



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 30, 2026 – 10:46 PM UTC

PDB ID : 7AZO / pdb\_00007azo  
Title : 70S thermus thermophilus ribosome with bound antibiotic lead SEQ-977  
Authors : Jenner, L.B.; Yusupov, M.; Yusupova, G.  
Deposited on : 2020-11-17  
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

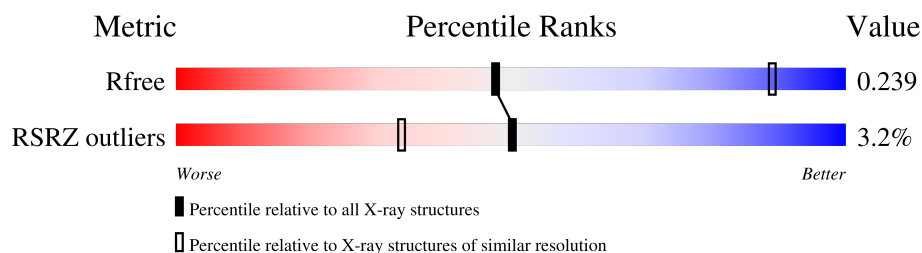
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



| Metric        | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|---------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$    | 180053                      | 1169 (3.32-3.28)                                      |
| RSRZ outliers | 180081                      | 1169 (3.32-3.28)                                      |

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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

| Mol | Type | Chain | Res     | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|---------|-----------|----------|---------|------------------|
| 58  | MG   | 16SB  | 2304[A] | -         | -        | -       | X                |
| 58  | MG   | 16SB  | 2304[B] | -         | -        | -       | X                |
| 58  | MG   | 23SA  | 3015    | -         | -        | -       | X                |

## 2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 306403 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | 16SA  | 1512     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32509 | 14478 | 6016 | 10503 | 1512 |         |         |       |
| 1   | 16SB  | 1508     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32429 | 14442 | 6008 | 10471 | 1508 |         |         |       |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | S2A   | 237      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1924  | 1228 | 344 | 347 | 5 |         |         |       |
| 2   | S2B   | 237      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1924  | 1228 | 344 | 347 | 5 |         |         |       |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | S3A   | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1605  | 1011 | 313 | 280 | 1 |         |         |       |
| 3   | S3B   | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1612  | 1016 | 314 | 281 | 1 |         |         |       |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | S4A   | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1702  | 1066 | 339 | 290 | 7 |         |         |       |
| 4   | S4B   | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1702  | 1066 | 339 | 290 | 7 |         |         |       |

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | S5A   | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1155  | 729 | 218 | 204 | 4 |         |         |       |
| 5   | S5B   | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1155  | 729 | 218 | 204 | 4 |         |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | S6A   | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 842   | 531 | 155 | 153 | 3 |         |         |       |
| 6   | S6B   | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 842   | 531 | 155 | 153 | 3 |         |         |       |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | S7A   | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1256  | 781 | 252 | 217 | 6 |         |         |       |
| 7   | S7B   | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1256  | 781 | 252 | 217 | 6 |         |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | S8A   | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1115  | 705 | 215 | 192 | 3 |         |         |       |
| 8   | S8B   | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1115  | 705 | 215 | 192 | 3 |         |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 9   | S9A   | 127      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1009  | 639 | 197 | 173 |  |         |         |       |
| 9   | S9B   | 127      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1009  | 639 | 197 | 173 |  |         |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | S10A  | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 801   | 504 | 157 | 139 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | S10B  | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 801   | 504 | 157 | 139 | 1 |         |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | S11A  | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 864   | 537 | 164 | 160 | 3 |         |         |       |
| 11  | S11B  | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 873   | 543 | 166 | 161 | 3 |         |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | S12A  | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 977   | 615 | 196 | 164 | 2 |         |         |       |
| 12  | S12B  | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 977   | 615 | 196 | 164 | 2 |         |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | S13A  | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 946   | 585 | 195 | 164 | 2 |         |         |       |
| 13  | S13B  | 121      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 597 | 199 | 166 | 2 |         |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14  | S14A  | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 491   | 312 | 104 | 71 | 4 |         |         |       |
| 14  | S14B  | 59       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 486   | 309 | 103 | 70 | 4 |         |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | S15A  | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 733   | 459 | 147 | 125 | 2 |         |         |       |
| 15  | S15B  | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 733   | 459 | 147 | 125 | 2 |         |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | S16A  | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 700   | 443 | 139 | 117 | 1 |         |         |       |
| 16  | S16B  | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 705   | 446 | 140 | 118 | 1 |         |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | S17A  | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 834   | 534 | 155 | 143 | 2 |         |         |       |
| 17  | S17B  | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 834   | 534 | 155 | 143 | 2 |         |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | S18A  | 71       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 584   | 373 | 116 | 95 |         |         |       |
| 18  | S18B  | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 573   | 367 | 112 | 94 |         |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | S19A  | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 674   | 430 | 126 | 116 | 2 |         |         |       |
| 19  | S19B  | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 684   | 436 | 126 | 120 | 2 |         |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | S20A  | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 470 | 162 | 128 | 2 |         |         |       |
| 20  | S20B  | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 470 | 162 | 128 | 2 |         |         |       |

- Molecule 21 is a protein called 30S ribosomal protein Thx.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21  | THXA  | 24       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 208   | 128 | 50 | 30 |         |         |       |
| 21  | THXB  | 25       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 217   | 134 | 52 | 31 |         |         |       |

- Molecule 22 is a RNA chain called Phe-tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 22  | ASIA  | 76       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1628  | 731 | 290 | 530 | 75 | 2 |         |         |       |

- Molecule 23 is a RNA chain called Phe-tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 23  | PSIA  | 76       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1635  | 735 | 291 | 532 | 75 | 2 |         |         |       |
| 23  | PSIB  | 76       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1635  | 735 | 291 | 532 | 75 | 2 |         |         |       |

- Molecule 24 is a RNA chain called Phe-tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 24  | ESIA  | 76       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1626  | 729 | 290 | 531 | 75 | 1 |         |         |       |
| 24  | ESIB  | 76       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1626  | 729 | 290 | 531 | 75 | 1 |         |         |       |

- Molecule 25 is a RNA chain called RNA (30-MER).

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 25  | MRNA  | 30       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 621   | 279 | 88 | 225 | 29 |         |         |       |
| 25  | MRNB  | 30       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 621   | 279 | 88 | 225 | 29 |         |         |       |

- Molecule 26 is a RNA chain called Phe-tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 26  | TRNA  | 73       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1565  | 702 | 279 | 510 | 72 | 2 |         |         |       |

- Molecule 27 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 27  | 23SA  | 2889     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62225 | 27699 | 11629 | 20008 | 2889 |         |         |       |
| 27  | 23SB  | 2873     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61886 | 27548 | 11574 | 19891 | 2873 |         |         |       |

- Molecule 28 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 28  | 5SA   | 122      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2617  | 1166 | 486 | 844 | 121 |         |         |       |
| 28  | 5SB   | 121      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2598  | 1156 | 481 | 840 | 121 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 29  | L2A   | 272      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2115  | 1335 | 420 | 357 | 3 |         |         |       |
| 29  | L2B   | 272      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2115  | 1335 | 420 | 357 | 3 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30  | L3A   | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1563  | 988 | 299 | 270 | 6 |         |         |       |
| 30  | L3B   | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1563  | 988 | 299 | 270 | 6 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 31  | L4A   | 202      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1585  | 1011 | 297 | 275 | 2 |         |         |       |
| 31  | L4B   | 202      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1585  | 1011 | 297 | 275 | 2 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | L5A   | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1473  | 942 | 268 | 259 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | L5B   | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1473  | 942 | 268 | 259 | 4 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | L6A   | 171      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1316  | 835 | 247 | 233 | 1 |         |         |       |
| 33  | L6B   | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1327  | 842 | 249 | 235 | 1 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | L9A   | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1131  | 723 | 200 | 207 | 1 |         |         |       |
| 34  | L9B   | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | L13A  | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |
| 35  | L13B  | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | L14A  | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 932   | 588 | 171 | 169 | 4 |         |         |       |
| 36  | L14B  | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 932   | 588 | 171 | 169 | 4 |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | L15A  | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1144  | 712 | 232 | 197 | 3 |         |         |       |
| 37  | L15B  | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1144  | 712 | 232 | 197 | 3 |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | L16A  | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1121  | 715 | 212 | 187 | 7 |         |         |       |
| 38  | L16B  | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1121  | 715 | 212 | 187 | 7 |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | L17A  | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 967   | 604 | 203 | 159 | 1 |         |         |       |
| 39  | L17B  | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 967   | 604 | 203 | 159 | 1 |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | L18A  | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 889   | 561 | 177 | 150 | 1 |         |         |       |
| 40  | L18B  | 111      | Total | C   | N   | O   |   | 0       | 0       | 0     |
|     |       |          | 881   | 556 | 176 | 149 |   |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | L19A  | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1141  | 710 | 234 | 196 | 1 |         |         |       |
| 41  | L19B  | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1141  | 710 | 234 | 196 | 1 |         |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | L20A  | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 963   | 610 | 202 | 150 | 1 |         |         |       |
| 42  | L20B  | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 963   | 610 | 202 | 150 | 1 |         |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | L21A  | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 778   | 501 | 142 | 134 | 1 |         |         |       |
| 43  | L21B  | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 778   | 501 | 142 | 134 | 1 |         |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | L22A  | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 899   | 566 | 177 | 154 | 2 |         |         |       |
| 44  | L22B  | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 899   | 566 | 177 | 154 | 2 |         |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | L23A  | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 738   | 480 | 133 | 124 | 1 |         |         |       |
| 45  | L23B  | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 742   | 482 | 134 | 125 | 1 |         |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | L24A  | 108      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 824   | 528 | 153 | 138 | 5 |         |         |       |
| 46  | L24B  | 106      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 775   | 494 | 147 | 129 | 5 |         |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | L25A  | 179      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1428  | 911 | 255 | 259 | 3 |         |         |       |
| 47  | L25B  | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1404  | 897 | 252 | 252 | 3 |         |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | L27A  | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 661   | 410 | 140 | 110 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | L27B  | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 661   | 410 | 140 | 110 | 1 |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49  | L28A  | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 481 | 150 | 130 | 1 |         |         |       |
| 49  | L28B  | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 481 | 150 | 130 | 1 |         |         |       |

- Molecule 50 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50  | L29A  | 69       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 583   | 363 | 117 | 101 | 2 |         |         |       |
| 50  | L29B  | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 590   | 367 | 119 | 103 | 1 |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 51  | L30A  | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 468   | 298 | 90 | 80 |         |         |       |
| 51  | L30B  | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 468   | 298 | 90 | 80 |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52  | L31A  | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 580   | 364 | 108 | 103 | 5 |         |         |       |
| 52  | L31B  | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 580   | 364 | 108 | 103 | 5 |         |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53  | L32A  | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 434   | 272 | 87 | 70 | 5 |         |         |       |
| 53  | L32B  | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 434   | 272 | 87 | 70 | 5 |         |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 54  | L33A  | 45       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 389   | 241 | 79 | 65 | 4 |         |         |       |
| 54  | L33B  | 45       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 389   | 241 | 79 | 65 | 4 |         |         |       |

- Molecule 55 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 55  | L34A  | 48       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 257 | 104 | 55 | 2 |         |         |       |
| 55  | L34B  | 49       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 429   | 263 | 108 | 56 | 2 |         |         |       |

- Molecule 56 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 56  | L35A  | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 516   | 331 | 102 | 81 | 2 |         |         |       |
| 56  | L35B  | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 516   | 331 | 102 | 81 | 2 |         |         |       |

- Molecule 57 is a RNA chain called Phe-tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 57  | ASIB  | 76       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1627  | 730 | 290 | 531 | 75 | 1 |         |         |       |

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

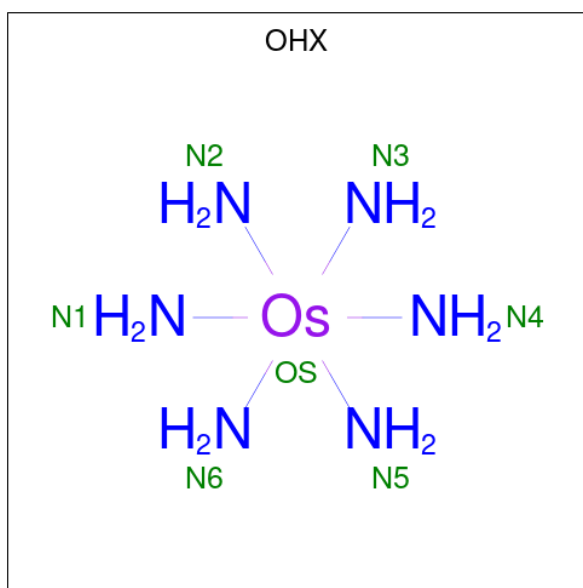
| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 58  | 16SA  | 92       | Total | Mg  | 0       | 0       |
|     |       |          | 92    | 92  |         |         |
| 58  | S4A   | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 58  | PSIA  | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 58  | 23SA  | 332      | Total | Mg  | 0       | 0       |
|     |       |          | 332   | 332 |         |         |
| 58  | 5SA   | 6        | Total | Mg  | 0       | 0       |
|     |       |          | 6     | 6   |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 58  | L3A   | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 58  | L4A   | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 58  | L5A   | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | L15A  | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 58  | L23A  | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | L27A  | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 58  | L30A  | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | L32A  | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | L33A  | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | L34A  | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | L35A  | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | 16SB  | 85       | Total<br>86  | Mg<br>86  | 0       | 1       |
| 58  | S5B   | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | PSIB  | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 58  | 23SB  | 240      | Total<br>241 | Mg<br>241 | 0       | 1       |
| 58  | 5SB   | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 58  | L3B   | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 58  | L4B   | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | L5B   | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | L15B  | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | L35B  | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |

- Molecule 59 is osmium (III) hexammine (CCD ID: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | S4A   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | S10A  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | S19A  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | ASIA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | ASIA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | ASIA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | PSIA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | ESIA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | MRNA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | TRNA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | TRNA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
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| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
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| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
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|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SA  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SA   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SA   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SA   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SA   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SA   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SA   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SA   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SA   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 5SA   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SA   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | L4A   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | L15A  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | L17A  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | L19A  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | L20A  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | L27A  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | L27A  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | L28A  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | L35A  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 16SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | S4B   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | S14B  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | ASIB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | ASIB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | ASIB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | PSIB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | PSIB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | ESIB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | MRNB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 23SB  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SB   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SB   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SB   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SB   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SB   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SB   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SB   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SB   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SB   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | 5SB   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | L4B   | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | L17B  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | L20B  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 59  | L35B  | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 60  | 16SA  | 46       | Total | K  | 0       | 0       |
|     |       |          | 46    | 46 |         |         |

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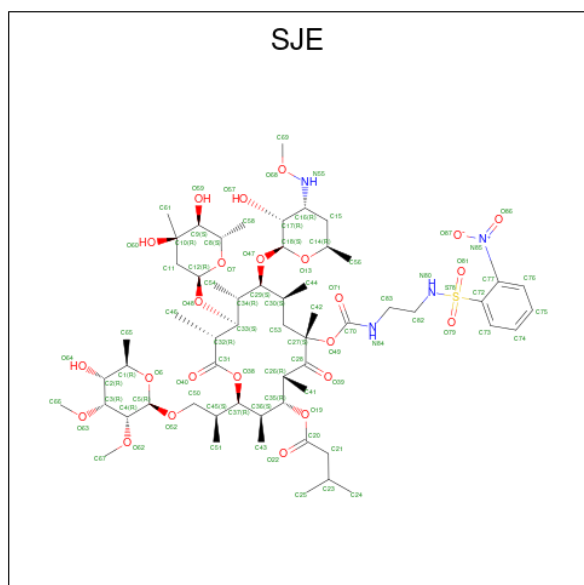
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 60  | S6A   | 1        | Total<br>1   | K<br>1   | 0       | 0       |
| 60  | S13A  | 1        | Total<br>1   | K<br>1   | 0       | 0       |
| 60  | S20A  | 1        | Total<br>1   | K<br>1   | 0       | 0       |
| 60  | PSIA  | 2        | Total<br>2   | K<br>2   | 0       | 0       |
| 60  | 23SA  | 102      | Total<br>102 | K<br>102 | 0       | 0       |
| 60  | 5SA   | 2        | Total<br>2   | K<br>2   | 0       | 0       |
| 60  | L2A   | 1        | Total<br>1   | K<br>1   | 0       | 0       |
| 60  | L3A   | 1        | Total<br>1   | K<br>1   | 0       | 0       |
| 60  | L4A   | 1        | Total<br>1   | K<br>1   | 0       | 0       |
| 60  | L5A   | 1        | Total<br>1   | K<br>1   | 0       | 0       |
| 60  | 16SB  | 35       | Total<br>35  | K<br>35  | 0       | 0       |
| 60  | S4B   | 1        | Total<br>1   | K<br>1   | 0       | 0       |
| 60  | S6B   | 1        | Total<br>1   | K<br>1   | 0       | 0       |
| 60  | S13B  | 1        | Total<br>1   | K<br>1   | 0       | 0       |
| 60  | S14B  | 1        | Total<br>1   | K<br>1   | 0       | 0       |
| 60  | S20B  | 1        | Total<br>1   | K<br>1   | 0       | 0       |
| 60  | 23SB  | 81       | Total<br>81  | K<br>81  | 0       | 0       |
| 60  | 5SB   | 1        | Total<br>1   | K<br>1   | 0       | 0       |
| 60  | L2B   | 1        | Total<br>1   | K<br>1   | 0       | 0       |
| 60  | L3B   | 1        | Total<br>1   | K<br>1   | 0       | 0       |
| 60  | L4B   | 1        | Total<br>1   | K<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 60  | L5B   | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 60  | L15B  | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 60  | L16B  | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

- Molecule 61 is (2R,3S,4R,5R,7S,9S,10S,11R,12S,13R)-12-(((2R,4R,5S,6S)-4,5-dihydroxy-4,6-dimethyltetrahydro-2H-pyran-2-yl)oxy)-2-(((S)-1-(((2R,3R,4R,5R,6R)-5-hydroxy-3,4-dimethoxy-6-methyltetrahydro-2H-pyran-2-yl)oxy)propan-2-yl)-10-(((2S,3R,4R,6R)-3-hydroxy-4-(methoxyamino)-6-methyltetrahydro-2H-pyran-2-yl)oxy)-3,5,7,9,11,13-hexamethyl-7-((2-((2-nitrophenyl)sulfonamido)ethyl)carbamoyl)oxy)-6,14-dioxooxacyclotetradecan-4-yl 3-methylbutanoate (CCD ID: SJE) (formula: C<sub>58</sub>H<sub>96</sub>N<sub>4</sub>O<sub>24</sub>S).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 61  | 23SA  | 1        | Total | C  | N | O  | S | 0       | 0       |
|     |       |          | 87    | 58 | 4 | 24 | 1 |         |         |
| 61  | 23SB  | 1        | Total | C  | N | O  | S | 0       | 0       |
|     |       |          | 87    | 58 | 4 | 24 | 1 |         |         |

- Molecule 62 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 62  | 16SA  | 172      | Total | O   | 0       | 0       |
|     |       |          | 172   | 172 |         |         |
| 62  | S4A   | 3        | Total | O   | 0       | 0       |
|     |       |          | 3     | 3   |         |         |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 62  | S5A   | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | S12A  | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | S13A  | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | S14A  | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | S16A  | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | THXA  | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 62  | PSIA  | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 62  | ESIA  | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | 23SA  | 788      | Total<br>788 | O<br>788 | 0       | 0       |
| 62  | 5SA   | 14       | Total<br>14  | O<br>14  | 0       | 0       |
| 62  | L2A   | 10       | Total<br>10  | O<br>10  | 0       | 0       |
| 62  | L3A   | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 62  | L4A   | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 62  | L15A  | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 62  | L16A  | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | L17A  | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 62  | L18A  | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 62  | L19A  | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | L23A  | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | L27A  | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 62  | L30A  | 1        | Total<br>1   | O<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 62  | L34A  | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | L35A  | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | 16SB  | 157      | Total<br>157 | O<br>157 | 0       | 0       |
| 62  | S4B   | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 62  | S5B   | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | S9B   | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | S12B  | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 62  | S14B  | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 62  | 23SB  | 519      | Total<br>519 | O<br>519 | 0       | 0       |
| 62  | 5SB   | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 62  | L2B   | 12       | Total<br>12  | O<br>12  | 0       | 0       |
| 62  | L3B   | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 62  | L4B   | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | L15B  | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 62  | L19B  | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | L27B  | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 62  | L28B  | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | L30B  | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | L35B  | 6        | Total<br>6   | O<br>6   | 0       | 0       |

