | 89/89 (100%)     | 0.77   | 7 (7%) 13 11   | 26, 44, 78, 101       | 0     |
| 1   | M     | 89/89 (100%)     | 0.84   | 8 (8%) 10 8    | 26, 47, 78, 101       | 0     |
| 1   | N     | 89/89 (100%)     | 0.64   | 7 (7%) 13 11   | 27, 49, 80, 105       | 0     |
| 1   | O     | 89/89 (100%)     | 0.65   | 8 (8%) 10 8    | 30, 48, 77, 118       | 0     |
| 1   | P     | 89/89 (100%)     | 0.47   | 3 (3%) 46 42   | 29, 47, 90, 107       | 0     |
| 1   | Q     | 89/89 (100%)     | 0.76   | 12 (13%) 3 2   | 25, 50, 89, 111       | 0     |
| 1   | R     | 89/89 (100%)     | 0.93   | 16 (17%) 2 1   | 29, 47, 83, 121       | 0     |
| 1   | S     | 89/89 (100%)     | 0.70   | 6 (6%) 19 16   | 26, 45, 74, 105       | 0     |
| 1   | T     | 89/89 (100%)     | 0.76   | 6 (6%) 19 16   | 26, 42, 76, 103       | 0     |
| 1   | U     | 89/89 (100%)     | 1.07   | 16 (17%) 2 1   | 23, 40, 82, 109       | 0     |
| 1   | V     | 89/89 (100%)     | 0.68   | 4 (4%) 34 30   | 22, 43, 64, 87        | 0     |
| All | All   | 1958/1958 (100%) | 0.41   | 112 (5%) 24 22 | 21, 39, 74, 121       | 0     |

All (112) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 89  | GLY  | 8.9  |
| 1   | F     | 89  | GLY  | 6.5  |
| 1   | M     | 89  | GLY  | 6.1  |
| 1   | N     | 48  | GLU  | 5.1  |
| 1   | R     | 48  | GLU  | 4.9  |
| 1   | N     | 49  | ALA  | 4.8  |
| 1   | O     | 47  | PRO  | 4.7  |
| 1   | U     | 48  | GLU  | 4.6  |
| 1   | R     | 51  | GLY  | 4.4  |
| 1   | T     | 48  | GLU  | 4.3  |
| 1   | Q     | 81  | ALA  | 4.2  |
| 1   | M     | 48  | GLU  | 4.2  |
| 1   | M     | 47  | PRO  | 4.0  |
| 1   | M     | 86  | SER  | 4.0  |
| 1   | R     | 49  | ALA  | 4.0  |
| 1   | U     | 80  | TYR  | 3.9  |
| 1   | N     | 89  | GLY  | 3.8  |
| 1   | O     | 45  | ARG  | 3.8  |
| 1   | P     | 45  | ARG  | 3.5  |
| 1   | Q     | 45  | ARG  | 3.5  |
| 1   | M     | 44  | ALA  | 3.5  |
| 1   | R     | 28  | PRO  | 3.4  |
| 1   | N     | 53  | ILE  | 3.4  |
| 1   | T     | 86  | SER  | 3.4  |
| 1   | C     | 89  | GLY  | 3.3  |
| 1   | S     | 81  | ALA  | 3.3  |
| 1   | U     | 43  | VAL  | 3.2  |
| 1   | R     | 81  | ALA  | 3.2  |
| 1   | T     | 81  | ALA  | 3.2  |
| 1   | O     | 53  | ILE  | 3.1  |
| 1   | R     | 47  | PRO  | 3.1  |
| 1   | U     | 52  | SER  | 3.1  |
| 1   | L     | 80  | TYR  | 3.1  |
| 1   | L     | 81  | ALA  | 3.1  |
| 1   | K     | 1   | MET  | 3.0  |
| 1   | R     | 59  | LEU  | 3.0  |
| 1   | H     | 89  | GLY  | 3.0  |
| 1   | V     | 48  | GLU  | 2.9  |
| 1   | G     | 45  | ARG  | 2.9  |
| 1   | U     | 51  | GLY  | 2.9  |
| 1   | R     | 50  | ARG  | 2.9  |
| 1   | G     | 1   | MET  | 2.8  |
| 1   | E     | 46  | GLN  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | P     | 52  | SER  | 2.8  |
| 1   | G     | 89  | GLY  | 2.8  |
| 1   | A     | 48  | GLU  | 2.8  |
| 1   | A     | 89  | GLY  | 2.8  |
| 1   | O     | 80  | TYR  | 2.7  |
| 1   | R     | 1   | MET  | 2.7  |
| 1   | S     | 80  | TYR  | 2.7  |
| 1   | R     | 45  | ARG  | 2.7  |
| 1   | Q     | 50  | ARG  | 2.7  |
| 1   | N     | 44  | ALA  | 2.6  |
| 1   | Q     | 51  | GLY  | 2.6  |
| 1   | U     | 49  | ALA  | 2.6  |
| 1   | R     | 42  | SER  | 2.6  |
| 1   | L     | 47  | PRO  | 2.6  |
