



# wwPDB X-ray Structure Validation Summary Report

Jul 22, 2014 – 01:57 PM EDT

PDB ID : 4V99  
Title : The Crystallographic Structure of Panicum Mosaic Virus  
Authors : Makino, D.L.; Larson, S.B.; McPherson, A.  
Deposited on : 2012-07-04  
Resolution : 2.90 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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

MolProbity : **NOT EXECUTED**  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : **NOT EXECUTED**  
Percentile statistics : **NOT EXECUTED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 Å.

There are no percentiles available for this entry.

MolProbity and EDS were not executed - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 588120 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Capsid protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | AA    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | AB    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | AC    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | AF    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | AG    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | AH    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | AK    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | AL    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | AM    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | AP    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | AQ    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | AR    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | AU    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | AV    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | AW    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | AZ    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | Aa    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Ab    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Ae    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Af    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Ag    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Aj    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Ak    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Al    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Ao    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Ap    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Aq    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | At    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Au    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Av    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Ay    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Az    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | A1    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | A4    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | A5    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | A6    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | BA    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | BB    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | BC    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | BF    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | BG    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | BH    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | BK    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | BL    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | BM    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | BP    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | BQ    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | BR    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | BU    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | BV    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | BW    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | BZ    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Ba    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Bb    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Be    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Bf    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Bg    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Bj    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | Bk    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Bl    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Bo    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Bp    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Bq    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Bt    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Bu    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Bv    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | By    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Bz    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | B1    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | B4    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | B5    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | B6    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | CA    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | CB    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | CC    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | CF    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | CG    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | CH    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | CK    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | CL    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | CM    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | CP    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | CQ    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | CR    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | CU    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | CV    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | CW    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | CZ    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Ca    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Cb    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Ce    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Cf    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Cg    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Cj    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Ck    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Cl    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Co    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Cp    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Cq    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Ct    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | Cu    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Cv    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Cy    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Cz    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | C1    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | C4    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | C5    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | C6    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | DA    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | DB    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | DC    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | DF    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | DG    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | DH    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | DK    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | DL    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | DM    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | DP    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | DQ    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | DR    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | DU    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | DV    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | DW    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | DZ    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Da    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Db    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | De    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Df    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Dg    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Dj    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Dk    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Di    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Do    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Dp    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Dq    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Dt    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Du    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Dv    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Dy    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Dz    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | D1    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | D4    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | D5    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | D6    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | EA    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | EB    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | EC    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | EF    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | EG    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | EH    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | EK    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | EL    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | EM    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | EP    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | EQ    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | ER    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | EU    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | EV    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | EW    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | EZ    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Ea    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Eb    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Ee    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | Ef    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Eg    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Ej    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Ek    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | El    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Eo    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Ep    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Eq    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Et    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Eu    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Ev    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Ey    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Ez    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | E1    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | E4    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | E5    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | E6    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | FA    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | FB    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | FC    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | FF    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | FG    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | FH    