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### 3 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 209.77Å 446.87Å 616.97Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 253.87 – 3.30<br>253.87 – 3.30                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (253.87-3.30)<br>100.0 (253.87-3.30)                  | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.15 (at 3.33Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.18.2_3874                                          | Depositor        |
| R, $R_{free}$                                                           | 0.214 , 0.238<br>0.215 , 0.239                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 25661 reflections (2.98%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 93.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.299                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 51.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 306403                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 94.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

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### 4.3 Torsion angles [i](#)

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

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

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

87 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 1   | 5MC  | 16SB  | 2028 | 1    | 19,22,23     | 4.10 | 8 (42%)     | 26,32,35    | 1.19 | 3 (11%)     |
| 1   | 5MC  | 16SA  | 2032 | 1    | 19,22,23     | 4.08 | 8 (42%)     | 26,32,35    | 0.89 | 3 (11%)     |
| 23  | 5MU  | PSIB  | 54   | 23   | 19,22,23     | 3.96 | 5 (26%)     | 27,32,35    | 3.10 | 9 (33%)     |

| Mol | Type | Chain | Res  | Link     | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|----------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |          | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | 5MC  | 16SB  | 1590 | 1        | 19,22,23     | 4.10 | 8 (42%)  | 26,32,35    | 1.00 | 1 (3%)   |
| 26  | H2U  | TRNA  | 20   | 28,26    | 18,21,22     | 2.32 | 4 (22%)  | 19,30,33    | 1.62 | 4 (21%)  |
| 24  | MIA  | ESIA  | 37   | 24       | 28,31,32     | 2.32 | 4 (14%)  | 38,44,47    | 3.11 | 14 (36%) |
| 26  | MIA  | TRNA  | 37   | 26,27    | 28,31,32     | 2.69 | 8 (28%)  | 38,44,47    | 4.52 | 15 (39%) |
| 27  | 2MA  | 23SA  | 2518 | 60,27    | 22,25,26     | 3.45 | 7 (31%)  | 32,37,40    | 2.20 | 11 (34%) |
| 23  | G7M  | PSIB  | 46   | 23       | 23,26,27     | 4.72 | 8 (34%)  | 34,39,42    | 3.33 | 13 (38%) |
| 26  | PSU  | TRNA  | 39   | 26       | 18,21,22     | 1.19 | 1 (5%)   | 21,30,33    | 1.95 | 5 (23%)  |
| 24  | MIA  | ESIB  | 37   | 24       | 28,31,32     | 2.33 | 4 (14%)  | 38,44,47    | 3.86 | 13 (34%) |
| 22  | 4SU  | ASIA  | 8    | 22       | 18,21,22     | 1.88 | 5 (27%)  | 25,30,33    | 2.45 | 6 (24%)  |
| 27  | PSU  | 23SA  | 2620 | 27       | 18,21,22     | 1.18 | 2 (11%)  | 21,30,33    | 1.96 | 4 (19%)  |
| 27  | OMG  | 23SA  | 2266 | 60,27,23 | 23,26,27     | 4.94 | 11 (47%) | 32,38,41    | 4.63 | 18 (56%) |
| 27  | 5MC  | 23SA  | 1987 | 60,27    | 19,22,23     | 3.91 | 8 (42%)  | 26,32,35    | 0.95 | 1 (3%)   |
| 23  | PSU  | PSIB  | 55   | 23       | 18,21,22     | 1.15 | 1 (5%)   | 21,30,33    | 1.80 | 3 (14%)  |
| 27  | PSU  | 23SA  | 1936 | 27       | 18,21,22     | 1.09 | 1 (5%)   | 21,30,33    | 1.96 | 4 (19%)  |
| 26  | 5MU  | TRNA  | 54   | 26       | 19,22,23     | 3.99 | 5 (26%)  | 27,32,35    | 3.22 | 9 (33%)  |
| 23  | G7M  | PSIA  | 46   | 23       | 23,26,27     | 4.59 | 8 (34%)  | 34,39,42    | 3.43 | 13 (38%) |
| 26  | H2U  | TRNA  | 16   | 26       | 18,21,22     | 2.08 | 4 (22%)  | 19,30,33    | 1.69 | 4 (21%)  |
| 23  | PSU  | PSIA  | 55   | 23       | 18,21,22     | 1.25 | 1 (5%)   | 21,30,33    | 1.79 | 4 (19%)  |
| 23  | MIA  | PSIA  | 37   | 23       | 28,31,32     | 2.23 | 4 (14%)  | 38,44,47    | 2.66 | 12 (31%) |
| 1   | MA6  | 16SB  | 2141 | 1        | 23,26,27     | 1.46 | 5 (21%)  | 33,38,41    | 2.58 | 11 (33%) |
| 1   | 2MG  | 16SA  | 1834 | 60,1     | 23,26,27     | 2.96 | 8 (34%)  | 33,38,41    | 2.24 | 12 (36%) |
| 27  | PSU  | 23SA  | 1942 | 27       | 18,21,22     | 1.07 | 1 (5%)   | 21,30,33    | 1.93 | 5 (23%)  |
| 1   | 2MG  | 16SB  | 1834 | 1        | 23,26,27     | 3.03 | 8 (34%)  | 33,38,41    | 2.29 | 12 (36%) |
| 27  | 5MU  | 23SB  | 1964 | 60,27    | 19,22,23     | 3.87 | 5 (26%)  | 27,32,35    | 3.31 | 9 (33%)  |
| 57  | MIA  | ASIB  | 37   | 57       | 28,31,32     | 2.24 | 4 (14%)  | 38,44,47    | 3.13 | 15 (39%) |
| 22  | PSU  | ASIA  | 55   | 22       | 18,21,22     | 1.08 | 1 (5%)   | 21,30,33    | 1.84 | 4 (19%)  |
| 1   | G7M  | 16SA  | 1156 | 60,1     | 23,26,27     | 4.59 | 8 (34%)  | 34,39,42    | 3.36 | 13 (38%) |
| 22  | MIA  | ASIA  | 37   | 22       | 28,31,32     | 2.20 | 4 (14%)  | 38,44,47    | 3.16 | 12 (31%) |
| 23  | PSU  | PSIA  | 32   | 23       | 18,21,22     | 1.06 | 1 (5%)   | 21,30,33    | 1.71 | 4 (19%)  |
| 1   | G7M  | 16SB  | 1156 | 60,1     | 23,26,27     | 4.65 | 8 (34%)  | 34,39,42    | 3.36 | 13 (38%) |
| 1   | 5MC  | 16SA  | 2028 | 1        | 19,22,23     | 4.06 | 8 (42%)  | 26,32,35    | 1.08 | 1 (3%)   |
| 1   | 5MC  | 16SA  | 1590 | 1        | 19,22,23     | 4.02 | 8 (42%)  | 26,32,35    | 1.06 | 1 (3%)   |
| 22  | 5MU  | ASIA  | 54   | 22       | 19,22,23     | 3.90 | 5 (26%)  | 27,32,35    | 3.27 | 10 (37%) |
| 27  | 5MC  | 23SA  | 1967 | 27       | 19,22,23     | 4.02 | 8 (42%)  | 26,32,35    | 1.14 | 2 (7%)   |
| 27  | OMU  | 23SB  | 2567 | 58,27    | 19,22,23     | 3.02 | 8 (42%)  | 25,31,34    | 1.95 | 5 (20%)  |

| Mol | Type | Chain | Res  | Link     | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|----------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |          | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 22  | PSU  | ASIA  | 32   | 22       | 18,21,22     | 1.16 | 1 (5%)   | 21,30,33    | 1.65 | 4 (19%)  |
| 1   | MA6  | 16SA  | 2141 | 1        | 23,26,27     | 1.49 | 5 (21%)  | 33,38,41    | 2.75 | 12 (36%) |
| 1   | UR3  | 16SB  | 2121 | 1        | 19,22,23     | 2.90 | 7 (36%)  | 26,32,35    | 1.67 | 4 (15%)  |
| 27  | 5MU  | 23SA  | 1964 | 60,27    | 19,22,23     | 3.83 | 5 (26%)  | 27,32,35    | 3.40 | 10 (37%) |
| 27  | OMC  | 23SB  | 1945 | 27       | 19,22,23     | 1.78 | 4 (21%)  | 25,31,34    | 0.94 | 1 (4%)   |
| 23  | PSU  | PSIB  | 39   | 23       | 18,21,22     | 1.16 | 1 (5%)   | 21,30,33    | 1.76 | 4 (19%)  |
| 1   | 5MC  | 16SB  | 2035 | 1        | 19,22,23     | 4.12 | 8 (42%)  | 26,32,35    | 1.12 | 3 (11%)  |
| 23  | H2U  | PSIB  | 16   | 23       | 18,21,22     | 2.11 | 4 (22%)  | 19,30,33    | 1.59 | 4 (21%)  |
| 23  | 4SU  | PSIB  | 8    | 58,23    | 18,21,22     | 1.94 | 5 (27%)  | 25,30,33    | 3.04 | 7 (28%)  |
| 12  | 0TD  | S12B  | 89   | 12       | 8,9,10       | 1.61 | 1 (12%)  | 6,11,13     | 2.00 | 2 (33%)  |
| 23  | PSU  | PSIA  | 39   | 23       | 18,21,22     | 1.10 | 1 (5%)   | 21,30,33    | 1.78 | 4 (19%)  |
| 1   | PSU  | 16SA  | 1145 | 58,1     | 18,21,22     | 1.18 | 1 (5%)   | 21,30,33    | 1.84 | 5 (23%)  |
| 22  | G7M  | ASIA  | 46   | 22       | 23,26,27     | 4.64 | 8 (34%)  | 34,39,42    | 3.42 | 13 (38%) |
| 1   | UR3  | 16SA  | 2121 | 1        | 19,22,23     | 2.86 | 8 (42%)  | 26,32,35    | 1.81 | 4 (15%)  |
| 26  | PSU  | TRNA  | 55   | 26       | 18,21,22     | 1.13 | 1 (5%)   | 21,30,33    | 1.91 | 4 (19%)  |
| 23  | 4SU  | PSIA  | 8    | 23       | 18,21,22     | 1.85 | 3 (16%)  | 25,30,33    | 2.60 | 5 (20%)  |
| 27  | OMU  | 23SA  | 2567 | 58,27    | 19,22,23     | 2.97 | 8 (42%)  | 25,31,34    | 1.98 | 5 (20%)  |
| 23  | 3AU  | PSIA  | 47   | 23       | 24,28,29     | 2.83 | 8 (33%)  | 30,40,43    | 1.61 | 5 (16%)  |
| 27  | 5MC  | 23SB  | 1987 | 60,27    | 19,22,23     | 4.05 | 8 (42%)  | 26,32,35    | 0.93 | 2 (7%)   |
| 1   | M2G  | 16SB  | 1589 | 1        | 24,27,28     | 2.93 | 8 (33%)  | 33,40,43    | 1.71 | 7 (21%)  |
| 1   | PSU  | 16SB  | 1145 | 58,1     | 18,21,22     | 1.15 | 1 (5%)   | 21,30,33    | 1.80 | 5 (23%)  |
| 57  | PSU  | ASIB  | 32   | 57       | 18,21,22     | 1.06 | 1 (5%)   | 21,30,33    | 1.82 | 4 (19%)  |
| 27  | 5MC  | 23SB  | 1967 | 27       | 19,22,23     | 4.08 | 8 (42%)  | 26,32,35    | 1.05 | 3 (11%)  |
| 27  | PSU  | 23SB  | 1936 | 27       | 18,21,22     | 1.19 | 1 (5%)   | 21,30,33    | 1.63 | 4 (19%)  |
| 27  | OMG  | 23SB  | 2266 | 60,27,23 | 23,26,27     | 5.03 | 11 (47%) | 32,38,41    | 4.73 | 17 (53%) |
| 27  | 5MU  | 23SA  | 1940 | 27       | 19,22,23     | 4.17 | 5 (26%)  | 27,32,35    | 3.50 | 10 (37%) |
| 1   | 5MC  | 16SB  | 2032 | 1        | 19,22,23     | 4.13 | 8 (42%)  | 26,32,35    | 0.95 | 2 (7%)   |
| 1   | 4OC  | 16SA  | 2030 | 1        | 20,23,24     | 3.12 | 8 (40%)  | 25,32,35    | 0.89 | 1 (4%)   |
| 27  | OMC  | 23SA  | 1945 | 60,27    | 19,22,23     | 1.71 | 4 (21%)  | 25,31,34    | 0.85 | 1 (4%)   |
| 27  | PSU  | 23SB  | 2620 | 27       | 18,21,22     | 1.22 | 2 (11%)  | 21,30,33    | 1.90 | 4 (19%)  |
| 26  | 4SU  | TRNA  | 8    | 26       | 18,21,22     | 1.87 | 3 (16%)  | 25,30,33    | 2.48 | 5 (20%)  |
| 12  | 0TD  | S12A  | 89   | 12       | 8,9,10       | 1.47 | 1 (12%)  | 6,11,13     | 1.88 | 1 (16%)  |
| 23  | PSU  | PSIB  | 32   | 23       | 18,21,22     | 1.06 | 1 (5%)   | 21,30,33    | 1.82 | 4 (19%)  |
| 23  | MIA  | PSIB  | 37   | 23       | 28,31,32     | 2.22 | 3 (10%)  | 38,44,47    | 2.80 | 13 (34%) |
| 1   | 5MC  | 16SA  | 2035 | 1        | 19,22,23     | 4.02 | 8 (42%)  | 26,32,35    | 1.05 | 1 (3%)   |

| Mol | Type | Chain | Res  | Link     | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|----------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |          | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 23  | 5MU  | PSIA  | 54   | 23       | 19,22,23     | 3.84 | 5 (26%)  | 27,32,35    | 3.17 | 7 (25%)  |
| 57  | 5MU  | ASIB  | 54   | 57       | 19,22,23     | 3.95 | 5 (26%)  | 27,32,35    | 3.18 | 8 (29%)  |
| 57  | PSU  | ASIB  | 39   | 57       | 18,21,22     | 1.15 | 1 (5%)   | 21,30,33    | 1.81 | 4 (19%)  |
| 23  | 3AU  | PSIB  | 47   | 23       | 24,28,29     | 2.88 | 8 (33%)  | 30,40,43    | 2.09 | 8 (26%)  |
| 27  | 2MA  | 23SB  | 2518 | 58,60,27 | 22,25,26     | 3.47 | 7 (31%)  | 32,37,40    | 2.27 | 12 (37%) |
| 22  | PSU  | ASIA  | 39   | 22       | 18,21,22     | 1.17 | 1 (5%)   | 21,30,33    | 1.71 | 3 (14%)  |
| 26  | PSU  | TRNA  | 32   | 26       | 18,21,22     | 1.19 | 1 (5%)   | 21,30,33    | 1.85 | 4 (19%)  |
| 1   | 4OC  | 16SB  | 2030 | 58,1     | 20,23,24     | 2.86 | 8 (40%)  | 25,32,35    | 1.44 | 4 (16%)  |
| 1   | M2G  | 16SA  | 1589 | 1        | 24,27,28     | 2.86 | 8 (33%)  | 33,40,43    | 1.57 | 8 (24%)  |
| 1   | MA6  | 16SB  | 2142 | 1        | 23,26,27     | 1.43 | 5 (21%)  | 33,38,41    | 2.73 | 12 (36%) |
| 1   | MA6  | 16SA  | 2142 | 1        | 23,26,27     | 1.48 | 5 (21%)  | 33,38,41    | 2.77 | 13 (39%) |
| 27  | 5MU  | 23SB  | 1940 | 27       | 19,22,23     | 4.05 | 5 (26%)  | 27,32,35    | 3.36 | 9 (33%)  |
| 23  | H2U  | PSIA  | 16   | 23       | 18,21,22     | 2.07 | 4 (22%)  | 19,30,33    | 1.64 | 4 (21%)  |
| 27  | PSU  | 23SB  | 1942 | 27       | 18,21,22     | 1.17 | 1 (5%)   | 21,30,33    | 1.77 | 4 (19%)  |