| 1   | U     | 39  | ALA  | 2.6  |
| 1   | U     | 20  | LEU  | 2.6  |
| 1   | Q     | 80  | TYR  | 2.6  |
| 1   | U     | 3   | LEU  | 2.6  |
| 1   | S     | 47  | PRO  | 2.5  |
| 1   | M     | 80  | TYR  | 2.5  |
| 1   | T     | 50  | ARG  | 2.5  |
| 1   | O     | 52  | SER  | 2.5  |
| 1   | O     | 41  | GLU  | 2.5  |
| 1   | A     | 47  | PRO  | 2.5  |
| 1   | Q     | 31  | GLY  | 2.5  |
| 1   | R     | 63  | VAL  | 2.5  |
| 1   | T     | 55  | SER  | 2.5  |
| 1   | L     | 1   | MET  | 2.4  |
| 1   | B     | 49  | ALA  | 2.4  |
| 1   | R     | 80  | TYR  | 2.4  |
| 1   | E     | 48  | GLU  | 2.4  |
| 1   | U     | 1   | MET  | 2.4  |
| 1   | L     | 64  | ALA  | 2.4  |
| 1   | S     | 48  | GLU  | 2.4  |
| 1   | H     | 45  | ARG  | 2.4  |
| 1   | G     | 80  | TYR  | 2.3  |
| 1   | V     | 80  | TYR  | 2.3  |
| 1   | R     | 52  | SER  | 2.3  |
| 1   | P     | 47  | PRO  | 2.3  |
| 1   | N     | 47  | PRO  | 2.3  |
| 1   | Q     | 49  | ALA  | 2.3  |
| 1   | T     | 80  | TYR  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | Q     | 52  | SER  | 2.2  |
| 1   | U     | 89  | GLY  | 2.2  |
| 1   | V     | 23  | ILE  | 2.2  |
| 1   | Q     | 46  | GLN  | 2.2  |
| 1   | M     | 50  | ARG  | 2.2  |
| 1   | U     | 62  | ALA  | 2.2  |
| 1   | O     | 23  | ILE  | 2.2  |
| 1   | H     | 86  | SER  | 2.1  |
| 1   | L     | 51  | GLY  | 2.1  |
| 1   | R     | 60  | GLY  | 2.1  |
| 1   | S     | 52  | SER  | 2.1  |
| 1   | E     | 47  | PRO  | 2.1  |
| 1   | Q     | 60  | GLY  | 2.1  |
| 1   | Q     | 89  | GLY  | 2.1  |
| 1   | I     | 1   | MET  | 2.1  |
| 1   | O     | 46  | GLN  | 2.1  |
| 1   | N     | 45  | ARG  | 2.1  |
| 1   | U     | 55  | SER  | 2.1  |
| 1   | S     | 55  | SER  | 2.1  |
| 1   | L     | 37  | GLY  | 2.1  |
| 1   | U     | 47  | PRO  | 2.1  |
| 1   | M     | 55  | SER  | 2.1  |
| 1   | R     | 31  | GLY  | 2.0  |
| 1   | U     | 23  | ILE  | 2.0  |
| 1   | Q     | 56  | THR  | 2.0  |
| 1   | V     | 3   | LEU  | 2.0  |
| 1   | U     | 40  | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 3   | DMU  | F     | 92  | 33/33 | 0.45 | 0.45 | 14.29 | 52,129,181,189             | 0     |
| 3   | DMU  | T     | 92  | 33/33 | 0.55 | 0.51 | 11.50 | 54,132,173,178             | 0     |
| 3   | DMU  | E     | 92  | 33/33 | 0.45 | 0.52 | 10.97 | 63,146,179,179             | 0     |
| 3   | DMU  | J     | 92  | 33/33 | 0.58 | 0.62 | 9.96  | 62,151,200,204             | 0     |
| 3   | DMU  | O     | 92  | 33/33 | 0.66 | 0.48 | 9.08  | 49,108,141,142             | 0     |
| 3   | DMU  | Q     | 92  | 33/33 | 0.50 | 0.52 | 9.05  | 59,117,165,169             | 0     |
| 3   | DMU  | D     | 92  | 33/33 | 0.73 | 0.40 | 8.15  | 40,114,167,170             | 0     |
| 3   | DMU  | N     | 92  | 33/33 | 0.59 | 0.46 | 6.96  | 41,126,163,170             | 0     |
| 3   | DMU  | P     | 92  | 33/33 | 0.64 | 0.44 | 6.74  | 62,133,158,159             | 0     |
| 3   | DMU  | B     | 92  | 33/33 | 0.65 | 0.46 | 6.70  | 57,129,151,152             | 0     |
| 3   | DMU  | S     | 92  | 33/33 | 0.64 | 0.48 | 6.24  | 46,140,173,178             | 0     |
| 3   | DMU  | C     | 92  | 33/33 | 0.66 | 0.38 | 6.12  | 55,135,173,176             | 0     |