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | FK    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | FL    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | FM    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | FP    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | FQ    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | FR    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | FU    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | FV    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | FW    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | FZ    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Fa    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Fb    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Fe    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Ff    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Fg    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Fj    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Fk    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Fl    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Fo    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | Fp    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Fq    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Ft    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Fu    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Fv    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Fy    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Fz    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | F1    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | F4    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | F5    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | F6    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | GA    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | GB    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | GC    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | GF    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | GG    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | GH    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | GK    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | GL    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | GM    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | GP    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | GQ    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | GR    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | GU    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | GV    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | GW    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | GZ    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Ga    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Gb    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Ge    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Gf    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Gg    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Gj    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Gk    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Gl    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Go    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Gp    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Gq    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Gt    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Gu    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Gv    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Gy    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | Gz    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | G1    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | G4    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | G5    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | G6    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | HA    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | HB    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | HC    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | HF    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | HG    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | HH    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | HK    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | HL    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | HM    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | HP    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | HQ    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | HR    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | HU    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | HV    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | HW    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | HZ    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | Ha    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Hb    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | He    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Hf    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Hg    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Hj    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Hk    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Hi    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Ho    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Hp    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Hq    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Ht    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Hu    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Hv    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Hy    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Hx    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | H1    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | H4    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | H5    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | H6    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | IA    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | IB    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | IC    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | IF    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | IG    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | IH    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | IK    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | IL    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | IM    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | IP    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | IQ    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | IR    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | IU    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | IV    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | IW    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | IZ    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Ia    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Ib    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Ie    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | If    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Ig    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Ij    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms         |           |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| 1   | Ik    | 189      | Total<br>1451 | C<br>915  | N<br>253 | O<br>278 | S<br>5 | 0       | 0       | 0     |
| 1   | Il    | 217      | Total<br>1674 | C<br>1049 | N<br>304 | O<br>316 | S<br>5 | 0       | 0       | 0     |
| 1   | Io    | 185      | Total<br>1426 | C<br>901  | N<br>248 | O<br>273 | S<br>4 | 0       | 0       | 0     |
| 1   | Ip    | 189      | Total<br>1451 | C<br>915  | N<br>253 | O<br>278 | S<br>5 | 0       | 0       | 0     |
| 1   | Iq    | 217      | Total<br>1674 | C<br>1049 | N<br>304 | O<br>316 | S<br>5 | 0       | 0       | 0     |
| 1   | It    | 185      | Total<br>1426 | C<br>901  | N<br>248 | O<br>273 | S<br>4 | 0       | 0       | 0     |
| 1   | Iu    | 189      | Total<br>1451 | C<br>915  | N<br>253 | O<br>278 | S<br>5 | 0       | 0       | 0     |
| 1   | Iv    | 217      | Total<br>1674 | C<br>1049 | N<br>304 | O<br>316 | S<br>5 | 0       | 0       | 0     |
| 1   | Iy    | 185      | Total<br>1426 | C<br>901  | N<br>248 | O<br>273 | S<br>4 | 0       | 0       | 0     |
| 1   | Iz    | 189      | Total<br>1451 | C<br>915  | N<br>253 | O<br>278 | S<br>5 | 0       | 0       | 0     |
| 1   | I1    | 217      | Total<br>1674 | C<br>1049 | N<br>304 | O<br>316 | S<br>5 | 0       | 0       | 0     |
| 1   | I4    | 185      | Total<br>1426 | C<br>901  | N<br>248 | O<br>273 | S<br>4 | 0       | 0       | 0     |
| 1   | I5    | 189      | Total<br>1451 | C<br>915  | N<br>253 | O<br>278 | S<br>5 | 0       | 0       | 0     |
| 1   | I6    | 217      | Total<br>1674 | C<br>1049 | N<br>304 | O<br>316 | S<br>5 | 0       | 0       | 0     |
| 1   | JA    | 185      | Total<br>1426 | C<br>901  | N<br>248 | O<br>273 | S<br>4 | 0       | 0       | 0     |
| 1   | JB    | 189      | Total<br>1451 | C<br>915  | N<br>253 | O<br>278 | S<br>5 | 0       | 0       | 0     |
| 1   | JC    | 217      | Total<br>1674 | C<br>1049 | N<br>304 | O<br>316 | S<br>5 | 0       | 0       | 0     |
| 1   | JF    | 185      | Total<br>1426 | C<br>901  | N<br>248 | O<br>273 | S<br>4 | 0       | 0       | 0     |
| 1   | JG    | 189      | Total<br>1451 | C<br>915  | N<br>253 | O<br>278 | S<br>5 | 0       | 0       | 0     |
| 1   | JH    | 217      | Total<br>1674 | C<br>1049 | N<br>304 | O<br>316 | S<br>5 | 0       | 0       | 0     |
| 1   | JK    | 185      | Total<br>1426 | C<br>901  | N<br>248 | O<br>273 | S<br>4 | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | JL    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | JM    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | JP    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | JQ    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | JR    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | JU    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | JV    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | JW    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | JZ    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Ja    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Jb    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Je    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Jf    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Jg    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Jj    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Jk    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Jl    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Jo    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Jp    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Jq    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Jt    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | Ju    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | Jv    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | Jy    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | Jz    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | J1    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |
| 1   | J4    | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 901  | 248 | 273 | 4 |         |         |       |
| 1   | J5    | 189      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 915  | 253 | 278 | 5 |         |         |       |
| 1   | J6    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1049 | 304 | 316 | 5 |         |         |       |