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

| Mol | Type | Chain | Res  | Link     | Chirals | Torsions   | Rings   |
|-----|------|-------|------|----------|---------|------------|---------|
| 1   | 5MC  | 16SB  | 2028 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 16SA  | 2032 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 23  | 5MU  | PSIB  | 54   | 23       | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 16SB  | 1590 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 26  | H2U  | TRNA  | 20   | 28,26    | -       | 5/7/38/39  | 0/2/2/2 |
| 24  | MIA  | ESIA  | 37   | 24       | -       | 7/15/33/34 | 0/3/3/3 |
| 26  | MIA  | TRNA  | 37   | 26,27    | -       | 6/15/33/34 | 0/3/3/3 |
| 27  | 2MA  | 23SA  | 2518 | 60,27    | -       | 1/7/25/26  | 0/3/3/3 |
| 23  | G7M  | PSIB  | 46   | 23       | -       | 0/7/25/26  | 0/3/3/3 |
| 26  | PSU  | TRNA  | 39   | 26       | -       | 0/7/25/26  | 0/2/2/2 |
| 24  | MIA  | ESIB  | 37   | 24       | -       | 6/15/33/34 | 0/3/3/3 |
| 22  | 4SU  | ASIA  | 8    | 22       | -       | 1/7/25/26  | 0/2/2/2 |
| 27  | PSU  | 23SA  | 2620 | 27       | -       | 0/7/25/26  | 0/2/2/2 |
| 27  | OMG  | 23SA  | 2266 | 60,27,23 | -       | 1/9/27/28  | 0/3/3/3 |
| 27  | 5MC  | 23SA  | 1987 | 60,27    | -       | 0/7/25/26  | 0/2/2/2 |
| 23  | PSU  | PSIB  | 55   | 23       | -       | 0/7/25/26  | 0/2/2/2 |
| 27  | PSU  | 23SA  | 1936 | 27       | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 26  | 5MU  | TRNA  | 54   | 26    | -       | 2/7/25/26  | 0/2/2/2 |
| 23  | G7M  | PSIA  | 46   | 23    | -       | 2/7/25/26  | 0/3/3/3 |
| 26  | H2U  | TRNA  | 16   | 26    | -       | 3/7/38/39  | 0/2/2/2 |
| 23  | PSU  | PSIA  | 55   | 23    | -       | 3/7/25/26  | 0/2/2/2 |
| 23  | MIA  | PSIA  | 37   | 23    | -       | 5/15/33/34 | 0/3/3/3 |
| 1   | MA6  | 16SB  | 2141 | 1     | -       | 0/11/29/30 | 0/3/3/3 |
| 1   | 2MG  | 16SA  | 1834 | 60,1  | -       | 0/9/27/28  | 0/3/3/3 |
| 27  | PSU  | 23SA  | 1942 | 27    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 2MG  | 16SB  | 1834 | 1     | -       | 2/9/27/28  | 0/3/3/3 |
| 27  | 5MU  | 23SB  | 1964 | 60,27 | -       | 2/7/25/26  | 0/2/2/2 |
| 57  | MIA  | ASIB  | 37   | 57    | -       | 3/15/33/34 | 0/3/3/3 |
| 22  | PSU  | ASIA  | 55   | 22    | -       | 3/7/25/26  | 0/2/2/2 |
| 1   | G7M  | 16SA  | 1156 | 60,1  | -       | 2/7/25/26  | 0/3/3/3 |
| 22  | MIA  | ASIA  | 37   | 22    | -       | 6/15/33/34 | 0/3/3/3 |
| 23  | PSU  | PSIA  | 32   | 23    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | G7M  | 16SB  | 1156 | 60,1  | -       | 2/7/25/26  | 0/3/3/3 |
| 1   | 5MC  | 16SA  | 2028 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 16SA  | 1590 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | 5MU  | ASIA  | 54   | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 27  | 5MC  | 23SA  | 1967 | 27    | -       | 0/7/25/26  | 0/2/2/2 |
| 27  | OMU  | 23SB  | 2567 | 58,27 | -       | 2/9/27/28  | 0/2/2/2 |
| 22  | PSU  | ASIA  | 32   | 22    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | MA6  | 16SA  | 2141 | 1     | -       | 0/11/29/30 | 0/3/3/3 |
| 1   | UR3  | 16SB  | 2121 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 27  | 5MU  | 23SA  | 1964 | 60,27 | -       | 2/7/25/26  | 0/2/2/2 |
| 27  | OMC  | 23SB  | 1945 | 27    | -       | 0/9/27/28  | 0/2/2/2 |
| 23  | PSU  | PSIB  | 39   | 23    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 16SB  | 2035 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 23  | H2U  | PSIB  | 16   | 23    | -       | 0/7/38/39  | 0/2/2/2 |
| 23  | 4SU  | PSIB  | 8    | 58,23 | -       | 2/7/25/26  | 0/2/2/2 |
| 12  | 0TD  | S12B  | 89   | 12    | -       | 3/7/12/14  | -       |
| 23  | PSU  | PSIA  | 39   | 23    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 16SA  | 1145 | 58,1  | -       | 0/7/25/26  | 0/2/2/2 |
| 22  | G7M  | ASIA  | 46   | 22    | -       | 2/7/25/26  | 0/3/3/3 |
| 1   | UR3  | 16SA  | 2121 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 26  | PSU  | TRNA  | 55   | 26    | -       | 0/7/25/26  | 0/2/2/2 |
| 23  | 4SU  | PSIA  | 8    | 23    | -       | 0/7/25/26  | 0/2/2/2 |
| 27  | OMU  | 23SA  | 2567 | 58,27 | -       | 0/9/27/28  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link     | Chirals | Torsions   | Rings   |
|-----|------|-------|------|----------|---------|------------|---------|
| 23  | 3AU  | PSIA  | 47   | 23       | -       | 7/16/34/35 | 0/2/2/2 |
| 27  | 5MC  | 23SB  | 1987 | 60,27    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | M2G  | 16SB  | 1589 | 1        | -       | 0/11/29/30 | 0/3/3/3 |
| 1   | PSU  | 16SB  | 1145 | 58,1     | -       | 0/7/25/26  | 0/2/2/2 |
| 57  | PSU  | ASIB  | 32   | 57       | -       | 0/7/25/26  | 0/2/2/2 |
| 27  | 5MC  | 23SB  | 1967 | 27       | -       | 0/7/25/26  | 0/2/2/2 |
| 27  | PSU  | 23SB  | 1936 | 27       | -       | 0/7/25/26  | 0/2/2/2 |
| 27  | OMG  | 23SB  | 2266 | 60,27,23 | -       | 1/9/27/28  | 0/3/3/3 |
| 27  | 5MU  | 23SA  | 1940 | 27       | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 16SB  | 2032 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 4OC  | 16SA  | 2030 | 1        | -       | 2/9/29/30  | 0/2/2/2 |
| 27  | OMC  | 23SA  | 1945 | 60,27    | -       | 1/9/27/28  | 0/2/2/2 |
| 27  | PSU  | 23SB  | 2620 | 27       | -       | 0/7/25/26  | 0/2/2/2 |
| 26  | 4SU  | TRNA  | 8    | 26       | -       | 2/7/25/26  | 0/2/2/2 |
| 12  | 0TD  | S12A  | 89   | 12       | -       | 2/7/12/14  | -       |
| 23  | PSU  | PSIB  | 32   | 23       | -       | 0/7/25/26  | 0/2/2/2 |
| 23  | MIA  | PSIB  | 37   | 23       | -       | 6/15/33/34 | 0/3/3/3 |
| 1   | 5MC  | 16SA  | 2035 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 23  | 5MU  | PSIA  | 54   | 23       | -       | 0/7/25/26  | 0/2/2/2 |
| 57  | 5MU  | ASIB  | 54   | 57       | -       | 0/7/25/26  | 0/2/2/2 |
| 57  | PSU  | ASIB  | 39   | 57       | -       | 0/7/25/26  | 0/2/2/2 |
| 23  | 3AU  | PSIB  | 47   | 23       | -       | 7/16/34/35 | 0/2/2/2 |
| 27  | 2MA  | 23SB  | 2518 | 58,60,27 | -       | 3/7/25/26  | 0/3/3/3 |
| 22  | PSU  | ASIA  | 39   | 22       | -       | 0/7/25/26  | 0/2/2/2 |
| 26  | PSU  | TRNA  | 32   | 26       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 4OC  | 16SB  | 2030 | 58,1     | -       | 2/9/29/30  | 0/2/2/2 |
| 1   | M2G  | 16SA  | 1589 | 1        | -       | 0/11/29/30 | 0/3/3/3 |
| 1   | MA6  | 16SB  | 2142 | 1        | -       | 3/11/29/30 | 0/3/3/3 |
| 1   | MA6  | 16SA  | 2142 | 1        | -       | 3/11/29/30 | 0/3/3/3 |
| 27  | 5MU  | 23SB  | 1940 | 27       | -       | 0/7/25/26  | 0/2/2/2 |
| 23  | H2U  | PSIA  | 16   | 23       | -       | 0/7/38/39  | 0/2/2/2 |
| 27  | PSU  | 23SB  | 1942 | 27       | -       | 0/7/25/26  | 0/2/2/2 |

The worst 5 of 429 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23  | PSIB  | 46   | G7M  | C8-N7 | 18.74 | 1.65        | 1.33     |
| 22  | ASIA  | 46   | G7M  | C8-N7 | 18.53 | 1.64        | 1.33     |
| 1   | 16SB  | 1156 | G7M  | C8-N7 | 18.48 | 1.64        | 1.33     |
| 23  | PSIA  | 46   | G7M  | C8-N7 | 18.38 | 1.64        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | 16SA  | 1156 | G7M  | C8-N7 | 18.31 | 1.64        | 1.33     |

The worst 5 of 578 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 24  | ESIB  | 37   | MIA  | C11-S10-C2 | 15.30  | 113.73      | 102.25   |
| 26  | TRNA  | 37   | MIA  | C5-C4-N3   | -13.66 | 112.79      | 127.18   |
| 26  | TRNA  | 37   | MIA  | N3-C4-N9   | 12.69  | 143.09      | 126.99   |
| 1   | 16SB  | 1156 | G7M  | CN7-N7-C5  | 12.30  | 142.13      | 126.80   |
| 22  | ASIA  | 46   | G7M  | CN7-N7-C5  | 12.18  | 141.98      | 126.80   |

There are no chirality outliers.

5 of 116 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | 16SA  | 1156 | G7M  | O4'-C4'-C5'-O5' |
| 1   | 16SA  | 2142 | MA6  | O4'-C4'-C5'-O5' |
| 12  | S12A  | 89   | 0TD  | CG-CB-SB-CSB    |
| 22  | ASIA  | 37   | MIA  | O4'-C4'-C5'-O5' |
| 22  | ASIA  | 37   | MIA  | C12-C13-C14-C15 |

There are no ring outliers.

1 monomer is involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 26  | TRNA  | 37  | MIA  | 0       | 4            |

## 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 4.6 Ligand geometry [i](#)

Of 1698 ligands modelled in this entry, 1077 are monoatomic - leaving 621 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 59  | OHX  | 16SB  | 2217 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3132 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3350 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 16SB  | 2248 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3100 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3272 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 16SB  | 2228 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 16SB  | 2267 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3367 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 16SA  | 2322 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3234 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3247 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3056 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 16SA  | 2275 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3081 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3088 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 16SA  | 2324 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 16SA  | 2311 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 16SB  | 2261 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3075 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3262 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3117 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3194 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3336 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3375 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 16SA  | 2288 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 16SB  | 2237 | 1    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3208 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3280 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3382 | -    | 0,6,6        | -    | -           | -           |      |             |
| 61  | SJE  | 23SA  | 3640 | -    | 88,91,91     | 4.09 | 26 (29%)    | 118,134,134 | 2.03 | 28 (23%)    |
| 59  | OHX  | 23SB  | 3045 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 5SB   | 211  | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3111 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 16SA  | 2341 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3344 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 16SA  | 2272 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3028 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3179 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3221 | -    | 0,6,6        | -    | -           | -           |      |             |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 59  | OHX  | S10A  | 201  | 1    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3235 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3366 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3225 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3027 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | PSIB  | 102  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2328 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3118 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2224 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2241 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2222 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3303 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2300 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3195 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3073 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3250 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3339 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2203 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3018 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3201 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3237 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3069 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3302 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3211 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | L4A   | 302  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3227 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | ASIA  | 102  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2265 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2225 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 5SA   | 207  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3223 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3087 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3187 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3148 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3177 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3195 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3325 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3057 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3082 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3169 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3364 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3053 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | MRNB  | 101  | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 59  | OHX  | 23SB  | 3015 | 27   | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2291 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 5SB   | 206  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2299 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3306 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3121 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3219 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3022 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3182 | 27   | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2211 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2205 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3086 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3220 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3183 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2337 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3282 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3023 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3193 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 5SA   | 209  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3158 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3352 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3379 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3226 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2334 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2223 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3189 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3157 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3335 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3048 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3060 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3012 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3084 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2275 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3212 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3186 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3304 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3290 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3149 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | L15A  | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3194 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | L17B  | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3070 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3155 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 59  | OHX  | 23SA  | 3213 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3200 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3108 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3188 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3196 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3299 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3095 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3274 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3041 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3380 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2260 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3089 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3363 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 5SA   | 211  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3256 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3214 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3310 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3029 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3008 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3035 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3273 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3168 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2326 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3093 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3099 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2298 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2312 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3196 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3362 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | L35B  | 101  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2318 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3033 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2214 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2209 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2202 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2302 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3202 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3333 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3318 | 27   | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3266 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3269 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3378 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3183 | 27   | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 59  | OHX  | 16SA  | 2267 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3359 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3170 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2272 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3197 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2262 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2310 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3358 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2321 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2213 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2240 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3245 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3098 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3186 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3078 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3232 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | ASIB  | 102  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3040 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3271 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3046 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3309 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3361 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2212 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3120 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3024 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3268 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3171 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3349 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3374 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3284 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3146 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | ASIA  | 101  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3156 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 5SA   | 208  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2226 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3181 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2323 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3338 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3019 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3124 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3017 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3175 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3210 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 59  | OHX  | 16SB  | 2210 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2249 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3127 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | S14B  | 101  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3229 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3179 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3332 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | L4B   | 301  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3216 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2287 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3207 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3373 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2221 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3135 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3311 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 5SB   | 204  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3275 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3327 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3296 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3365 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3203 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2254 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3110 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | TRNA  | 102  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3114 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2273 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 5SA   | 205  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3036 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2278 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3292 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3356 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2278 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3184 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | ESIB  | 101  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3167 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | S19A  | 101  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2250 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2308 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | ESIA  | 101  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3206 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3067 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3300 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3125 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 59  | OHX  | 16SB  | 2266 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3289 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2236 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3025 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3259 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3162 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2233 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2263 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3368 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3279 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2294 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3371 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3077 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3139 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | S4A   | 301  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3267 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3004 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3324 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2245 | 1    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3376 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2229 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3113 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 5SA   | 210  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3116 | 27   | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3054 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2252 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3051 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3287 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3381 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2274 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3109 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2305 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2338 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3096 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | L28A  | 101  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3319 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3058 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2329 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3005 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2295 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2336 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3163 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2231 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 59  | OHX  | 16SA  | 2280 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3360 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3316 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3218 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2290 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3285 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3312 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3107 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3126 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2320 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2335 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3255 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3134 | -    | 0,6,6        | -    | -        | -           |      |          |
| 61  | SJE  | 23SB  | 3521 | -    | 88,91,91     | 4.07 | 22 (25%) | 118,134,134 | 2.01 | 23 (19%) |
| 59  | OHX  | 23SB  | 3034 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3277 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3343 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3080 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | ASIA  | 103  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | L27A  | 102  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | L20B  | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3191 | 27   | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3151 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3115 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3278 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2325 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | MRNA  | 101  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3141 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2282 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3003 | 27   | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3123 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2307 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3128 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2303 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3283 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 5SA   | 214  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2277 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2301 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2230 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3043 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3129 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2313 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3261 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 59  | OHX  | 23SA  | 3314 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | ASIB  | 103  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3131 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2273 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2279 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3248 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 5SA   | 212  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | PSIB  | 101  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3301 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3049 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3076 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3313 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3143 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 5SB   | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3236 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3199 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3133 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3260 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2281 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3026 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3153 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3230 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2293 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3251 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3182 | 27   | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3065 | 62   | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3369 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2271 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 5SB   | 207  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3037 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3209 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3105 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3104 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3150 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3083 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3293 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2208 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3106 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3185 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2296 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2330 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3265 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3323 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 59  | OHX  | 23SB  | 3119 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | TRNA  | 101  | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3145 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3228 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3192 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 16SA  | 2333 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 16SB  | 2234 | 1    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 16SB  | 2274 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3347 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3264 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 16SA  | 2262 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3346 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3011 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3122 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3174 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3052 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3345 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3291 | 27   | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3370 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3039 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3064 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3217 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3021 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3281 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 16SB  | 2204 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3224 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3322 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3002 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3328 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3197 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3342 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3136 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 5SB   | 208  | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3091 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 5SA   | 213  | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3340 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | S4B   | 301  | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | L19A  | 201  | 41   | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 16SB  | 2239 | 1    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3198 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SA  | 3353 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 23SB  | 3112 | -    | 0,6,6        | -    | -           | -           |      |             |
| 59  | OHX  | 5SA   | 206  | -    | 0,6,6        | -    | -           | -           |      |             |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 59  | OHX  | 16SB  | 2215 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2235 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3239 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3166 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3348 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2268 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3032 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3137 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3341 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3331 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3062 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2309 | 1    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2286 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3044 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3190 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3038 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3377 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3242 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3059 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2317 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2201 | 1    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3016 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2263 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2216 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2206 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2264 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3193 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2266 | 1    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3204 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3187 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2283 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2314 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2292 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | L35A  | 102  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3320 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3102 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2246 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3101 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3007 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3142 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3298 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3013 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3263 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 59  | OHX  | L20A  | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2227 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3161 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 5SB   | 209  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3253 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 5SB   | 205  | 28   | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2256 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2261 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2244 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2306 | 1    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2340 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | PSIA  | 102  | 23   | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3286 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3205 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3351 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3326 | 27   | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2269 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3144 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3354 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3042 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3090 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2258 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2270 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3180 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3330 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3072 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3241 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2339 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2327 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3249 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3184 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3317 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3329 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3020 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3321 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3164 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3159 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3308 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2253 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3238 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3178 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3001 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2284 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 59  | OHX  | 23SA  | 3246 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3010 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | L17A  | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3192 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3188 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3337 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3165 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2276 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2304 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | ASIB  | 101  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | L27A  | 103  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2265 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3270 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3231 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2255 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2277 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3130 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3372 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3050 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3258 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2289 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3189 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3185 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3097 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3030 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3222 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3357 | 27   | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3176 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2268 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3244 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3031 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2285 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3257 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2319 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3009 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3154 | 27   | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 5SB   | 210  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3079 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2271 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3180 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3355 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3191 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3147 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 59  | OHX  | 23SA  | 3305 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2232 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2260 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2242 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3160 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3103 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2264 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3294 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3071 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2297 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2259 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3243 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3254 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 5SB   | 203  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3172 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2332 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3240 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2219 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3252 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3295 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3094 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3068 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 5SB   | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2251 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3063 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3181 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2207 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2243 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3199 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3334 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 5SA   | 204  | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2218 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3178 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3297 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3066 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3074 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3173 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3061 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3215 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3047 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3140 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2269 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3152 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 59  | OHX  | 16SA  | 2316 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3307 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2257 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3014 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2270 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3288 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3198 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3315 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3138 | 27   | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3006 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3233 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3055 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3276 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2276 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2238 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2220 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2315 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SA  | 2331 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 16SB  | 2247 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3092 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SB  | 3085 | -    | 0,6,6        | -    | -        | -           |      |          |
| 59  | OHX  | 23SA  | 3190 | 27   | 0,6,6        | -    | -        | -           |      |          |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|------|------|---------|----------------|---------|
| 61  | SJE  | 23SA  | 3640 | -    | -       | 41/101/161/161 | 0/5/5/5 |
| 61  | SJE  | 23SB  | 3521 | -    | -       | 41/101/161/161 | 0/5/5/5 |

The worst 5 of 48 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 61  | 23SA  | 3640 | SJE  | O81-S78 | 20.31 | 1.67        | 1.43     |
| 61  | 23SB  | 3521 | SJE  | O79-S78 | 20.16 | 1.66        | 1.43     |
| 61  | 23SB  | 3521 | SJE  | O81-S78 | 20.07 | 1.66        | 1.43     |
| 61  | 23SA  | 3640 | SJE  | O79-S78 | 19.86 | 1.66        | 1.43     |
| 61  | 23SB  | 3521 | SJE  | O86-N85 | 11.01 | 1.41        | 1.22     |

The worst 5 of 51 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 61  | 23SA  | 3640 | SJE  | O81-S78-O79 | -10.71 | 106.52      | 119.52   |
| 61  | 23SB  | 3521 | SJE  | O81-S78-O79 | -9.47  | 108.02      | 119.52   |
| 61  | 23SA  | 3640 | SJE  | O49-C70-N84 | 6.76   | 119.59      | 110.00   |
| 61  | 23SB  | 3521 | SJE  | C18-C17-C16 | 6.32   | 119.28      | 109.15   |
| 61  | 23SB  | 3521 | SJE  | O49-C70-N84 | 6.32   | 118.97      | 110.00   |

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 61  | 23SA  | 3640 | SJE  | C21-C20-O19-C35 |
| 61  | 23SA  | 3640 | SJE  | O22-C20-O19-C35 |
| 61  | 23SA  | 3640 | SJE  | C28-C26-C35-O19 |
| 61  | 23SA  | 3640 | SJE  | C41-C26-C35-O19 |
| 61  | 23SA  | 3640 | SJE  | C42-C27-C28-C26 |

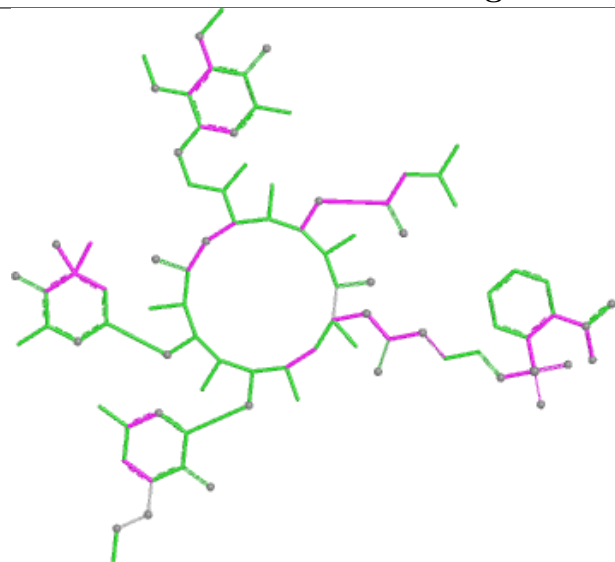
There are no ring outliers.