| 3   | DMU  | M     | 92  | 33/33 | 0.68 | 0.39 | 4.83  | 55,121,185,195             | 0     |
| 3   | DMU  | K     | 92  | 33/33 | 0.62 | 0.52 | 4.79  | 39,118,175,189             | 0     |
| 3   | DMU  | A     | 92  | 33/33 | 0.72 | 0.37 | 4.73  | 53,117,171,175             | 0     |
| 3   | DMU  | L     | 92  | 33/33 | 0.47 | 0.47 | 4.63  | 71,137,166,172             | 0     |
| 3   | DMU  | I     | 92  | 33/33 | 0.74 | 0.39 | 3.90  | 58,126,153,175             | 0     |
| 3   | DMU  | G     | 92  | 33/33 | 0.58 | 0.42 | 3.28  | 43,122,176,179             | 0     |
| 3   | DMU  | H     | 92  | 33/33 | 0.63 | 0.35 | 3.23  | 36,135,177,179             | 0     |
| 3   | DMU  | V     | 92  | 33/33 | 0.64 | 0.38 | 3.11  | 57,119,157,168             | 0     |
| 3   | DMU  | U     | 92  | 33/33 | 0.69 | 0.37 | 2.86  | 43,150,170,170             | 0     |
| 3   | DMU  | A     | 93  | 33/33 | 0.80 | 0.34 | 2.40  | 66,82,99,109               | 0     |
| 3   | DMU  | R     | 92  | 33/33 | 0.68 | 0.27 | 0.82  | 58,119,202,202             | 0     |
| 2   | NA   | U     | 90  | 1/1   | 0.73 | 0.23 | 0.18  | 44,44,44,44                | 0     |
| 2   | NA   | T     | 90  | 1/1   | 0.78 | 0.20 | -0.38 | 46,46,46,46                | 0     |
| 2   | NA   | H     | 90  | 1/1   | 0.91 | 0.12 | -0.77 | 41,41,41,41                | 0     |
| 2   | NA   | L     | 90  | 1/1   | 0.90 | 0.20 | -1.04 | 32,32,32,32                | 0     |
| 2   | NA   | Q     | 90  | 1/1   | 0.85 | 0.14 | -1.12 | 65,65,65,65                | 0     |
| 2   | NA   | D     | 90  | 1/1   | 0.96 | 0.09 | -1.77 | 33,33,33,33                | 0     |
| 2   | NA   | A     | 90  | 1/1   | 0.89 | 0.12 | -1.79 | 46,46,46,46                | 0     |
| 2   | NA   | R     | 90  | 1/1   | 0.91 | 0.09 | -1.79 | 49,49,49,49                | 0     |
| 2   | NA   | I     | 90  | 1/1   | 0.90 | 0.08 | -1.86 | 45,45,45,45                | 0     |
| 2   | NA   | S     | 90  | 1/1   | 0.89 | 0.12 | -1.98 | 39,39,39,39                | 0     |
| 2   | NA   | E     | 90  | 1/1   | 0.97 | 0.09 | -2.16 | 33,33,33,33                | 0     |
| 2   | NA   | M     | 90  | 1/1   | 0.90 | 0.09 | -2.25 | 37,37,37,37                | 0     |
| 2   | NA   | N     | 90  | 1/1   | 0.85 | 0.09 | -2.36 | 35,35,35,35                | 0     |
| 2   | NA   | B     | 90  | 1/1   | 0.97 | 0.09 | -2.39 | 40,40,40,40                | 0     |
| 2   | NA   | K     | 90  | 1/1   | 0.91 | 0.12 | -2.59 | 32,32,32,32                | 0     |
| 2   | NA   | F     | 90  | 1/1   | 0.94 | 0.08 | -2.61 | 42,42,42,42                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 2   | NA   | O     | 90  | 1/1   | 0.94 | 0.08 | -2.68 | 40,40,40,40                 | 0     |
| 2   | NA   | J     | 90  | 1/1   | 0.90 | 0.09 | -2.71 | 33,33,33,33                 | 0     |
| 2   | NA   | V     | 90  | 1/1   | 0.95 | 0.13 | -3.06 | 29,29,29,29                 | 0     |
| 2   | NA   | G     | 90  | 1/1   | 0.95 | 0.06 | -3.37 | 29,29,29,29                 | 0     |
| 2   | NA   | C     | 90  | 1/1   | 0.95 | 0.06 | -3.62 | 33,33,33,33                 | 0     |
| 2   | NA   | P     | 90  | 1/1   | 0.89 | 0.09 | -4.29 | 48,48,48,48                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.