- Molecule 2 is a RNA chain called 5'-R(P\*UP\*UP\*AP\*AP\*UP\*AP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*UP\*UP\*UP\*U)-3'.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 2   | AD    | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 349   | 157 | 46 | 129 | 17 |         |         |       |
| 2   | AI    | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 349   | 157 | 46 | 129 | 17 |         |         |       |
| 2   | AN    | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 349   | 157 | 46 | 129 | 17 |         |         |       |
| 2   | AS    | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 349   | 157 | 46 | 129 | 17 |         |         |       |
| 2   | AX    | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 349   | 157 | 46 | 129 | 17 |         |         |       |
| 2   | Ac    | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 349   | 157 | 46 | 129 | 17 |         |         |       |
| 2   | Ah    | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 349   | 157 | 46 | 129 | 17 |         |         |       |
| 2   | Am    | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 349   | 157 | 46 | 129 | 17 |         |         |       |
| 2   | Ar    | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 349   | 157 | 46 | 129 | 17 |         |         |       |
| 2   | Aw    | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 349   | 157 | 46 | 129 | 17 |         |         |       |
| 2   | A2    | 17       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 349   | 157 | 46 | 129 | 17 |         |         |       |

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| Mol | Chain | Residues | Atoms        |          |         |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|----------|---------|---------|---------|-------|
| 2   | A7    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | BD    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | BI    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | BN    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | BS    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | BX    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Bc    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Bh    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Bm    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Br    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Bw    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | B2    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | B7    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | CD    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | CI    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | CN    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | CS    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | CX    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Cc    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Ch    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Cm    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms        |          |         |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|----------|---------|---------|---------|-------|
| 2   | Cr    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Cw    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | C2    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | C7    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | DD    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | DI    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | DN    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | DS    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | DX    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Dc    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Dh    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Dm    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Dr    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Dw    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | D2    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | D7    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | ED    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | EI    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | EN    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | ES    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | EX    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms        |          |         |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|----------|---------|---------|---------|-------|
| 2   | Ec    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Eh    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Em    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Er    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Ew    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | E2    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | E7    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | FD    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | FI    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | FN    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | FS    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | FX    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Fc    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Fh    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Fm    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Fr    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Fw    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | F2    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | F7    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | GD    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | GI    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms        |          |         |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|----------|---------|---------|---------|-------|
| 2   | GN    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | GS    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | GX    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Gc    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Gh    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Gm    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Gr    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Gw    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | G2    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | G7    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | HD    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | HI    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | HN    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | HS    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | HX    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Hc    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Hh    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Hm    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Hr    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Hw    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | H2    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms        |          |         |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|----------|---------|---------|---------|-------|
| 2   | H7    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | ID    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | II    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | IN    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | IS    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | IX    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Ic    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Ih    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Im    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Ir    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Iw    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | I2    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | I7    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | JD    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | JI    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | JN    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | JS    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | JX    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Jc    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Jh    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Jm    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms        |          |         |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|----------|---------|---------|---------|-------|
| 2   | Jr    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | Jw    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | J2    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |
| 2   | J7    | 17       | Total<br>349 | C<br>157 | N<br>46 | O<br>129 | P<br>17 | 0       | 0       | 0     |