1 monomer is involved in 2 short contacts:

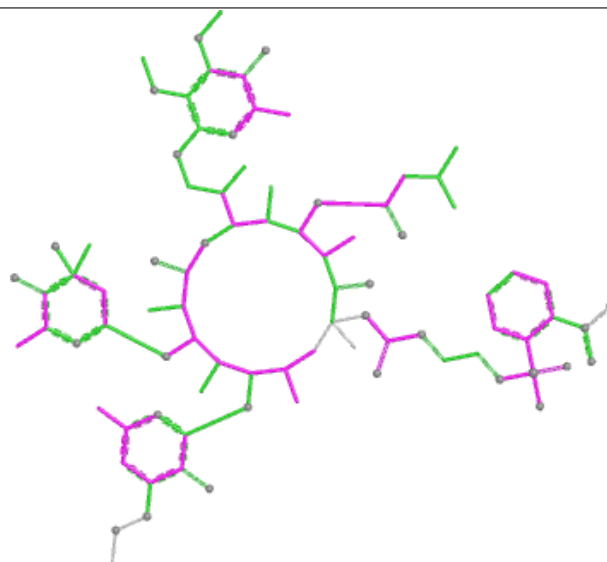
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 59  | 23SA  | 3304 | OHX  | 0       | 2            |

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

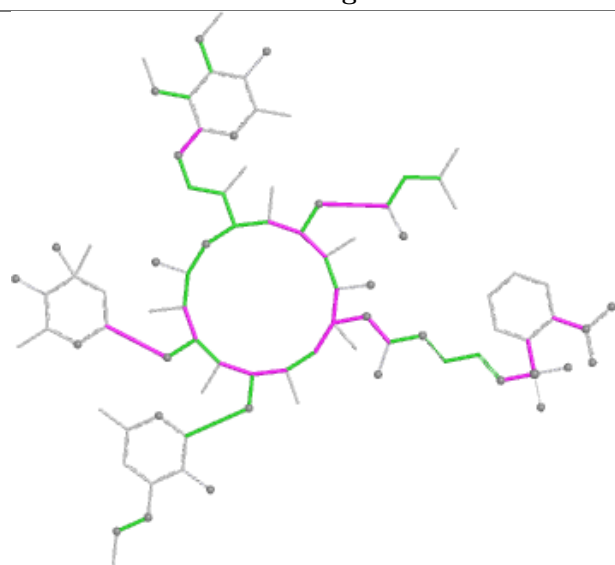
## Ligand SJE 23SA 3640



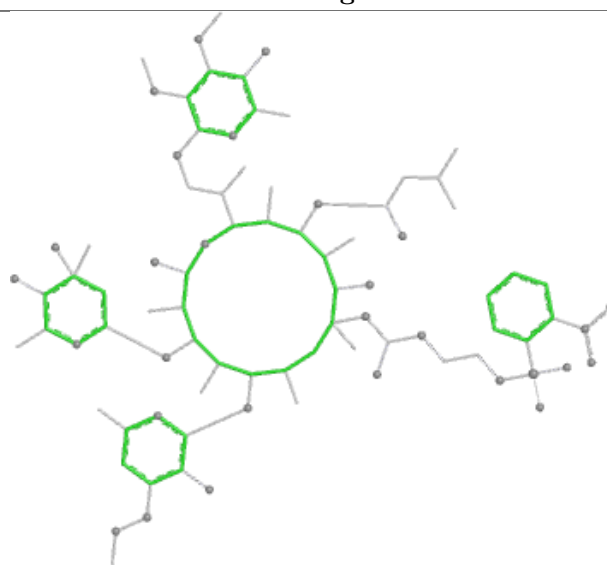
Bond lengths



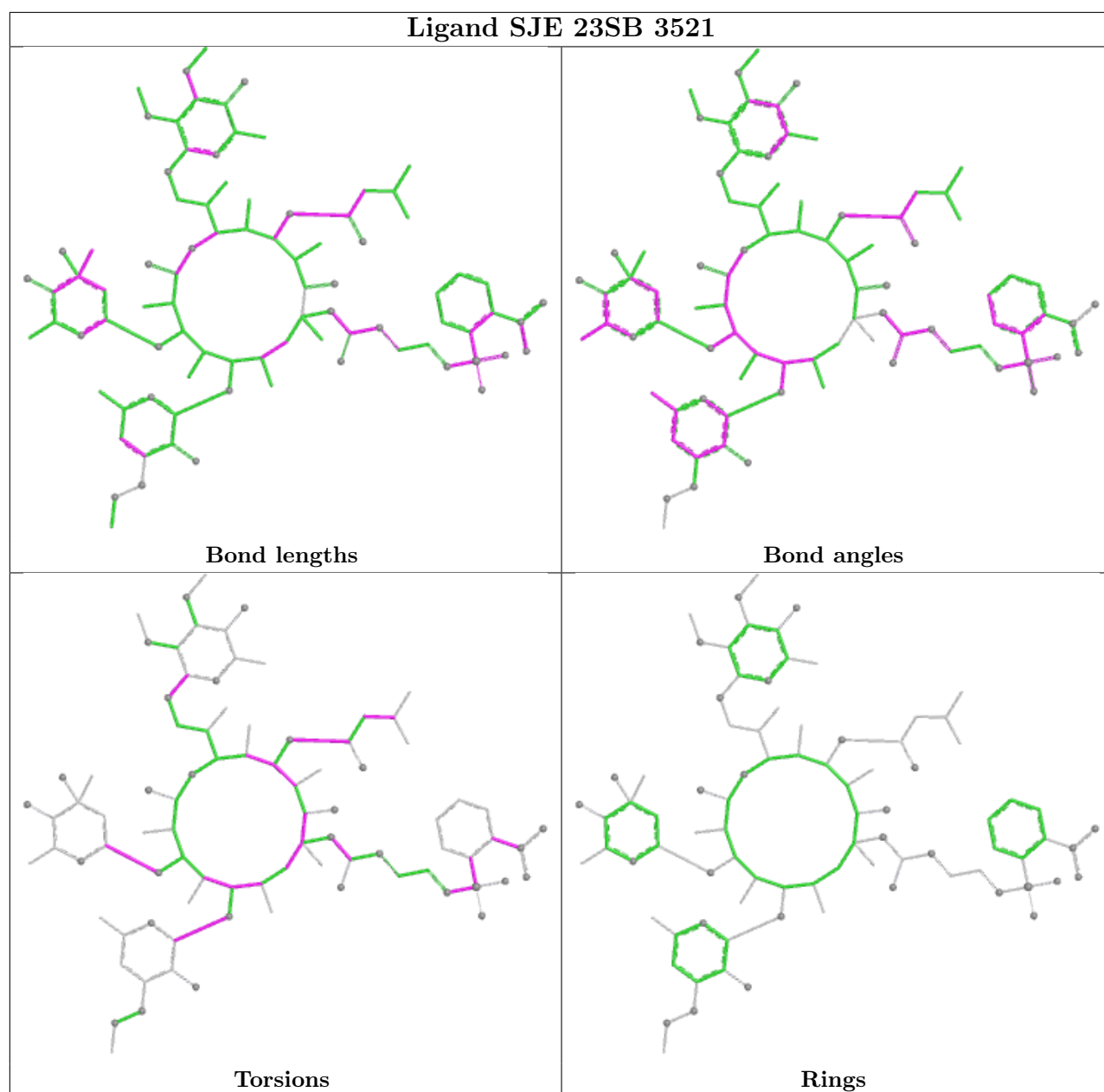
Bond angles



Torsions



Rings



#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 5 Fit of model and data ⓘ

### 5.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | 16SA  | 1500/1512 (99%) | -0.43  | 4 (0%) 90 82  | 45, 89, 170, 260      | 0     |
| 1   | 16SB  | 1496/1512 (98%) | -0.61  | 2 (0%) 92 90  | 57, 100, 164, 267     | 0     |
| 2   | S2A   | 237/256 (92%)   | 0.57   | 10 (4%) 40 26 | 91, 125, 164, 178     | 0     |
| 2   | S2B   | 237/256 (92%)   | 0.73   | 12 (5%) 33 22 | 105, 153, 186, 205    | 0     |
| 3   | S3A   | 205/239 (85%)   | 0.58   | 6 (2%) 53 35  | 80, 100, 141, 168     | 0     |
| 3   | S3B   | 206/239 (86%)   | 0.50   | 8 (3%) 43 29  | 104, 128, 157, 161    | 0     |
| 4   | S4A   | 208/209 (99%)   | 0.60   | 14 (6%) 24 16 | 75, 97, 119, 128      | 0     |
| 4   | S4B   | 208/209 (99%)   | 0.71   | 14 (6%) 24 16 | 79, 96, 117, 138      | 0     |
| 5   | S5A   | 151/162 (93%)   | 0.47   | 4 (2%) 57 38  | 65, 87, 108, 132      | 0     |
| 5   | S5B   | 151/162 (93%)   | 0.39   | 4 (2%) 57 38  | 86, 105, 123, 151     | 0     |
| 6   | S6A   | 101/101 (100%)  | 0.52   | 3 (2%) 52 35  | 70, 91, 107, 124      | 0     |
| 6   | S6B   | 101/101 (100%)  | 0.58   | 6 (5%) 28 19  | 73, 94, 109, 132      | 0     |
| 7   | S7A   | 155/156 (99%)   | 0.30   | 7 (4%) 38 25  | 90, 105, 129, 138     | 0     |
| 7   | S7B   | 155/156 (99%)   | 0.21   | 2 (1%) 75 56  | 30, 115, 151, 175     | 0     |
| 8   | S8A   | 138/138 (100%)  | 0.15   | 0 100 100     | 75, 92, 104, 114      | 0     |
| 8   | S8B   | 138/138 (100%)  | -0.05  | 1 (0%) 84 70  | 83, 104, 115, 125     | 0     |
| 9   | S9A   | 127/128 (99%)   | 0.23   | 5 (3%) 43 29  | 72, 121, 140, 144     | 0     |
| 9   | S9B   | 127/128 (99%)   | -0.13  | 1 (0%) 82 68  | 77, 136, 152, 156     | 0     |
| 10  | S10A  | 99/105 (94%)    | 0.28   | 5 (5%) 33 22  | 72, 124, 151, 154     | 0     |
| 10  | S10B  | 99/105 (94%)    | 0.20   | 1 (1%) 79 63  | 104, 144, 159, 166    | 0     |
| 11  | S11A  | 116/129 (89%)   | 0.41   | 2 (1%) 69 50  | 63, 90, 113, 142      | 0     |
| 11  | S11B  | 117/129 (90%)   | 0.28   | 5 (4%) 40 25  | 76, 97, 122, 156      | 0     |
| 12  | S12A  | 124/132 (93%)   | 0.55   | 10 (8%) 18 13 | 57, 66, 98, 162       | 0     |
| 12  | S12B  | 124/132 (93%)   | 0.60   | 11 (8%) 15 12 | 69, 86, 112, 167      | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13  | S13A  | 119/126 (94%)   | 0.37   | 8 (6%) 24 16  | 77, 113, 129, 138     | 0     |
| 13  | S13B  | 121/126 (96%)   | 0.20   | 5 (4%) 41 27  | 100, 138, 150, 159    | 0     |
| 14  | S14A  | 60/61 (98%)     | 0.21   | 1 (1%) 69 50  | 78, 90, 103, 117      | 0     |
| 14  | S14B  | 59/61 (96%)     | 0.11   | 1 (1%) 69 50  | 106, 119, 143, 146    | 0     |
| 15  | S15A  | 88/89 (98%)     | 0.13   | 0 100 100     | 65, 84, 108, 115      | 0     |
| 15  | S15B  | 88/89 (98%)     | -0.10  | 0 100 100     | 73, 96, 112, 119      | 0     |
| 16  | S16A  | 83/88 (94%)     | 0.32   | 3 (3%) 46 31  | 86, 98, 118, 146      | 0     |
| 16  | S16B  | 84/88 (95%)     | 0.20   | 1 (1%) 76 58  | 79, 88, 106, 144      | 0     |
| 17  | S17A  | 100/105 (95%)   | 0.17   | 2 (2%) 65 46  | 74, 90, 101, 104      | 0     |
| 17  | S17B  | 100/105 (95%)   | 0.09   | 2 (2%) 65 46  | 80, 97, 114, 126      | 0     |
| 18  | S18A  | 71/88 (80%)     | 0.50   | 4 (5%) 30 20  | 72, 88, 121, 148      | 0     |
| 18  | S18B  | 70/88 (79%)     | 0.54   | 3 (4%) 40 25  | 80, 97, 125, 148      | 0     |
| 19  | S19A  | 84/93 (90%)     | 0.77   | 10 (11%) 9 7  | 30, 114, 133, 139     | 0     |
| 19  | S19B  | 86/93 (92%)     | 0.43   | 7 (8%) 18 13  | 125, 151, 177, 188    | 0     |
| 20  | S20A  | 99/106 (93%)    | 0.27   | 1 (1%) 79 63  | 58, 105, 133, 139     | 0     |
| 20  | S20B  | 99/106 (93%)    | -0.03  | 1 (1%) 79 63  | 60, 103, 127, 133     | 0     |
| 21  | THXA  | 24/27 (88%)     | -0.19  | 0 100 100     | 92, 102, 114, 129     | 0     |
| 21  | THXB  | 25/27 (92%)     | -0.10  | 0 100 100     | 113, 127, 143, 148    | 0     |
| 22  | ASIA  | 69/76 (90%)     | 1.90   | 30 (43%) 0 0  | 71, 185, 223, 237     | 0     |
| 23  | PSIA  | 67/76 (88%)     | 0.28   | 6 (8%) 15 11  | 62, 86, 106, 154      | 0     |
| 23  | PSIB  | 67/76 (88%)     | 0.01   | 3 (4%) 38 25  | 73, 103, 134, 167     | 0     |
| 24  | ESIA  | 75/76 (98%)     | 0.78   | 8 (10%) 11 9  | 61, 191, 216, 221     | 0     |
| 24  | ESIB  | 75/76 (98%)     | 0.26   | 0 100 100     | 72, 196, 221, 233     | 0     |
| 25  | MRNA  | 30/30 (100%)    | 0.98   | 5 (16%) 4 4   | 60, 150, 238, 250     | 0     |
| 25  | MRNB  | 30/30 (100%)    | 0.25   | 2 (6%) 24 16  | 79, 168, 237, 243     | 0     |
| 26  | TRNA  | 65/76 (85%)     | 0.38   | 3 (4%) 37 25  | 106, 176, 202, 216    | 0     |
| 27  | 23SA  | 2878/2911 (98%) | -0.72  | 13 (0%) 87 76 | 33, 60, 190, 262      | 0     |
| 27  | 23SB  | 2862/2911 (98%) | -0.50  | 20 (0%) 84 70 | 40, 76, 213, 270      | 0     |
| 28  | 5SA   | 122/124 (98%)   | -0.77  | 0 100 100     | 57, 76, 92, 167       | 0     |
| 28  | 5SB   | 121/124 (97%)   | -0.44  | 1 (0%) 82 68  | 80, 105, 137, 192     | 0     |
| 29  | L2A   | 272/276 (98%)   | -0.07  | 0 100 100     | 35, 52, 68, 81        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 29  | L2B   | 272/276 (98%)  | -0.11  | 2 (0%) 84 70  | 41, 62, 81, 92        | 0     |
| 30  | L3A   | 204/206 (99%)  | 0.05   | 4 (1%) 65 46  | 41, 68, 95, 114       | 0     |
| 30  | L3B   | 204/206 (99%)  | 0.54   | 12 (5%) 28 19 | 49, 86, 115, 128      | 0     |
| 31  | L4A   | 202/210 (96%)  | -0.18  | 2 (0%) 79 63  | 35, 64, 94, 117       | 0     |
| 31  | L4B   | 202/210 (96%)  | 0.28   | 7 (3%) 47 31  | 48, 85, 113, 129      | 0     |
| 32  | L5A   | 181/182 (99%)  | 0.17   | 2 (1%) 78 60  | 70, 87, 114, 130      | 0     |
| 32  | L5B   | 181/182 (99%)  | 0.26   | 3 (1%) 69 50  | 100, 119, 142, 152    | 0     |
| 33  | L6A   | 171/180 (95%)  | 0.82   | 14 (8%) 17 13 | 30, 94, 113, 136      | 0     |
| 33  | L6B   | 173/180 (96%)  | 2.07   | 86 (49%) 0 0  | 154, 201, 242, 260    | 0     |
| 34  | L9A   | 145/148 (97%)  | 1.00   | 24 (16%) 4 4  | 61, 116, 131, 146     | 0     |
| 34  | L9B   | 146/148 (98%)  | 1.07   | 31 (21%) 2 2  | 75, 116, 137, 150     | 0     |
| 35  | L13A  | 138/140 (98%)  | 0.15   | 4 (2%) 53 35  | 51, 70, 102, 112      | 0     |
| 35  | L13B  | 138/140 (98%)  | 1.22   | 24 (17%) 4 4  | 68, 101, 130, 136     | 0     |
| 36  | L14A  | 122/122 (100%) | 0.24   | 3 (2%) 58 39  | 44, 62, 75, 84        | 0     |
| 36  | L14B  | 122/122 (100%) | 0.60   | 4 (3%) 49 33  | 62, 81, 101, 112      | 0     |
| 37  | L15A  | 150/150 (100%) | -0.08  | 0 100 100     | 38, 69, 99, 141       | 0     |
| 37  | L15B  | 150/150 (100%) | 0.05   | 2 (1%) 75 56  | 49, 95, 127, 145      | 0     |
| 38  | L16A  | 141/141 (100%) | 0.26   | 6 (4%) 40 25  | 48, 66, 89, 120       | 0     |
| 38  | L16B  | 141/141 (100%) | 0.39   | 7 (4%) 34 23  | 58, 73, 93, 123       | 0     |
| 39  | L17A  | 118/118 (100%) | -0.20  | 1 (0%) 82 68  | 49, 66, 85, 94        | 0     |
| 39  | L17B  | 118/118 (100%) | -0.00  | 0 100 100     | 57, 75, 94, 111       | 0     |
| 40  | L18A  | 112/112 (100%) | 0.12   | 1 (0%) 81 65  | 57, 72, 99, 115       | 0     |
| 40  | L18B  | 111/112 (99%)  | 0.02   | 0 100 100     | 73, 104, 141, 150     | 0     |
| 41  | L19A  | 137/146 (93%)  | 0.28   | 2 (1%) 72 53  | 56, 73, 129, 158      | 0     |
| 41  | L19B  | 137/146 (93%)  | 0.48   | 4 (2%) 53 35  | 72, 90, 167, 185      | 0     |
| 42  | L20A  | 117/118 (99%)  | -0.28  | 1 (0%) 81 65  | 43, 60, 88, 115       | 0     |
| 42  | L20B  | 117/118 (99%)  | 0.80   | 21 (17%) 3 3  | 57, 94, 136, 149      | 0     |
| 43  | L21A  | 101/101 (100%) | 0.05   | 1 (0%) 79 63  | 44, 81, 98, 110       | 0     |
| 43  | L21B  | 101/101 (100%) | 1.59   | 31 (30%) 1 1  | 58, 112, 128, 142     | 0     |
| 44  | L22A  | 113/113 (100%) | -0.33  | 1 (0%) 81 65  | 43, 57, 88, 128       | 0     |
| 44  | L22B  | 113/113 (100%) | 0.33   | 4 (3%) 47 31  | 52, 65, 114, 147      | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 45  | L23A  | 93/96 (96%)       | -0.21  | 0 100 100      | 44, 57, 75, 98        | 0     |
| 45  | L23B  | 94/96 (97%)       | 0.07   | 2 (2%) 63 44   | 58, 73, 98, 121       | 0     |
| 46  | L24A  | 108/110 (98%)     | 0.16   | 2 (1%) 66 48   | 61, 87, 135, 151      | 0     |
| 46  | L24B  | 106/110 (96%)     | 1.01   | 15 (14%) 6 5   | 66, 99, 145, 153      | 0     |
| 47  | L25A  | 179/206 (86%)     | 0.53   | 11 (6%) 27 18  | 70, 104, 181, 189     | 0     |
| 47  | L25B  | 176/206 (85%)     | 0.86   | 11 (6%) 26 17  | 107, 145, 224, 228    | 0     |
| 48  | L27A  | 84/85 (98%)       | -0.09  | 1 (1%) 76 58   | 45, 59, 84, 104       | 0     |
| 48  | L27B  | 84/85 (98%)       | 0.02   | 4 (4%) 35 24   | 63, 79, 100, 128      | 0     |
| 49  | L28A  | 97/98 (98%)       | 0.25   | 7 (7%) 21 15   | 43, 63, 110, 132      | 0     |
| 49  | L28B  | 97/98 (98%)       | 0.28   | 4 (4%) 41 27   | 52, 75, 118, 132      | 0     |
| 50  | L29A  | 69/72 (95%)       | 0.13   | 0 100 100      | 50, 66, 81, 105       | 0     |
| 50  | L29B  | 71/72 (98%)       | 0.17   | 2 (2%) 55 36   | 70, 89, 109, 138      | 0     |
| 51  | L30A  | 59/60 (98%)       | -0.16  | 0 100 100      | 48, 66, 96, 115       | 0     |
| 51  | L30B  | 59/60 (98%)       | 0.54   | 2 (3%) 48 32   | 69, 90, 130, 146      | 0     |
| 52  | L31A  | 71/71 (100%)      | 0.61   | 3 (4%) 40 26   | 95, 137, 172, 175     | 0     |
| 52  | L31B  | 71/71 (100%)      | 0.27   | 0 100 100      | 123, 160, 188, 194    | 0     |
| 53  | L32A  | 56/60 (93%)       | -0.14  | 2 (3%) 46 31   | 38, 70, 126, 133      | 0     |
| 53  | L32B  | 56/60 (93%)       | 0.60   | 3 (5%) 31 21   | 47, 78, 139, 150      | 0     |
| 54  | L33A  | 45/54 (83%)       | 1.52   | 12 (26%) 1 1   | 106, 130, 157, 160    | 0     |
| 54  | L33B  | 45/54 (83%)       | 0.54   | 0 100 100      | 129, 157, 182, 188    | 0     |
| 55  | L34A  | 48/49 (97%)       | -0.43  | 1 (2%) 63 44   | 37, 42, 57, 78        | 0     |
| 55  | L34B  | 49/49 (100%)      | -0.21  | 1 (2%) 65 46   | 42, 51, 97, 109       | 0     |
| 56  | L35A  | 64/65 (98%)       | -0.36  | 1 (1%) 70 52   | 38, 54, 71, 93        | 0     |
| 56  | L35B  | 64/65 (98%)       | 0.03   | 0 100 100      | 30, 70, 91, 116       | 0     |
| 57  | ASIB  | 72/76 (94%)       | 0.79   | 10 (13%) 6 5   | 98, 216, 254, 258     | 0     |
| All | All   | 21108/21740 (97%) | -0.04  | 675 (3%) 50 34 | 30, 88, 176, 270      | 0     |

The worst 5 of 675 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 33  | L6B   | 72  | ILE  | 7.5  |
| 4   | S4A   | 9   | CYS  | 6.4  |
| 34  | L9A   | 129 | THR  | 6.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 22  | ASIA  | 1   | G    | 6.2  |
| 12  | S12A  | 44  | LYS  | 6.0  |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 26  | H2U  | TRNA  | 16   | 20/21 | 0.50 | 0.12 | 145,157,174,175            | 0     |
| 23  | H2U  | PSIB  | 16   | 20/21 | 0.60 | 0.12 | 109,134,154,162            | 0     |
| 26  | PSU  | TRNA  | 32   | 20/21 | 0.63 | 0.11 | 182,188,194,195            | 0     |
| 26  | H2U  | TRNA  | 20   | 20/21 | 0.63 | 0.10 | 145,163,173,181            | 0     |
| 22  | PSU  | ASIA  | 55   | 20/21 | 0.67 | 0.12 | 146,160,172,173            | 0     |
| 26  | PSU  | TRNA  | 55   | 20/21 | 0.67 | 0.09 | 143,151,170,173            | 0     |
| 26  | 4SU  | TRNA  | 8    | 20/21 | 0.67 | 0.12 | 169,174,178,181            | 0     |
| 26  | PSU  | TRNA  | 39   | 20/21 | 0.68 | 0.10 | 134,167,176,179            | 0     |
| 57  | 5MU  | ASIB  | 54   | 21/22 | 0.68 | 0.13 | 145,183,189,193            | 0     |
| 23  | 3AU  | PSIB  | 47   | 27/28 | 0.69 | 0.13 | 127,146,156,158            | 0     |
| 23  | 5MU  | PSIB  | 54   | 21/22 | 0.71 | 0.11 | 102,108,115,117            | 0     |
| 26  | 5MU  | TRNA  | 54   | 21/22 | 0.73 | 0.09 | 151,158,162,164            | 0     |
| 22  | 4SU  | ASIA  | 8    | 20/21 | 0.74 | 0.14 | 200,203,207,208            | 0     |
| 23  | PSU  | PSIB  | 55   | 20/21 | 0.76 | 0.10 | 100,105,112,112            | 0     |
| 24  | MIA  | ESIB  | 37   | 29/30 | 0.78 | 0.18 | 130,151,154,154            | 0     |
| 26  | MIA  | TRNA  | 37   | 29/30 | 0.79 | 0.17 | 115,135,154,162            | 0     |
| 23  | G7M  | PSIB  | 46   | 24/25 | 0.81 | 0.10 | 109,119,139,142            | 0     |
| 23  | 4SU  | PSIB  | 8    | 20/21 | 0.81 | 0.10 | 101,106,116,120            | 0     |
| 22  | G7M  | ASIA  | 46   | 24/25 | 0.82 | 0.15 | 201,205,216,222            | 0     |
| 23  | PSU  | PSIA  | 55   | 20/21 | 0.84 | 0.09 | 84,89,100,103              | 0     |
| 23  | 3AU  | PSIA  | 47   | 27/28 | 0.84 | 0.14 | 94,118,133,135             | 0     |
| 22  | 5MU  | ASIA  | 54   | 21/22 | 0.85 | 0.12 | 113,137,147,148            | 0     |
| 1   | 2MG  | 16SB  | 1834 | 24/25 | 0.86 | 0.09 | 111,120,124,126            | 0     |
| 27  | 5MU  | 23SB  | 1940 | 21/22 | 0.87 | 0.10 | 85,92,102,106              | 0     |
| 57  | PSU  | ASIB  | 32   | 20/21 | 0.87 | 0.08 | 111,121,129,135            | 0     |
| 24  | MIA  | ESIA  | 37   | 29/30 | 0.87 | 0.14 | 120,144,148,150            | 0     |
| 12  | 0TD  | S12B  | 89   | 10/11 | 0.88 | 0.14 | 82,85,91,98                | 0     |
| 12  | 0TD  | S12A  | 89   | 10/11 | 0.89 | 0.17 | 59,65,68,72                | 0     |
| 57  | PSU  | ASIB  | 39   | 20/21 | 0.89 | 0.09 | 102,120,127,130            | 0     |
| 22  | PSU  | ASIA  | 39   | 20/21 | 0.89 | 0.14 | 77,88,95,99                | 0     |
| 23  | 5MU  | PSIA  | 54   | 21/22 | 0.90 | 0.09 | 88,91,100,107              | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 1   | M2G  | 16SB  | 1589 | 25/26 | 0.90 | 0.09 | 81,91,96,102                | 0     |
| 23  | G7M  | PSIA  | 46   | 24/25 | 0.91 | 0.11 | 77,88,112,114               | 0     |
| 23  | H2U  | PSIA  | 16   | 20/21 | 0.91 | 0.10 | 91,111,134,148              | 0     |
| 1   | PSU  | 16SB  | 1145 | 20/21 | 0.92 | 0.07 | 85,90,95,97                 | 0     |
| 1   | 4OC  | 16SB  | 2030 | 22/23 | 0.92 | 0.09 | 68,75,81,95                 | 0     |
| 27  | 5MC  | 23SB  | 1987 | 21/22 | 0.92 | 0.11 | 57,67,74,81                 | 0     |
| 1   | G7M  | 16SB  | 1156 | 24/25 | 0.92 | 0.10 | 78,83,90,91                 | 0     |
| 1   | PSU  | 16SA  | 1145 | 20/21 | 0.92 | 0.11 | 69,74,79,81                 | 0     |
| 1   | 5MC  | 16SB  | 1590 | 21/22 | 0.92 | 0.08 | 83,90,96,102                | 0     |
| 22  | PSU  | ASIA  | 32   | 20/21 | 0.93 | 0.11 | 82,90,97,98                 | 0     |
| 23  | PSU  | PSIA  | 32   | 20/21 | 0.93 | 0.08 | 67,71,75,79                 | 0     |
| 27  | OMU  | 23SB  | 2567 | 21/22 | 0.93 | 0.11 | 57,64,67,71                 | 0     |
| 1   | 5MC  | 16SB  | 2028 | 21/22 | 0.93 | 0.09 | 78,84,87,90                 | 0     |
| 27  | PSU  | 23SB  | 1936 | 20/21 | 0.93 | 0.07 | 72,79,83,85                 | 0     |
| 27  | 5MU  | 23SA  | 1940 | 21/22 | 0.93 | 0.11 | 60,67,75,81                 | 0     |
| 27  | PSU  | 23SB  | 1942 | 20/21 | 0.94 | 0.07 | 76,81,86,87                 | 0     |
| 22  | MIA  | ASIA  | 37   | 29/30 | 0.94 | 0.12 | 64,70,77,79                 | 0     |
| 27  | PSU  | 23SA  | 1936 | 20/21 | 0.94 | 0.11 | 57,59,62,70                 | 0     |
| 23  | PSU  | PSIB  | 32   | 20/21 | 0.94 | 0.08 | 86,91,97,102                | 0     |
| 57  | MIA  | ASIB  | 37   | 29/30 | 0.94 | 0.08 | 83,96,107,111               | 0     |
| 23  | PSU  | PSIB  | 39   | 20/21 | 0.94 | 0.06 | 80,86,90,93                 | 0     |
| 1   | 5MC  | 16SA  | 1590 | 21/22 | 0.94 | 0.09 | 65,69,73,81                 | 0     |
| 27  | 5MC  | 23SA  | 1967 | 21/22 | 0.95 | 0.10 | 51,55,61,69                 | 0     |
| 1   | 5MC  | 16SA  | 2032 | 21/22 | 0.95 | 0.13 | 51,53,60,61                 | 0     |
| 27  | OMG  | 23SB  | 2266 | 24/25 | 0.95 | 0.09 | 53,58,63,65                 | 0     |
| 23  | 4SU  | PSIA  | 8    | 20/21 | 0.95 | 0.07 | 72,75,81,83                 | 0     |
| 27  | PSU  | 23SB  | 2620 | 20/21 | 0.95 | 0.09 | 48,54,60,64                 | 0     |
| 1   | G7M  | 16SA  | 1156 | 24/25 | 0.95 | 0.12 | 58,67,71,77                 | 0     |
| 23  | MIA  | PSIB  | 37   | 29/30 | 0.95 | 0.09 | 82,87,100,103               | 0     |
| 1   | 2MG  | 16SA  | 1834 | 24/25 | 0.95 | 0.07 | 77,83,87,89                 | 0     |
| 27  | 5MU  | 23SA  | 1964 | 21/22 | 0.95 | 0.09 | 38,44,49,54                 | 0     |
| 27  | OMC  | 23SB  | 1945 | 21/22 | 0.96 | 0.07 | 69,77,79,81                 | 0     |
| 1   | UR3  | 16SA  | 2121 | 21/22 | 0.96 | 0.11 | 51,54,60,68                 | 0     |
| 27  | 5MU  | 23SB  | 1964 | 21/22 | 0.96 | 0.08 | 55,59,67,70                 | 0     |
| 23  | PSU  | PSIA  | 39   | 20/21 | 0.96 | 0.07 | 59,66,69,69                 | 0     |
| 27  | 5MC  | 23SB  | 1967 | 21/22 | 0.96 | 0.07 | 66,73,78,88                 | 0     |
| 27  | 5MC  | 23SA  | 1987 | 21/22 | 0.96 | 0.10 | 46,50,55,59                 | 0     |
| 1   | 5MC  | 16SA  | 2028 | 21/22 | 0.96 | 0.09 | 54,65,68,71                 | 0     |
| 1   | M2G  | 16SA  | 1589 | 25/26 | 0.96 | 0.07 | 59,65,72,74                 | 0     |
| 27  | 2MA  | 23SA  | 2518 | 23/24 | 0.96 | 0.09 | 34,40,44,50                 | 0     |
| 1   | 5MC  | 16SB  | 2032 | 21/22 | 0.96 | 0.07 | 63,69,74,76                 | 0     |
| 1   | UR3  | 16SB  | 2121 | 21/22 | 0.96 | 0.09 | 59,66,70,72                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 1   | MA6  | 16SB  | 2141 | 24/25 | 0.96 | 0.08 | 68,74,77,79                 | 0     |
| 1   | MA6  | 16SB  | 2142 | 24/25 | 0.96 | 0.09 | 65,71,74,77                 | 0     |
| 23  | MIA  | PSIA  | 37   | 29/30 | 0.96 | 0.09 | 57,65,80,85                 | 0     |
| 27  | OMC  | 23SA  | 1945 | 21/22 | 0.96 | 0.09 | 53,55,58,61                 | 0     |
| 27  | 2MA  | 23SB  | 2518 | 23/24 | 0.97 | 0.09 | 45,48,52,53                 | 0     |
| 27  | OMU  | 23SA  | 2567 | 21/22 | 0.97 | 0.09 | 42,48,52,58                 | 0     |
| 1   | 4OC  | 16SA  | 2030 | 22/23 | 0.97 | 0.10 | 56,60,64,67                 | 0     |
| 27  | PSU  | 23SA  | 2620 | 20/21 | 0.97 | 0.06 | 44,47,53,57                 | 0     |
| 1   | MA6  | 16SA  | 2142 | 24/25 | 0.97 | 0.09 | 49,52,54,59                 | 0     |
| 1   | 5MC  | 16SB  | 2035 | 21/22 | 0.97 | 0.07 | 64,69,73,76                 | 0     |
| 27  | OMG  | 23SA  | 2266 | 24/25 | 0.97 | 0.07 | 40,45,49,51                 | 0     |
| 27  | PSU  | 23SA  | 1942 | 20/21 | 0.97 | 0.11 | 57,63,68,68                 | 0     |
| 1   | 5MC  | 16SA  | 2035 | 21/22 | 0.97 | 0.12 | 45,54,59,62                 | 0     |
| 1   | MA6  | 16SA  | 2141 | 24/25 | 0.98 | 0.08 | 49,52,55,56                 | 0     |