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3   | Jt    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | FU    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | CA    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | IZ    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Eo    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | FK    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | DZ    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Ce    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Af    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | EF    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | JL    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | C4    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Gt    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Df    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | HF    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3   | Be    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | AA    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Hj    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | JA    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | A4    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | D4    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | AL    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | JZ    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | DP    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Hg    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | GK    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | HZ    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | JF    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | EU    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | AF    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | CZ    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Ek    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Bo    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | DK    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | DF    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | GA    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3   | DU    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Ao    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Jy    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | CU    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Co    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Gj    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Et    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Cy    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | BU    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Aj    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | HP    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | FF    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | CP    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | DA    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | AU    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Ht    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | GZ    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | EK    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Fo    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Ct    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | BZ    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3   | FP    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Bk    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | GP    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | AP    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | I1    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Ft    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | At    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | B5    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | IR    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | BF    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | BQ    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | I4    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | CG    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | HK    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | G1    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | A1    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | FZ    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | AZ    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Ho    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | BK    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | If    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3   | G4    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | J4    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Jj    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Ey    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Je    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | IA    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | JP    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | GF    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Dj    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | EP    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Dy    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | HA    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Dt    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | H4    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Jo    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Go    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | IK    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | BB    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | JU    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | EZ    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Do    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3   | Io    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Fk    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | CK    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Ge    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | IU    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | FA    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Bt    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | IF    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | F4    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Fe    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | HU    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Ij    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Cj    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Hy    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | Ee    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | By    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | GU    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | F1    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | E4    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | EC    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 3   | It    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |

### 3 Residue-property plots

MolProbity and EDS were not executed - this section will therefore be empty.



## 4 Data and refinement statistics

EDS was not executed - this section will therefore be incomplete.

| Property   | Value   | Source    |
|--|---|-----------|
| Space group  | P 1 21 1  | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 411.74Å 403.90Å 412.46Å<br>90.00° 89.65° 90.00°   | Depositor |
| Resolution (Å)   | 50.01 – 2.90  | Depositor |
| % Data completeness<br>(in resolution range)             | 74.9 (50.01-2.90)   | Depositor |
| $R_{merge}$  | 0.14  | Depositor |
| $R_{sym}$  | (Not available)   | Depositor |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>               | 2.99 (at 2.91Å)   | Xtriage   |
| Refinement program                                       | CNS 1.3   | Depositor |
| R, $R_{free}$  | 0.251 , 0.285   | Depositor |
| Wilson B-factor (Å <sup>2</sup> )                        | 45.5  | Xtriage   |
| Anisotropy   | 0.138   | Xtriage   |
| Estimated twinning fraction                              | 0.025 for -l,k,h<br>0.034 for -h,-l,-k<br>0.024 for -h,l,k<br>0.044 for -k,-h,-l<br>0.024 for k,h,-l<br>0.017 for -l,-h,k<br>0.030 for -k,l,-h<br>0.038 for l,h,k<br>0.027 for k,-l,-h<br>0.035 for h,-k,-l<br>0.030 for -l,-k,-h | Xtriage   |
| L-test for twinning                                      | $\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$   | Xtriage   |
| Outliers   | 0 of 2217465 reflections  | Xtriage   |
| Total number of atoms                                    | 588120  | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 73.0  | wwPDB-VP  |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

MolProbity was not executed - this section will therefore be empty.

### 5.2 Close contacts ⓘ

MolProbity was not executed - this section will therefore be empty.

### 5.3 Torsion angles

#### 5.3.1 Protein backbone ⓘ

MolProbity was not executed - this section will therefore be empty.

#### 5.3.2 Protein sidechains ⓘ

MolProbity was not executed - this section will therefore be empty.

#### 5.3.3 RNA ⓘ

MolProbity was not executed - this section will therefore be empty.

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

validation-pack was not executed - this section will therefore be empty.

### 5.5 Carbohydrates ⓘ

validation-pack was not executed - this section will therefore be empty.

### 5.6 Ligand geometry ⓘ

validation-pack was not executed - this section will therefore be empty.

### 5.7 Other polymers ⓘ

validation-pack was not executed - this section will therefore be empty.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.