### 5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res     | Atoms | RSCC  | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|---------|-------|-------|------|-----------------------------|-------|
| 58  | MG   | 23SB  | 3320    | 1/1   | -0.16 | 0.15 | 112,112,112,112             | 0     |
| 58  | MG   | 16SA  | 2250    | 1/1   | 0.25  | 0.15 | 114,114,114,114             | 0     |
| 60  | K    | 23SA  | 3594    | 1/1   | 0.27  | 0.30 | 127,127,127,127             | 0     |
| 58  | MG   | 16SB  | 2304[A] | 1/1   | 0.30  | 0.45 | 59,59,59,59                 | 1     |
| 58  | MG   | 16SB  | 2304[B] | 1/1   | 0.30  | 0.45 | 56,56,56,56                 | 1     |
| 58  | MG   | 23SB  | 3328    | 1/1   | 0.31  | 0.37 | 102,102,102,102             | 0     |
| 58  | MG   | 23SA  | 3152    | 1/1   | 0.40  | 0.27 | 95,95,95,95                 | 0     |
| 60  | K    | S4B   | 302     | 1/1   | 0.44  | 0.21 | 115,115,115,115             | 0     |
| 58  | MG   | 16SA  | 2213    | 1/1   | 0.47  | 0.29 | 103,103,103,103             | 0     |
| 58  | MG   | 16SB  | 2313    | 1/1   | 0.48  | 0.19 | 142,142,142,142             | 0     |
| 58  | MG   | 23SB  | 3318    | 1/1   | 0.51  | 0.16 | 88,88,88,88                 | 0     |
| 58  | MG   | 23SB  | 3262[B] | 1/1   | 0.54  | 0.38 | 59,59,59,59                 | 1     |
| 58  | MG   | 23SB  | 3262[A] | 1/1   | 0.54  | 0.38 | 55,55,55,55                 | 1     |
| 58  | MG   | 23SA  | 3137    | 1/1   | 0.57  | 0.11 | 89,89,89,89                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 60  | K    | 23SA  | 3634 | 1/1   | 0.57 | 0.14 | 104,104,104,104            | 0     |
| 60  | K    | 23SA  | 3539 | 1/1   | 0.57 | 0.10 | 125,125,125,125            | 0     |
| 58  | MG   | 23SB  | 3314 | 1/1   | 0.58 | 0.16 | 89,89,89,89                | 0     |
| 58  | MG   | 23SB  | 3212 | 1/1   | 0.58 | 0.23 | 83,83,83,83                | 0     |
| 58  | MG   | 16SA  | 2242 | 1/1   | 0.58 | 0.15 | 93,93,93,93                | 0     |
| 58  | MG   | 16SB  | 2343 | 1/1   | 0.58 | 0.12 | 148,148,148,148            | 0     |
| 60  | K    | 16SA  | 2383 | 1/1   | 0.59 | 0.14 | 123,123,123,123            | 0     |
| 60  | K    | 23SB  | 3519 | 1/1   | 0.59 | 0.15 | 119,119,119,119            | 0     |
| 60  | K    | 16SA  | 2403 | 1/1   | 0.60 | 0.15 | 84,84,84,84                | 0     |
| 58  | MG   | 16SA  | 2245 | 1/1   | 0.60 | 0.29 | 71,71,71,71                | 0     |
| 60  | K    | S20B  | 201  | 1/1   | 0.61 | 0.10 | 121,121,121,121            | 0     |
| 60  | K    | 23SB  | 3492 | 1/1   | 0.61 | 0.09 | 146,146,146,146            | 0     |
| 58  | MG   | 23SB  | 3285 | 1/1   | 0.61 | 0.29 | 77,77,77,77                | 0     |
| 58  | MG   | 23SA  | 3110 | 1/1   | 0.62 | 0.27 | 109,109,109,109            | 0     |
| 58  | MG   | 23SA  | 3015 | 1/1   | 0.63 | 0.46 | 91,91,91,91                | 0     |
| 60  | K    | 23SA  | 3549 | 1/1   | 0.64 | 0.10 | 104,104,104,104            | 0     |
| 60  | K    | 16SB  | 2364 | 1/1   | 0.64 | 0.10 | 132,132,132,132            | 0     |
| 60  | K    | 16SA  | 2395 | 1/1   | 0.65 | 0.14 | 105,105,105,105            | 0     |
| 60  | K    | L15B  | 202  | 1/1   | 0.65 | 0.14 | 96,96,96,96                | 0     |
| 60  | K    | 23SA  | 3548 | 1/1   | 0.66 | 0.20 | 100,100,100,100            | 0     |
| 58  | MG   | 23SA  | 3127 | 1/1   | 0.66 | 0.18 | 107,107,107,107            | 0     |
| 58  | MG   | 16SA  | 2241 | 1/1   | 0.66 | 0.29 | 81,81,81,81                | 0     |
| 58  | MG   | 16SB  | 2322 | 1/1   | 0.66 | 0.16 | 99,99,99,99                | 0     |
| 60  | K    | 16SA  | 2376 | 1/1   | 0.66 | 0.12 | 106,106,106,106            | 0     |
| 58  | MG   | 16SB  | 2314 | 1/1   | 0.67 | 0.23 | 99,99,99,99                | 0     |
| 60  | K    | 23SA  | 3563 | 1/1   | 0.67 | 0.12 | 83,83,83,83                | 0     |
| 58  | MG   | 16SA  | 2223 | 1/1   | 0.68 | 0.15 | 102,102,102,102            | 0     |
| 58  | MG   | 23SA  | 3154 | 1/1   | 0.68 | 0.19 | 59,59,59,59                | 0     |
| 58  | MG   | 23SA  | 3013 | 1/1   | 0.68 | 0.32 | 69,69,69,69                | 0     |
| 60  | K    | 23SA  | 3575 | 1/1   | 0.68 | 0.12 | 68,68,68,68                | 0     |
| 58  | MG   | 16SA  | 2246 | 1/1   | 0.69 | 0.07 | 100,100,100,100            | 0     |
| 58  | MG   | 16SB  | 2323 | 1/1   | 0.69 | 0.15 | 92,92,92,92                | 0     |
| 60  | K    | 23SB  | 3515 | 1/1   | 0.69 | 0.08 | 88,88,88,88                | 0     |
| 58  | MG   | 16SA  | 2258 | 1/1   | 0.69 | 0.26 | 95,95,95,95                | 0     |
| 58  | MG   | 23SA  | 3103 | 1/1   | 0.69 | 0.17 | 85,85,85,85                | 0     |
| 60  | K    | 16SB  | 2395 | 1/1   | 0.70 | 0.12 | 103,103,103,103            | 0     |
| 58  | MG   | 16SA  | 2255 | 1/1   | 0.70 | 0.26 | 82,82,82,82                | 0     |
| 58  | MG   | 23SB  | 3293 | 1/1   | 0.70 | 0.33 | 71,71,71,71                | 0     |
| 58  | MG   | PSIB  | 105  | 1/1   | 0.70 | 0.23 | 78,78,78,78                | 0     |
| 58  | MG   | 16SB  | 2317 | 1/1   | 0.70 | 0.19 | 98,98,98,98                | 0     |
| 58  | MG   | 23SA  | 3159 | 1/1   | 0.70 | 0.16 | 83,83,83,83                | 0     |
| 58  | MG   | 23SA  | 3177 | 1/1   | 0.70 | 0.13 | 91,91,91,91                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 23SB  | 3283 | 1/1   | 0.71 | 0.33 | 72,72,72,72                 | 0     |
| 60  | K    | L3B   | 303  | 1/1   | 0.71 | 0.13 | 98,98,98,98                 | 0     |
| 58  | MG   | 23SB  | 3286 | 1/1   | 0.71 | 0.26 | 65,65,65,65                 | 0     |
| 58  | MG   | 23SA  | 3099 | 1/1   | 0.72 | 0.11 | 80,80,80,80                 | 0     |
| 58  | MG   | 23SB  | 3311 | 1/1   | 0.72 | 0.22 | 75,75,75,75                 | 0     |
| 58  | MG   | 16SA  | 2238 | 1/1   | 0.72 | 0.19 | 118,118,118,118             | 0     |
| 60  | K    | 16SB  | 2370 | 1/1   | 0.72 | 0.09 | 135,135,135,135             | 0     |
| 58  | MG   | S5B   | 201  | 1/1   | 0.73 | 0.19 | 96,96,96,96                 | 0     |
| 60  | K    | 23SA  | 3545 | 1/1   | 0.73 | 0.15 | 103,103,103,103             | 0     |
| 58  | MG   | 16SA  | 2234 | 1/1   | 0.73 | 0.28 | 83,83,83,83                 | 0     |
| 58  | MG   | 16SA  | 2249 | 1/1   | 0.73 | 0.24 | 77,77,77,77                 | 0     |
| 60  | K    | 23SA  | 3638 | 1/1   | 0.73 | 0.11 | 104,104,104,104             | 0     |
| 58  | MG   | 16SA  | 2237 | 1/1   | 0.74 | 0.32 | 62,62,62,62                 | 0     |
| 60  | K    | 23SB  | 3442 | 1/1   | 0.74 | 0.15 | 112,112,112,112             | 0     |
| 60  | K    | 23SB  | 3481 | 1/1   | 0.74 | 0.13 | 105,105,105,105             | 0     |
| 58  | MG   | 16SB  | 2324 | 1/1   | 0.74 | 0.17 | 86,86,86,86                 | 0     |
| 58  | MG   | 16SB  | 2309 | 1/1   | 0.74 | 0.26 | 77,77,77,77                 | 0     |
| 60  | K    | 23SA  | 3611 | 1/1   | 0.74 | 0.12 | 118,118,118,118             | 0     |
| 60  | K    | 16SB  | 2396 | 1/1   | 0.74 | 0.15 | 92,92,92,92                 | 0     |
| 60  | K    | 16SA  | 2408 | 1/1   | 0.74 | 0.17 | 89,89,89,89                 | 0     |
| 58  | MG   | 23SA  | 3106 | 1/1   | 0.75 | 0.23 | 60,60,60,60                 | 0     |
| 58  | MG   | 16SB  | 2315 | 1/1   | 0.75 | 0.25 | 85,85,85,85                 | 0     |
| 58  | MG   | 23SA  | 3100 | 1/1   | 0.75 | 0.15 | 66,66,66,66                 | 0     |
| 58  | MG   | 23SB  | 3309 | 1/1   | 0.75 | 0.33 | 77,77,77,77                 | 0     |
| 60  | K    | 23SB  | 3513 | 1/1   | 0.75 | 0.08 | 127,127,127,127             | 0     |
| 60  | K    | 23SA  | 3560 | 1/1   | 0.75 | 0.08 | 89,89,89,89                 | 0     |
| 58  | MG   | 23SA  | 3065 | 1/1   | 0.75 | 0.21 | 56,56,56,56                 | 0     |
| 58  | MG   | 23SB  | 3276 | 1/1   | 0.75 | 0.30 | 82,82,82,82                 | 0     |
| 58  | MG   | PSIB  | 104  | 1/1   | 0.75 | 0.30 | 79,79,79,79                 | 0     |
| 58  | MG   | 16SA  | 2230 | 1/1   | 0.76 | 0.28 | 60,60,60,60                 | 0     |
| 58  | MG   | 23SB  | 3315 | 1/1   | 0.76 | 0.09 | 58,58,58,58                 | 0     |
| 60  | K    | 16SA  | 2384 | 1/1   | 0.76 | 0.16 | 106,106,106,106             | 0     |
| 58  | MG   | 16SA  | 2252 | 1/1   | 0.76 | 0.21 | 86,86,86,86                 | 0     |
| 58  | MG   | 23SA  | 3034 | 1/1   | 0.76 | 0.12 | 60,60,60,60                 | 0     |
| 58  | MG   | 16SB  | 2284 | 1/1   | 0.76 | 0.19 | 84,84,84,84                 | 0     |
| 58  | MG   | 23SB  | 3419 | 1/1   | 0.76 | 0.15 | 99,99,99,99                 | 0     |
| 60  | K    | 23SA  | 3542 | 1/1   | 0.76 | 0.10 | 105,105,105,105             | 0     |
| 58  | MG   | L32A  | 101  | 1/1   | 0.77 | 0.12 | 67,67,67,67                 | 0     |
| 58  | MG   | 16SA  | 2211 | 1/1   | 0.77 | 0.28 | 70,70,70,70                 | 0     |
| 58  | MG   | 16SA  | 2224 | 1/1   | 0.77 | 0.17 | 73,73,73,73                 | 0     |
| 60  | K    | 16SA  | 2415 | 1/1   | 0.77 | 0.08 | 89,89,89,89                 | 0     |
| 60  | K    | 23SB  | 3493 | 1/1   | 0.77 | 0.16 | 98,98,98,98                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 60  | K    | 23SB  | 3511 | 1/1   | 0.77 | 0.09 | 119,119,119,119            | 0     |
| 60  | K    | 16SB  | 2388 | 1/1   | 0.77 | 0.08 | 119,119,119,119            | 0     |
| 60  | K    | 16SB  | 2393 | 1/1   | 0.77 | 0.09 | 96,96,96,96                | 0     |
| 58  | MG   | 23SB  | 3268 | 1/1   | 0.77 | 0.14 | 66,66,66,66                | 0     |
| 58  | MG   | 16SB  | 2333 | 1/1   | 0.77 | 0.26 | 88,88,88,88                | 0     |
| 60  | K    | 16SA  | 2386 | 1/1   | 0.77 | 0.15 | 117,117,117,117            | 0     |
| 60  | K    | 23SA  | 3632 | 1/1   | 0.78 | 0.11 | 116,116,116,116            | 0     |
| 58  | MG   | 23SB  | 3310 | 1/1   | 0.78 | 0.31 | 79,79,79,79                | 0     |
| 58  | MG   | 16SB  | 2294 | 1/1   | 0.78 | 0.21 | 77,77,77,77                | 0     |
| 58  | MG   | 23SB  | 3272 | 1/1   | 0.78 | 0.26 | 57,57,57,57                | 0     |
| 58  | MG   | 16SB  | 2316 | 1/1   | 0.78 | 0.20 | 80,80,80,80                | 0     |
| 60  | K    | 16SA  | 2404 | 1/1   | 0.78 | 0.09 | 114,114,114,114            | 0     |
| 58  | MG   | 16SA  | 2218 | 1/1   | 0.78 | 0.39 | 78,78,78,78                | 0     |
| 58  | MG   | 23SA  | 3088 | 1/1   | 0.78 | 0.14 | 72,72,72,72                | 0     |
| 60  | K    | 16SA  | 2416 | 1/1   | 0.78 | 0.14 | 86,86,86,86                | 0     |
| 60  | K    | 16SA  | 2418 | 1/1   | 0.78 | 0.17 | 97,97,97,97                | 0     |
| 60  | K    | S14B  | 102  | 1/1   | 0.78 | 0.08 | 116,116,116,116            | 0     |
| 60  | K    | S20A  | 201  | 1/1   | 0.78 | 0.08 | 123,123,123,123            | 0     |
| 58  | MG   | 16SA  | 2243 | 1/1   | 0.78 | 0.22 | 89,89,89,89                | 0     |
| 58  | MG   | 16SB  | 2287 | 1/1   | 0.78 | 0.19 | 103,103,103,103            | 0     |
| 58  | MG   | 5SB   | 213  | 1/1   | 0.78 | 0.12 | 79,79,79,79                | 0     |
| 59  | OHX  | 16SA  | 2315 | 7/7   | 0.78 | 0.11 | 101,111,120,229            | 0     |
| 59  | OHX  | 23SA  | 3308 | 7/7   | 0.78 | 0.12 | 78,95,108,232              | 0     |
| 59  | OHX  | 23SA  | 3352 | 7/7   | 0.78 | 0.12 | 140,147,169,246            | 0     |
| 59  | OHX  | 23SB  | 3192 | 7/7   | 0.78 | 0.10 | 169,174,178,271            | 0     |
| 59  | OHX  | 23SB  | 3193 | 7/7   | 0.78 | 0.11 | 132,147,161,243            | 0     |
| 58  | MG   | 23SB  | 3300 | 1/1   | 0.78 | 0.16 | 67,67,67,67                | 0     |
| 60  | K    | L5B   | 202  | 1/1   | 0.78 | 0.09 | 110,110,110,110            | 0     |
| 58  | MG   | 16SB  | 2292 | 1/1   | 0.78 | 0.33 | 59,59,59,59                | 0     |
| 60  | K    | 23SA  | 3586 | 1/1   | 0.79 | 0.09 | 73,73,73,73                | 0     |
| 58  | MG   | 23SA  | 3023 | 1/1   | 0.79 | 0.20 | 77,77,77,77                | 0     |
| 59  | OHX  | 23SB  | 3163 | 7/7   | 0.79 | 0.11 | 127,143,150,243            | 0     |
| 58  | MG   | 16SB  | 2288 | 1/1   | 0.79 | 0.28 | 70,70,70,70                | 0     |
| 58  | MG   | 16SA  | 2239 | 1/1   | 0.79 | 0.14 | 84,84,84,84                | 0     |
| 58  | MG   | 23SB  | 3316 | 1/1   | 0.79 | 0.15 | 62,62,62,62                | 0     |
| 60  | K    | 23SB  | 3501 | 1/1   | 0.79 | 0.12 | 84,84,84,84                | 0     |
| 58  | MG   | 16SA  | 2254 | 1/1   | 0.79 | 0.31 | 67,67,67,67                | 0     |
| 58  | MG   | 23SA  | 3427 | 1/1   | 0.79 | 0.12 | 53,53,53,53                | 0     |
| 58  | MG   | 23SB  | 3239 | 1/1   | 0.79 | 0.26 | 50,50,50,50                | 0     |
| 58  | MG   | 23SA  | 3142 | 1/1   | 0.79 | 0.28 | 36,36,36,36                | 0     |
| 58  | MG   | 23SB  | 3303 | 1/1   | 0.79 | 0.15 | 66,66,66,66                | 0     |
| 58  | MG   | 16SB  | 2281 | 1/1   | 0.79 | 0.23 | 81,81,81,81                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 58  | MG   | 23SA  | 3017 | 1/1   | 0.79 | 0.14 | 73,73,73,73                | 0     |
| 58  | MG   | 23SB  | 3297 | 1/1   | 0.80 | 0.25 | 68,68,68,68                | 0     |
| 58  | MG   | 23SB  | 3281 | 1/1   | 0.80 | 0.20 | 77,77,77,77                | 0     |
| 60  | K    | 16SA  | 2405 | 1/1   | 0.80 | 0.10 | 115,115,115,115            | 0     |
| 60  | K    | 23SA  | 3547 | 1/1   | 0.80 | 0.11 | 72,72,72,72                | 0     |
| 58  | MG   | 23SB  | 3265 | 1/1   | 0.80 | 0.24 | 57,57,57,57                | 0     |
| 58  | MG   | 23SA  | 3089 | 1/1   | 0.80 | 0.16 | 77,77,77,77                | 0     |
| 58  | MG   | 23SA  | 3128 | 1/1   | 0.80 | 0.17 | 62,62,62,62                | 0     |
| 59  | OHX  | 16SB  | 2261 | 7/7   | 0.80 | 0.10 | 136,151,159,251            | 0     |
| 58  | MG   | 23SA  | 3067 | 1/1   | 0.80 | 0.32 | 71,71,71,71                | 0     |
| 58  | MG   | 23SB  | 3284 | 1/1   | 0.81 | 0.32 | 69,69,69,69                | 0     |
| 58  | MG   | 23SB  | 3399 | 1/1   | 0.81 | 0.11 | 88,88,88,88                | 0     |
| 58  | MG   | 23SA  | 3095 | 1/1   | 0.81 | 0.12 | 67,67,67,67                | 0     |
| 58  | MG   | 23SB  | 3234 | 1/1   | 0.81 | 0.24 | 55,55,55,55                | 0     |
| 58  | MG   | 16SB  | 2295 | 1/1   | 0.81 | 0.27 | 66,66,66,66                | 0     |
| 58  | MG   | 23SB  | 3253 | 1/1   | 0.81 | 0.10 | 78,78,78,78                | 0     |
| 58  | MG   | 23SB  | 3257 | 1/1   | 0.81 | 0.26 | 62,62,62,62                | 0     |
| 59  | OHX  | 23SA  | 3362 | 7/7   | 0.81 | 0.12 | 102,109,127,232            | 0     |
| 58  | MG   | 23SB  | 3301 | 1/1   | 0.81 | 0.16 | 75,75,75,75                | 0     |
| 58  | MG   | 23SB  | 3258 | 1/1   | 0.81 | 0.18 | 72,72,72,72                | 0     |
| 59  | OHX  | 23SB  | 3177 | 7/7   | 0.81 | 0.12 | 117,128,145,232            | 0     |
| 60  | K    | 23SB  | 3467 | 1/1   | 0.81 | 0.24 | 106,106,106,106            | 0     |
| 58  | MG   | 23SA  | 3006 | 1/1   | 0.81 | 0.24 | 50,50,50,50                | 0     |
| 60  | K    | 23SA  | 3554 | 1/1   | 0.81 | 0.14 | 87,87,87,87                | 0     |
| 58  | MG   | 23SA  | 3130 | 1/1   | 0.81 | 0.14 | 61,61,61,61                | 0     |
| 58  | MG   | 16SA  | 2232 | 1/1   | 0.81 | 0.33 | 66,66,66,66                | 0     |
| 60  | K    | 23SB  | 3509 | 1/1   | 0.81 | 0.28 | 102,102,102,102            | 0     |
| 58  | MG   | 23SA  | 3101 | 1/1   | 0.81 | 0.32 | 73,73,73,73                | 0     |
| 58  | MG   | 23SA  | 3086 | 1/1   | 0.81 | 0.19 | 71,71,71,71                | 0     |
| 58  | MG   | 16SA  | 2222 | 1/1   | 0.81 | 0.33 | 74,74,74,74                | 0     |
| 60  | K    | 23SA  | 3595 | 1/1   | 0.81 | 0.13 | 71,71,71,71                | 0     |
| 58  | MG   | 23SA  | 3059 | 1/1   | 0.81 | 0.20 | 77,77,77,77                | 0     |
| 58  | MG   | 23SB  | 3209 | 1/1   | 0.81 | 0.33 | 63,63,63,63                | 0     |
| 58  | MG   | 23SB  | 3322 | 1/1   | 0.81 | 0.17 | 72,72,72,72                | 0     |
| 58  | MG   | 16SB  | 2327 | 1/1   | 0.82 | 0.21 | 93,93,93,93                | 0     |
| 60  | K    | 16SB  | 2365 | 1/1   | 0.82 | 0.10 | 126,126,126,126            | 0     |
| 58  | MG   | 23SA  | 3002 | 1/1   | 0.82 | 0.25 | 58,58,58,58                | 0     |
| 59  | OHX  | 23SA  | 3353 | 7/7   | 0.82 | 0.11 | 128,135,151,244            | 0     |
| 60  | K    | PSIA  | 105  | 1/1   | 0.82 | 0.11 | 100,100,100,100            | 0     |
| 58  | MG   | 23SB  | 3263 | 1/1   | 0.82 | 0.33 | 56,56,56,56                | 0     |
| 59  | OHX  | 23SA  | 3382 | 7/7   | 0.82 | 0.10 | 86,97,101,238              | 0     |
| 60  | K    | 16SB  | 2398 | 1/1   | 0.82 | 0.09 | 101,101,101,101            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 60  | K    | 23SA  | 3544 | 1/1   | 0.82 | 0.08 | 91,91,91,91                | 0     |
| 58  | MG   | 16SA  | 2235 | 1/1   | 0.82 | 0.31 | 80,80,80,80                | 0     |
| 58  | MG   | 23SB  | 3267 | 1/1   | 0.82 | 0.16 | 63,63,63,63                | 0     |
| 58  | MG   | 23SA  | 3532 | 1/1   | 0.82 | 0.08 | 100,100,100,100            | 0     |
| 58  | MG   | 5SA   | 202  | 1/1   | 0.82 | 0.07 | 67,67,67,67                | 0     |
| 58  | MG   | 16SA  | 2236 | 1/1   | 0.82 | 0.15 | 99,99,99,99                | 0     |
| 58  | MG   | 16SA  | 2247 | 1/1   | 0.82 | 0.25 | 66,66,66,66                | 0     |
| 58  | MG   | 23SA  | 3060 | 1/1   | 0.82 | 0.22 | 63,63,63,63                | 0     |
| 58  | MG   | 23SB  | 3230 | 1/1   | 0.82 | 0.23 | 66,66,66,66                | 0     |
| 58  | MG   | 23SA  | 3148 | 1/1   | 0.82 | 0.05 | 64,64,64,64                | 0     |
| 58  | MG   | 23SB  | 3332 | 1/1   | 0.82 | 0.24 | 67,67,67,67                | 0     |
| 58  | MG   | 23SA  | 3063 | 1/1   | 0.82 | 0.18 | 66,66,66,66                | 0     |
| 60  | K    | 23SA  | 3608 | 1/1   | 0.82 | 0.09 | 80,80,80,80                | 0     |
| 58  | MG   | 16SB  | 2290 | 1/1   | 0.82 | 0.21 | 79,79,79,79                | 0     |
| 58  | MG   | 23SA  | 3117 | 1/1   | 0.82 | 0.11 | 81,81,81,81                | 0     |
| 58  | MG   | 23SA  | 3124 | 1/1   | 0.82 | 0.14 | 72,72,72,72                | 0     |
| 59  | OHX  | 16SA  | 2333 | 7/7   | 0.82 | 0.10 | 128,146,168,234            | 0     |
| 58  | MG   | 23SB  | 3201 | 1/1   | 0.83 | 0.23 | 72,72,72,72                | 0     |
| 58  | MG   | 23SA  | 3055 | 1/1   | 0.83 | 0.18 | 51,51,51,51                | 0     |
| 58  | MG   | 5SB   | 212  | 1/1   | 0.83 | 0.13 | 103,103,103,103            | 0     |
| 58  | MG   | 23SB  | 3210 | 1/1   | 0.83 | 0.28 | 60,60,60,60                | 0     |
| 58  | MG   | L5B   | 201  | 1/1   | 0.83 | 0.08 | 122,122,122,122            | 0     |
| 59  | OHX  | 16SA  | 2300 | 7/7   | 0.83 | 0.12 | 104,105,114,228            | 0     |
| 58  | MG   | 23SB  | 3307 | 1/1   | 0.83 | 0.19 | 71,71,71,71                | 0     |
| 59  | OHX  | 16SA  | 2325 | 7/7   | 0.83 | 0.10 | 137,144,157,243            | 0     |
| 58  | MG   | 23SA  | 3108 | 1/1   | 0.83 | 0.23 | 46,46,46,46                | 0     |
| 59  | OHX  | 23SA  | 3304 | 7/7   | 0.83 | 0.10 | 109,115,118,229            | 0     |
| 58  | MG   | 16SB  | 2326 | 1/1   | 0.83 | 0.39 | 78,78,78,78                | 0     |
| 60  | K    | 16SA  | 2419 | 1/1   | 0.83 | 0.13 | 95,95,95,95                | 0     |
| 58  | MG   | 5SA   | 201  | 1/1   | 0.83 | 0.16 | 67,67,67,67                | 0     |
| 58  | MG   | 16SB  | 2330 | 1/1   | 0.83 | 0.16 | 93,93,93,93                | 0     |
| 58  | MG   | 23SB  | 3240 | 1/1   | 0.83 | 0.22 | 54,54,54,54                | 0     |
| 59  | OHX  | 23SA  | 3363 | 7/7   | 0.83 | 0.10 | 109,126,158,239            | 0     |
| 60  | K    | 23SB  | 3462 | 1/1   | 0.83 | 0.13 | 102,102,102,102            | 0     |
| 59  | OHX  | 23SA  | 3369 | 7/7   | 0.83 | 0.10 | 125,136,152,237            | 0     |
| 59  | OHX  | 23SA  | 3381 | 7/7   | 0.83 | 0.24 | 74,88,105,228              | 0     |
| 58  | MG   | 23SA  | 3161 | 1/1   | 0.83 | 0.07 | 88,88,88,88                | 0     |
| 59  | OHX  | L28A  | 101  | 7/7   | 0.83 | 0.10 | 84,89,95,234               | 0     |
| 60  | K    | 23SB  | 3494 | 1/1   | 0.83 | 0.12 | 109,109,109,109            | 0     |
| 60  | K    | 23SB  | 3498 | 1/1   | 0.83 | 0.07 | 108,108,108,108            | 0     |
| 59  | OHX  | 16SB  | 2257 | 7/7   | 0.83 | 0.10 | 149,153,169,230            | 0     |
| 58  | MG   | 5SA   | 203  | 1/1   | 0.83 | 0.24 | 79,79,79,79                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 23SA  | 3176 | 1/1   | 0.83 | 0.34 | 63,63,63,63                 | 0     |
| 58  | MG   | L33A  | 101  | 1/1   | 0.83 | 0.26 | 95,95,95,95                 | 0     |
| 59  | OHX  | 23SB  | 3185 | 7/7   | 0.83 | 0.10 | 130,138,151,236             | 0     |
| 58  | MG   | 23SB  | 3295 | 1/1   | 0.83 | 0.20 | 57,57,57,57                 | 0     |
| 60  | K    | 23SB  | 3520 | 1/1   | 0.83 | 0.10 | 107,107,107,107             | 0     |
| 58  | MG   | 23SA  | 3036 | 1/1   | 0.83 | 0.18 | 53,53,53,53                 | 0     |
| 58  | MG   | 23SB  | 3360 | 1/1   | 0.83 | 0.18 | 111,111,111,111             | 0     |
| 60  | K    | 16SA  | 2380 | 1/1   | 0.83 | 0.14 | 91,91,91,91                 | 0     |
| 58  | MG   | 23SA  | 3118 | 1/1   | 0.84 | 0.14 | 59,59,59,59                 | 0     |
| 58  | MG   | 16SB  | 2344 | 1/1   | 0.84 | 0.09 | 107,107,107,107             | 0     |
| 60  | K    | 16SB  | 2367 | 1/1   | 0.84 | 0.11 | 115,115,115,115             | 0     |
| 58  | MG   | 23SB  | 3327 | 1/1   | 0.84 | 0.07 | 59,59,59,59                 | 0     |
| 60  | K    | 16SB  | 2375 | 1/1   | 0.84 | 0.08 | 106,106,106,106             | 0     |
| 60  | K    | 16SB  | 2387 | 1/1   | 0.84 | 0.17 | 93,93,93,93                 | 0     |
| 58  | MG   | 16SB  | 2363 | 1/1   | 0.84 | 0.10 | 89,89,89,89                 | 0     |
| 58  | MG   | 23SA  | 3422 | 1/1   | 0.84 | 0.13 | 63,63,63,63                 | 0     |
| 58  | MG   | 23SA  | 3143 | 1/1   | 0.84 | 0.19 | 69,69,69,69                 | 0     |
| 58  | MG   | 23SB  | 3299 | 1/1   | 0.84 | 0.16 | 68,68,68,68                 | 0     |
| 58  | MG   | 23SA  | 3147 | 1/1   | 0.84 | 0.11 | 76,76,76,76                 | 0     |
| 59  | OHX  | 23SB  | 3140 | 7/7   | 0.84 | 0.10 | 108,117,123,240             | 0     |
| 58  | MG   | 23SA  | 3037 | 1/1   | 0.84 | 0.15 | 88,88,88,88                 | 0     |
| 58  | MG   | 23SA  | 3051 | 1/1   | 0.84 | 0.29 | 53,53,53,53                 | 0     |
| 59  | OHX  | 23SB  | 3180 | 7/7   | 0.84 | 0.11 | 104,121,149,231             | 0     |
| 58  | MG   | 23SA  | 3109 | 1/1   | 0.84 | 0.18 | 55,55,55,55                 | 0     |
| 59  | OHX  | 23SB  | 3186 | 7/7   | 0.84 | 0.11 | 122,128,152,228             | 0     |
| 60  | K    | 23SB  | 3478 | 1/1   | 0.84 | 0.13 | 94,94,94,94                 | 0     |
| 58  | MG   | L30A  | 101  | 1/1   | 0.84 | 0.15 | 54,54,54,54                 | 0     |
| 58  | MG   | 23SB  | 3218 | 1/1   | 0.84 | 0.21 | 56,56,56,56                 | 0     |
| 58  | MG   | 23SB  | 3220 | 1/1   | 0.84 | 0.08 | 72,72,72,72                 | 0     |
| 60  | K    | 16SA  | 2377 | 1/1   | 0.84 | 0.09 | 101,101,101,101             | 0     |
| 60  | K    | 23SA  | 3584 | 1/1   | 0.84 | 0.06 | 85,85,85,85                 | 0     |
| 58  | MG   | 23SB  | 3280 | 1/1   | 0.84 | 0.17 | 59,59,59,59                 | 0     |
| 60  | K    | 23SB  | 3502 | 1/1   | 0.84 | 0.10 | 97,97,97,97                 | 0     |
| 60  | K    | 23SA  | 3588 | 1/1   | 0.84 | 0.27 | 70,70,70,70                 | 0     |
| 59  | OHX  | 23SA  | 3257 | 7/7   | 0.84 | 0.11 | 134,139,144,224             | 0     |
| 58  | MG   | 23SA  | 3092 | 1/1   | 0.84 | 0.07 | 60,60,60,60                 | 0     |
| 58  | MG   | 23SA  | 3131 | 1/1   | 0.84 | 0.11 | 63,63,63,63                 | 0     |
| 60  | K    | 23SB  | 3517 | 1/1   | 0.84 | 0.24 | 103,103,103,103             | 0     |
| 59  | OHX  | 23SA  | 3346 | 7/7   | 0.84 | 0.10 | 143,147,162,241             | 0     |
| 60  | K    | 23SA  | 3625 | 1/1   | 0.84 | 0.08 | 83,83,83,83                 | 0     |
| 58  | MG   | 16SA  | 2248 | 1/1   | 0.84 | 0.26 | 83,83,83,83                 | 0     |
| 58  | MG   | 23SB  | 3319 | 1/1   | 0.84 | 0.11 | 83,83,83,83                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 59  | OHX  | 23SA  | 3354 | 7/7   | 0.84 | 0.13 | 110,114,141,218            | 0     |
| 59  | OHX  | 23SB  | 3165 | 7/7   | 0.85 | 0.09 | 146,151,160,234            | 0     |
| 59  | OHX  | 23SB  | 3172 | 7/7   | 0.85 | 0.10 | 120,133,146,238            | 0     |
| 58  | MG   | 23SA  | 3116 | 1/1   | 0.85 | 0.20 | 62,62,62,62                | 0     |
| 59  | OHX  | 23SB  | 3179 | 7/7   | 0.85 | 0.11 | 154,162,169,245            | 0     |
| 58  | MG   | 16SB  | 2321 | 1/1   | 0.85 | 0.27 | 73,73,73,73                | 0     |
| 58  | MG   | 23SA  | 3080 | 1/1   | 0.85 | 0.17 | 57,57,57,57                | 0     |
| 58  | MG   | 23SA  | 3081 | 1/1   | 0.85 | 0.20 | 50,50,50,50                | 0     |
| 58  | MG   | 16SB  | 2279 | 1/1   | 0.85 | 0.20 | 68,68,68,68                | 0     |
| 60  | K    | S13B  | 201  | 1/1   | 0.85 | 0.08 | 139,139,139,139            | 0     |
| 58  | MG   | 16SB  | 2325 | 1/1   | 0.85 | 0.23 | 92,92,92,92                | 0     |
| 59  | OHX  | 23SB  | 3199 | 7/7   | 0.85 | 0.10 | 100,103,106,239            | 0     |
| 58  | MG   | 23SA  | 3445 | 1/1   | 0.85 | 0.12 | 43,43,43,43                | 0     |
| 60  | K    | 23SB  | 3448 | 1/1   | 0.85 | 0.17 | 104,104,104,104            | 0     |
| 58  | MG   | 16SB  | 2307 | 1/1   | 0.85 | 0.41 | 61,61,61,61                | 0     |
| 58  | MG   | 23SA  | 3156 | 1/1   | 0.85 | 0.09 | 69,69,69,69                | 0     |
| 58  | MG   | 16SB  | 2332 | 1/1   | 0.85 | 0.14 | 92,92,92,92                | 0     |
| 59  | OHX  | 23SA  | 3374 | 7/7   | 0.85 | 0.11 | 123,128,153,223            | 0     |
| 59  | OHX  | 23SA  | 3380 | 7/7   | 0.85 | 0.10 | 101,108,113,232            | 0     |
| 58  | MG   | 16SB  | 2312 | 1/1   | 0.85 | 0.12 | 71,71,71,71                | 0     |
| 60  | K    | 16SA  | 2398 | 1/1   | 0.85 | 0.12 | 67,67,67,67                | 0     |
| 58  | MG   | 23SA  | 3008 | 1/1   | 0.85 | 0.10 | 73,73,73,73                | 0     |
| 60  | K    | 23SA  | 3617 | 1/1   | 0.85 | 0.10 | 74,74,74,74                | 0     |
| 59  | OHX  | 5SA   | 213  | 7/7   | 0.85 | 0.10 | 118,123,145,229            | 0     |
| 58  | MG   | 16SA  | 2229 | 1/1   | 0.85 | 0.23 | 71,71,71,71                | 0     |
| 58  | MG   | 16SA  | 2209 | 1/1   | 0.85 | 0.09 | 86,86,86,86                | 0     |
| 59  | OHX  | 16SA  | 2328 | 7/7   | 0.85 | 0.11 | 143,155,166,234            | 0     |
| 60  | K    | L3A   | 303  | 1/1   | 0.85 | 0.11 | 88,88,88,88                | 0     |
| 60  | K    | L5A   | 302  | 1/1   | 0.85 | 0.12 | 83,83,83,83                | 0     |
| 59  | OHX  | 16SB  | 2272 | 7/7   | 0.85 | 0.10 | 140,141,165,247            | 0     |
| 58  | MG   | 16SB  | 2291 | 1/1   | 0.85 | 0.21 | 73,73,73,73                | 0     |
| 60  | K    | 16SB  | 2366 | 1/1   | 0.85 | 0.09 | 88,88,88,88                | 0     |
| 59  | OHX  | 23SB  | 3161 | 7/7   | 0.85 | 0.09 | 142,150,169,244            | 0     |
| 59  | OHX  | TRNA  | 102  | 7/7   | 0.85 | 0.09 | 125,127,144,247            | 0     |
| 58  | MG   | 16SA  | 2257 | 1/1   | 0.86 | 0.23 | 54,54,54,54                | 0     |
| 58  | MG   | L4B   | 302  | 1/1   | 0.86 | 0.29 | 94,94,94,94                | 0     |
| 60  | K    | 16SA  | 2391 | 1/1   | 0.86 | 0.12 | 86,86,86,86                | 0     |
| 58  | MG   | 16SA  | 2220 | 1/1   | 0.86 | 0.20 | 47,47,47,47                | 0     |
| 58  | MG   | 16SA  | 2201 | 1/1   | 0.86 | 0.24 | 73,73,73,73                | 0     |
| 58  | MG   | 23SA  | 3045 | 1/1   | 0.86 | 0.26 | 44,44,44,44                | 0     |
| 58  | MG   | 23SA  | 3499 | 1/1   | 0.86 | 0.14 | 56,56,56,56                | 0     |
| 59  | OHX  | 16SB  | 2264 | 7/7   | 0.86 | 0.09 | 140,157,163,237            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | K    | 16SB  | 2381 | 1/1   | 0.86 | 0.09 | 100,100,100,100             | 0     |
| 58  | MG   | 16SB  | 2289 | 1/1   | 0.86 | 0.12 | 89,89,89,89                 | 0     |
| 59  | OHX  | 16SB  | 2277 | 7/7   | 0.86 | 0.09 | 99,106,111,245              | 0     |
| 60  | K    | 16SB  | 2390 | 1/1   | 0.86 | 0.12 | 96,96,96,96                 | 0     |
| 59  | OHX  | 23SB  | 3110 | 7/7   | 0.86 | 0.09 | 104,110,117,225             | 0     |
| 59  | OHX  | 23SB  | 3119 | 7/7   | 0.86 | 0.10 | 86,94,113,210               | 0     |
| 59  | OHX  | 23SB  | 3126 | 7/7   | 0.86 | 0.10 | 110,115,124,217             | 0     |
| 59  | OHX  | 23SB  | 3135 | 7/7   | 0.86 | 0.11 | 81,95,103,232               | 0     |
| 58  | MG   | 23SA  | 3516 | 1/1   | 0.86 | 0.10 | 84,84,84,84                 | 0     |
| 59  | OHX  | 23SB  | 3148 | 7/7   | 0.86 | 0.10 | 111,126,143,215             | 0     |
| 59  | OHX  | 23SB  | 3157 | 7/7   | 0.86 | 0.10 | 120,135,155,223             | 0     |
| 59  | OHX  | ASIA  | 102  | 7/7   | 0.86 | 0.11 | 113,120,131,219             | 0     |
| 58  | MG   | 23SA  | 3071 | 1/1   | 0.86 | 0.19 | 77,77,77,77                 | 0     |
| 58  | MG   | 23SB  | 3279 | 1/1   | 0.86 | 0.23 | 82,82,82,82                 | 0     |
| 58  | MG   | 23SA  | 3049 | 1/1   | 0.86 | 0.23 | 57,57,57,57                 | 0     |
| 59  | OHX  | 23SB  | 3174 | 7/7   | 0.86 | 0.10 | 128,128,151,234             | 0     |
| 60  | K    | 23SA  | 3550 | 1/1   | 0.86 | 0.18 | 81,81,81,81                 | 0     |
| 60  | K    | 23SA  | 3553 | 1/1   | 0.86 | 0.13 | 92,92,92,92                 | 0     |
| 58  | MG   | 23SA  | 3005 | 1/1   | 0.86 | 0.18 | 54,54,54,54                 | 0     |
| 59  | OHX  | 23SA  | 3312 | 7/7   | 0.86 | 0.23 | 74,87,95,219                | 0     |
| 58  | MG   | 23SB  | 3223 | 1/1   | 0.86 | 0.17 | 79,79,79,79                 | 0     |
| 59  | OHX  | 23SB  | 3181 | 7/7   | 0.86 | 0.09 | 118,141,152,230             | 0     |
| 59  | OHX  | 23SA  | 3347 | 7/7   | 0.86 | 0.10 | 126,132,144,218             | 0     |
| 58  | MG   | 23SB  | 3224 | 1/1   | 0.86 | 0.17 | 68,68,68,68                 | 0     |
| 58  | MG   | 23SA  | 3083 | 1/1   | 0.86 | 0.18 | 41,41,41,41                 | 0     |
| 58  | MG   | 16SB  | 2301 | 1/1   | 0.86 | 0.28 | 68,68,68,68                 | 0     |
| 60  | K    | 23SB  | 3512 | 1/1   | 0.86 | 0.10 | 79,79,79,79                 | 0     |
| 59  | OHX  | 23SB  | 3194 | 7/7   | 0.86 | 0.09 | 133,151,170,230             | 0     |
| 59  | OHX  | 23SB  | 3196 | 7/7   | 0.86 | 0.10 | 157,162,174,238             | 0     |
| 58  | MG   | L5A   | 301  | 1/1   | 0.86 | 0.25 | 67,67,67,67                 | 0     |
| 58  | MG   | L23A  | 101  | 1/1   | 0.86 | 0.10 | 60,60,60,60                 | 0     |
| 58  | MG   | 23SA  | 3020 | 1/1   | 0.86 | 0.23 | 32,32,32,32                 | 0     |
| 60  | K    | 16SA  | 2379 | 1/1   | 0.86 | 0.07 | 111,111,111,111             | 0     |
| 58  | MG   | 23SA  | 3170 | 1/1   | 0.86 | 0.09 | 69,69,69,69                 | 0     |
| 58  | MG   | 16SA  | 2226 | 1/1   | 0.86 | 0.11 | 78,78,78,78                 | 0     |
| 58  | MG   | 23SB  | 3304 | 1/1   | 0.87 | 0.21 | 68,68,68,68                 | 0     |
| 60  | K    | 16SB  | 2379 | 1/1   | 0.87 | 0.11 | 121,121,121,121             | 0     |
| 58  | MG   | 16SB  | 2282 | 1/1   | 0.87 | 0.35 | 83,83,83,83                 | 0     |
| 60  | K    | 16SB  | 2382 | 1/1   | 0.87 | 0.09 | 94,94,94,94                 | 0     |
| 58  | MG   | 16SB  | 2296 | 1/1   | 0.87 | 0.19 | 71,71,71,71                 | 0     |
| 59  | OHX  | 23SA  | 3361 | 7/7   | 0.87 | 0.10 | 86,117,130,220              | 0     |
| 58  | MG   | 23SA  | 3096 | 1/1   | 0.87 | 0.09 | 70,70,70,70                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | K    | 16SB  | 2392 | 1/1   | 0.87 | 0.08 | 117,117,117,117             | 0     |
| 58  | MG   | 16SB  | 2361 | 1/1   | 0.87 | 0.08 | 122,122,122,122             | 0     |
| 58  | MG   | 16SB  | 2318 | 1/1   | 0.87 | 0.31 | 65,65,65,65                 | 0     |
| 58  | MG   | 16SB  | 2302 | 1/1   | 0.87 | 0.35 | 66,66,66,66                 | 0     |
| 58  | MG   | 16SA  | 2219 | 1/1   | 0.87 | 0.14 | 74,74,74,74                 | 0     |
| 59  | OHX  | 23SB  | 3189 | 7/7   | 0.87 | 0.10 | 147,159,176,238             | 0     |
| 59  | OHX  | 16SA  | 2326 | 7/7   | 0.87 | 0.10 | 127,136,164,238             | 0     |
| 58  | MG   | 23SB  | 3255 | 1/1   | 0.87 | 0.29 | 50,50,50,50                 | 0     |
| 58  | MG   | 23SA  | 3057 | 1/1   | 0.87 | 0.15 | 44,44,44,44                 | 0     |
| 60  | K    | 23SB  | 3441 | 1/1   | 0.87 | 0.12 | 88,88,88,88                 | 0     |
| 58  | MG   | 16SA  | 2221 | 1/1   | 0.87 | 0.28 | 62,62,62,62                 | 0     |
| 59  | OHX  | 16SB  | 2246 | 7/7   | 0.87 | 0.10 | 104,108,114,227             | 0     |
| 60  | K    | 23SA  | 3581 | 1/1   | 0.87 | 0.10 | 72,72,72,72                 | 0     |
| 58  | MG   | 23SB  | 3207 | 1/1   | 0.87 | 0.17 | 47,47,47,47                 | 0     |
| 58  | MG   | 23SB  | 3324 | 1/1   | 0.87 | 0.13 | 58,58,58,58                 | 0     |
| 59  | OHX  | 23SA  | 3258 | 7/7   | 0.87 | 0.09 | 90,100,113,211              | 0     |
| 59  | OHX  | 23SA  | 3272 | 7/7   | 0.87 | 0.10 | 84,96,103,208               | 0     |
| 59  | OHX  | 23SA  | 3288 | 7/7   | 0.87 | 0.18 | 82,88,106,207               | 0     |
| 60  | K    | 23SA  | 3597 | 1/1   | 0.87 | 0.13 | 87,87,87,87                 | 0     |
| 59  | OHX  | 23SA  | 3295 | 7/7   | 0.87 | 0.08 | 103,109,114,228             | 0     |
| 59  | OHX  | 23SA  | 3298 | 7/7   | 0.87 | 0.09 | 95,100,108,219              | 0     |
| 60  | K    | 16SA  | 2389 | 1/1   | 0.87 | 0.13 | 82,82,82,82                 | 0     |
| 59  | OHX  | 23SB  | 3122 | 7/7   | 0.87 | 0.11 | 93,97,102,223               | 0     |
| 58  | MG   | 23SA  | 3102 | 1/1   | 0.87 | 0.26 | 45,45,45,45                 | 0     |
| 59  | OHX  | 23SB  | 3127 | 7/7   | 0.87 | 0.09 | 109,115,122,246             | 0     |
| 58  | MG   | 16SB  | 2311 | 1/1   | 0.87 | 0.33 | 84,84,84,84                 | 0     |
| 58  | MG   | 23SA  | 3537 | 1/1   | 0.87 | 0.14 | 72,72,72,72                 | 0     |
| 59  | OHX  | 23SB  | 3144 | 7/7   | 0.87 | 0.08 | 103,111,118,233             | 0     |
| 59  | OHX  | 23SA  | 3336 | 7/7   | 0.87 | 0.10 | 112,116,141,218             | 0     |
| 59  | OHX  | 23SB  | 3151 | 7/7   | 0.87 | 0.09 | 135,140,158,248             | 0     |
| 58  | MG   | 23SA  | 3026 | 1/1   | 0.87 | 0.18 | 52,52,52,52                 | 0     |
| 58  | MG   | 23SA  | 3136 | 1/1   | 0.87 | 0.10 | 77,77,77,77                 | 0     |
| 59  | OHX  | 23SA  | 3349 | 7/7   | 0.87 | 0.09 | 115,126,155,229             | 0     |
| 60  | K    | 16SA  | 2385 | 1/1   | 0.88 | 0.16 | 107,107,107,107             | 0     |
| 58  | MG   | 16SA  | 2204 | 1/1   | 0.88 | 0.23 | 52,52,52,52                 | 0     |
| 60  | K    | 16SA  | 2387 | 1/1   | 0.88 | 0.10 | 93,93,93,93                 | 0     |
| 59  | OHX  | MRNB  | 101  | 7/7   | 0.88 | 0.09 | 144,148,154,235             | 0     |
| 58  | MG   | 23SB  | 3204 | 1/1   | 0.88 | 0.29 | 54,54,54,54                 | 0     |
| 59  | OHX  | 23SB  | 3114 | 7/7   | 0.88 | 0.08 | 96,100,108,207              | 0     |
| 58  | MG   | 23SB  | 3372 | 1/1   | 0.88 | 0.10 | 50,50,50,50                 | 0     |
| 59  | OHX  | 23SA  | 3307 | 7/7   | 0.88 | 0.09 | 108,113,123,223             | 0     |
| 58  | MG   | 23SB  | 3261 | 1/1   | 0.88 | 0.18 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 23SB  | 3205 | 1/1   | 0.88 | 0.23 | 54,54,54,54                 | 0     |
| 59  | OHX  | 23SB  | 3132 | 7/7   | 0.88 | 0.09 | 105,111,127,226             | 0     |
| 58  | MG   | 23SB  | 3420 | 1/1   | 0.88 | 0.11 | 62,62,62,62                 | 0     |
| 59  | OHX  | 23SA  | 3339 | 7/7   | 0.88 | 0.09 | 99,120,146,218              | 0     |
| 59  | OHX  | 23SB  | 3143 | 7/7   | 0.88 | 0.09 | 101,107,113,221             | 0     |
| 59  | OHX  | 23SA  | 3345 | 7/7   | 0.88 | 0.10 | 107,120,136,224             | 0     |
| 60  | K    | 16SA  | 2420 | 1/1   | 0.88 | 0.10 | 99,99,99,99                 | 0     |
| 58  | MG   | 23SA  | 3171 | 1/1   | 0.88 | 0.11 | 49,49,49,49                 | 0     |
| 59  | OHX  | 23SB  | 3149 | 7/7   | 0.88 | 0.09 | 111,128,143,208             | 0     |
| 58  | MG   | 23SA  | 3140 | 1/1   | 0.88 | 0.12 | 61,61,61,61                 | 0     |
| 58  | MG   | 5SB   | 214  | 1/1   | 0.88 | 0.31 | 56,56,56,56                 | 0     |
| 58  | MG   | 23SA  | 3097 | 1/1   | 0.88 | 0.25 | 50,50,50,50                 | 0     |
| 58  | MG   | L3A   | 301  | 1/1   | 0.88 | 0.19 | 57,57,57,57                 | 0     |
| 60  | K    | 23SA  | 3546 | 1/1   | 0.88 | 0.22 | 94,94,94,94                 | 0     |
| 59  | OHX  | 16SA  | 2290 | 7/7   | 0.88 | 0.18 | 82,92,113,204               | 0     |
| 59  | OHX  | 16SA  | 2292 | 7/7   | 0.88 | 0.11 | 88,100,116,196              | 0     |
| 58  | MG   | 23SA  | 3094 | 1/1   | 0.88 | 0.19 | 55,55,55,55                 | 0     |
| 58  | MG   | 23SA  | 3144 | 1/1   | 0.88 | 0.20 | 52,52,52,52                 | 0     |
| 58  | MG   | 23SB  | 3222 | 1/1   | 0.88 | 0.18 | 64,64,64,64                 | 0     |
| 59  | OHX  | 23SA  | 3373 | 7/7   | 0.88 | 0.10 | 92,109,134,230              | 0     |
| 60  | K    | 23SB  | 3471 | 1/1   | 0.88 | 0.14 | 106,106,106,106             | 0     |
| 60  | K    | 23SB  | 3475 | 1/1   | 0.88 | 0.09 | 90,90,90,90                 | 0     |
| 60  | K    | 23SB  | 3476 | 1/1   | 0.88 | 0.22 | 77,77,77,77                 | 0     |
| 58  | MG   | 16SA  | 2259 | 1/1   | 0.88 | 0.22 | 47,47,47,47                 | 0     |
| 60  | K    | 23SB  | 3479 | 1/1   | 0.88 | 0.09 | 76,76,76,76                 | 0     |
| 60  | K    | 23SA  | 3562 | 1/1   | 0.88 | 0.05 | 80,80,80,80                 | 0     |
| 58  | MG   | 23SA  | 3489 | 1/1   | 0.88 | 0.11 | 36,36,36,36                 | 0     |
| 59  | OHX  | 16SA  | 2332 | 7/7   | 0.88 | 0.10 | 133,137,152,236             | 0     |
| 58  | MG   | 23SA  | 3495 | 1/1   | 0.88 | 0.09 | 67,67,67,67                 | 0     |
| 59  | OHX  | 5SA   | 209  | 7/7   | 0.88 | 0.10 | 81,100,111,199              | 0     |
| 60  | K    | 23SB  | 3499 | 1/1   | 0.88 | 0.09 | 85,85,85,85                 | 0     |
| 59  | OHX  | 16SA  | 2335 | 7/7   | 0.88 | 0.09 | 127,136,156,226             | 0     |
| 58  | MG   | 16SB  | 2298 | 1/1   | 0.88 | 0.31 | 72,72,72,72                 | 0     |
| 58  | MG   | 23SA  | 3166 | 1/1   | 0.88 | 0.17 | 38,38,38,38                 | 0     |
| 59  | OHX  | 16SB  | 2249 | 7/7   | 0.88 | 0.09 | 102,104,116,221             | 0     |
| 58  | MG   | PSIB  | 103  | 1/1   | 0.88 | 0.23 | 52,52,52,52                 | 0     |
| 60  | K    | 23SA  | 3599 | 1/1   | 0.88 | 0.07 | 66,66,66,66                 | 0     |
| 58  | MG   | 23SB  | 3244 | 1/1   | 0.88 | 0.21 | 43,43,43,43                 | 0     |
| 60  | K    | 16SA  | 2378 | 1/1   | 0.88 | 0.09 | 93,93,93,93                 | 0     |
| 60  | K    | 23SA  | 3613 | 1/1   | 0.88 | 0.11 | 91,91,91,91                 | 0     |
| 58  | MG   | 23SA  | 3168 | 1/1   | 0.88 | 0.17 | 89,89,89,89                 | 0     |
| 58  | MG   | 23SA  | 3169 | 1/1   | 0.88 | 0.20 | 82,82,82,82                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 59  | OHX  | 16SB  | 2273 | 7/7   | 0.88 | 0.09 | 129,146,161,233            | 0     |
| 59  | OHX  | 16SB  | 2275 | 7/7   | 0.88 | 0.10 | 115,137,163,225            | 0     |
| 58  | MG   | L15B  | 201  | 1/1   | 0.89 | 0.15 | 58,58,58,58                | 0     |
| 59  | OHX  | 23SB  | 3035 | 7/7   | 0.89 | 0.14 | 65,93,108,150              | 0     |
| 60  | K    | 23SA  | 3635 | 1/1   | 0.89 | 0.04 | 69,69,69,69                | 0     |
| 59  | OHX  | 23SA  | 3341 | 7/7   | 0.89 | 0.10 | 113,122,146,225            | 0     |
| 58  | MG   | 16SA  | 2205 | 1/1   | 0.89 | 0.26 | 51,51,51,51                | 0     |
| 58  | MG   | 23SB  | 3282 | 1/1   | 0.89 | 0.22 | 64,64,64,64                | 0     |
| 58  | MG   | 23SB  | 3254 | 1/1   | 0.89 | 0.25 | 46,46,46,46                | 0     |
| 58  | MG   | 23SA  | 3068 | 1/1   | 0.89 | 0.09 | 64,64,64,64                | 0     |
| 59  | OHX  | 23SA  | 3350 | 7/7   | 0.89 | 0.08 | 121,138,153,230            | 0     |
| 60  | K    | 16SA  | 2396 | 1/1   | 0.89 | 0.07 | 103,103,103,103            | 0     |
| 59  | OHX  | 16SA  | 2316 | 7/7   | 0.89 | 0.08 | 114,126,153,236            | 0     |
| 60  | K    | 16SA  | 2402 | 1/1   | 0.89 | 0.17 | 89,89,89,89                | 0     |
| 59  | OHX  | 16SA  | 2318 | 7/7   | 0.89 | 0.08 | 113,116,137,211            | 0     |
| 58  | MG   | 23SA  | 3484 | 1/1   | 0.89 | 0.12 | 84,84,84,84                | 0     |
| 59  | OHX  | 23SA  | 3358 | 7/7   | 0.89 | 0.08 | 129,130,145,238            | 0     |
| 60  | K    | 16SB  | 2384 | 1/1   | 0.89 | 0.08 | 98,98,98,98                | 0     |
| 58  | MG   | 23SA  | 3069 | 1/1   | 0.89 | 0.18 | 70,70,70,70                | 0     |
| 58  | MG   | 23SB  | 3323 | 1/1   | 0.89 | 0.27 | 45,45,45,45                | 0     |
| 58  | MG   | 23SB  | 3259 | 1/1   | 0.89 | 0.33 | 35,35,35,35                | 0     |
| 59  | OHX  | 23SA  | 3365 | 7/7   | 0.89 | 0.08 | 184,185,193,269            | 0     |
| 58  | MG   | 16SB  | 2308 | 1/1   | 0.89 | 0.30 | 59,59,59,59                | 0     |
| 59  | OHX  | 23SB  | 3159 | 7/7   | 0.89 | 0.09 | 124,131,146,207            | 0     |
| 60  | K    | S13A  | 201  | 1/1   | 0.89 | 0.06 | 108,108,108,108            | 0     |
| 59  | OHX  | 23SA  | 3370 | 7/7   | 0.89 | 0.11 | 94,101,133,213             | 0     |
| 60  | K    | PSIA  | 104  | 1/1   | 0.89 | 0.11 | 80,80,80,80                | 0     |
| 60  | K    | S6B   | 201  | 1/1   | 0.89 | 0.09 | 85,85,85,85                | 0     |
| 59  | OHX  | 23SA  | 3371 | 7/7   | 0.89 | 0.09 | 130,141,155,222            | 0     |
| 58  | MG   | 23SA  | 3158 | 1/1   | 0.89 | 0.32 | 77,77,77,77                | 0     |
| 60  | K    | 23SA  | 3540 | 1/1   | 0.89 | 0.06 | 79,79,79,79                | 0     |
| 59  | OHX  | 23SB  | 3170 | 7/7   | 0.89 | 0.08 | 132,138,158,216            | 0     |
| 58  | MG   | 23SA  | 3139 | 1/1   | 0.89 | 0.17 | 58,58,58,58                | 0     |
| 60  | K    | 23SB  | 3446 | 1/1   | 0.89 | 0.13 | 85,85,85,85                | 0     |
| 60  | K    | 23SB  | 3447 | 1/1   | 0.89 | 0.08 | 97,97,97,97                | 0     |
| 58  | MG   | 23SA  | 3121 | 1/1   | 0.89 | 0.18 | 54,54,54,54                | 0     |
| 59  | OHX  | 23SB  | 3176 | 7/7   | 0.89 | 0.09 | 143,147,163,222            | 0     |
| 58  | MG   | 23SB  | 3366 | 1/1   | 0.89 | 0.15 | 39,39,39,39                | 0     |
| 59  | OHX  | 23SB  | 3178 | 7/7   | 0.89 | 0.10 | 103,113,139,232            | 0     |
| 58  | MG   | 23SB  | 3200 | 1/1   | 0.89 | 0.25 | 39,39,39,39                | 0     |
| 58  | MG   | 23SB  | 3388 | 1/1   | 0.89 | 0.12 | 38,38,38,38                | 0     |
| 59  | OHX  | 23SA  | 3274 | 7/7   | 0.89 | 0.08 | 95,102,117,215             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 59  | OHX  | 5SA   | 214  | 7/7   | 0.89 | 0.08 | 138,149,161,234            | 0     |
| 60  | K    | 23SB  | 3480 | 1/1   | 0.89 | 0.13 | 80,80,80,80                | 0     |
| 59  | OHX  | 23SA  | 3286 | 7/7   | 0.89 | 0.24 | 75,84,102,179              | 0     |
| 59  | OHX  | 23SB  | 3188 | 7/7   | 0.89 | 0.08 | 134,155,164,228            | 0     |
| 58  | MG   | 23SA  | 3162 | 1/1   | 0.89 | 0.26 | 62,62,62,62                | 0     |
| 59  | OHX  | 23SB  | 3190 | 7/7   | 0.89 | 0.09 | 112,126,151,218            | 0     |
| 58  | MG   | 23SB  | 3237 | 1/1   | 0.89 | 0.20 | 73,73,73,73                | 0     |
| 59  | OHX  | 16SB  | 2250 | 7/7   | 0.89 | 0.09 | 110,121,130,223            | 0     |
| 59  | OHX  | 16SB  | 2253 | 7/7   | 0.89 | 0.09 | 122,127,146,233            | 0     |
| 59  | OHX  | 23SB  | 3195 | 7/7   | 0.89 | 0.09 | 182,185,190,255            | 0     |
| 60  | K    | 23SB  | 3508 | 1/1   | 0.89 | 0.14 | 76,76,76,76                | 0     |
| 60  | K    | 23SA  | 3591 | 1/1   | 0.89 | 0.10 | 66,66,66,66                | 0     |
| 60  | K    | 23SA  | 3592 | 1/1   | 0.89 | 0.09 | 67,67,67,67                | 0     |
| 58  | MG   | 23SA  | 3402 | 1/1   | 0.89 | 0.12 | 49,49,49,49                | 0     |
| 58  | MG   | 23SB  | 3308 | 1/1   | 0.89 | 0.14 | 73,73,73,73                | 0     |
| 59  | OHX  | 5SB   | 210  | 7/7   | 0.89 | 0.09 | 125,130,151,226            | 0     |
| 58  | MG   | 23SB  | 3273 | 1/1   | 0.89 | 0.36 | 51,51,51,51                | 0     |
| 58  | MG   | 23SA  | 3421 | 1/1   | 0.89 | 0.10 | 63,63,63,63                | 0     |
| 59  | OHX  | 23SA  | 3311 | 7/7   | 0.89 | 0.09 | 99,101,117,228             | 0     |
| 58  | MG   | 23SA  | 3163 | 1/1   | 0.89 | 0.19 | 45,45,45,45                | 0     |
| 58  | MG   | 23SB  | 3245 | 1/1   | 0.89 | 0.22 | 45,45,45,45                | 0     |
| 60  | K    | 16SA  | 2382 | 1/1   | 0.89 | 0.10 | 88,88,88,88                | 0     |
| 61  | SJE  | 23SA  | 3640 | 87/87 | 0.89 | 0.14 | 44,53,86,93                | 0     |
| 58  | MG   | 23SB  | 3260 | 1/1   | 0.90 | 0.34 | 63,63,63,63                | 0     |
| 58  | MG   | 23SA  | 3016 | 1/1   | 0.90 | 0.12 | 59,59,59,59                | 0     |
| 59  | OHX  | 23SA  | 3302 | 7/7   | 0.90 | 0.13 | 83,91,106,208              | 0     |
| 59  | OHX  | 23SB  | 3197 | 7/7   | 0.90 | 0.09 | 100,101,110,231            | 0     |
| 59  | OHX  | 23SB  | 3198 | 7/7   | 0.90 | 0.08 | 107,108,121,238            | 0     |
| 59  | OHX  | 16SB  | 2256 | 7/7   | 0.90 | 0.08 | 125,127,138,219            | 0     |
| 59  | OHX  | 5SB   | 208  | 7/7   | 0.90 | 0.10 | 98,111,123,206             | 0     |
| 58  | MG   | 23SB  | 3431 | 1/1   | 0.90 | 0.08 | 113,113,113,113            | 0     |
| 60  | K    | 23SA  | 3636 | 1/1   | 0.90 | 0.07 | 85,85,85,85                | 0     |
| 58  | MG   | 23SA  | 3150 | 1/1   | 0.90 | 0.20 | 60,60,60,60                | 0     |
| 59  | OHX  | 16SB  | 2262 | 7/7   | 0.90 | 0.08 | 158,164,176,252            | 0     |
| 58  | MG   | 23SB  | 3219 | 1/1   | 0.90 | 0.17 | 61,61,61,61                | 0     |
| 59  | OHX  | 23SA  | 3310 | 7/7   | 0.90 | 0.07 | 99,106,111,224             | 0     |
| 58  | MG   | 23SA  | 3524 | 1/1   | 0.90 | 0.07 | 113,113,113,113            | 0     |
| 60  | K    | 16SA  | 2381 | 1/1   | 0.90 | 0.09 | 109,109,109,109            | 0     |
| 58  | MG   | 23SA  | 3064 | 1/1   | 0.90 | 0.17 | 55,55,55,55                | 0     |
| 59  | OHX  | 23SA  | 3317 | 7/7   | 0.90 | 0.08 | 107,109,120,235            | 0     |
| 60  | K    | 16SB  | 2374 | 1/1   | 0.90 | 0.07 | 94,94,94,94                | 0     |
| 59  | OHX  | ASIB  | 103  | 7/7   | 0.90 | 0.08 | 124,130,147,238            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | OHX  | 23SA  | 3318 | 7/7   | 0.90 | 0.09 | 138,157,165,234             | 0     |
| 58  | MG   | 23SA  | 3172 | 1/1   | 0.90 | 0.30 | 58,58,58,58                 | 0     |
| 59  | OHX  | 23SB  | 3063 | 7/7   | 0.90 | 0.10 | 90,104,112,182              | 0     |
| 59  | OHX  | 23SB  | 3095 | 7/7   | 0.90 | 0.09 | 94,97,104,213               | 0     |
| 60  | K    | 16SB  | 2386 | 1/1   | 0.90 | 0.08 | 94,94,94,94                 | 0     |
| 59  | OHX  | 23SB  | 3099 | 7/7   | 0.90 | 0.08 | 87,101,111,219              | 0     |
| 58  | MG   | 23SA  | 3175 | 1/1   | 0.90 | 0.09 | 52,52,52,52                 | 0     |
| 59  | OHX  | 16SA  | 2281 | 7/7   | 0.90 | 0.09 | 106,115,123,199             | 0     |
| 59  | OHX  | 23SB  | 3117 | 7/7   | 0.90 | 0.22 | 88,92,98,197                | 0     |
| 59  | OHX  | 23SB  | 3118 | 7/7   | 0.90 | 0.08 | 114,118,121,225             | 0     |
| 59  | OHX  | 23SA  | 3342 | 7/7   | 0.90 | 0.27 | 87,93,102,203               | 0     |
| 59  | OHX  | 23SA  | 3343 | 7/7   | 0.90 | 0.10 | 93,117,131,217              | 0     |
| 58  | MG   | 16SA  | 2227 | 1/1   | 0.90 | 0.18 | 56,56,56,56                 | 0     |
| 58  | MG   | 23SB  | 3312 | 1/1   | 0.90 | 0.17 | 41,41,41,41                 | 0     |
| 60  | K    | 16SA  | 2411 | 1/1   | 0.90 | 0.25 | 82,82,82,82                 | 0     |
| 59  | OHX  | 23SB  | 3131 | 7/7   | 0.90 | 0.08 | 114,116,124,216             | 0     |
| 58  | MG   | 23SB  | 3232 | 1/1   | 0.90 | 0.23 | 60,60,60,60                 | 0     |
| 60  | K    | 16SA  | 2417 | 1/1   | 0.90 | 0.09 | 81,81,81,81                 | 0     |
| 59  | OHX  | 16SA  | 2307 | 7/7   | 0.90 | 0.09 | 106,110,119,215             | 0     |
| 59  | OHX  | 16SA  | 2310 | 7/7   | 0.90 | 0.10 | 109,114,122,197             | 0     |
| 60  | K    | 23SB  | 3445 | 1/1   | 0.90 | 0.09 | 66,66,66,66                 | 0     |
| 59  | OHX  | 23SB  | 3141 | 7/7   | 0.90 | 0.08 | 98,103,118,228              | 0     |
| 59  | OHX  | 16SA  | 2314 | 7/7   | 0.90 | 0.08 | 119,126,128,235             | 0     |
| 58  | MG   | 23SA  | 3019 | 1/1   | 0.90 | 0.10 | 35,35,35,35                 | 0     |
| 60  | K    | 23SB  | 3449 | 1/1   | 0.90 | 0.08 | 63,63,63,63                 | 0     |
| 60  | K    | 23SB  | 3454 | 1/1   | 0.90 | 0.08 | 74,74,74,74                 | 0     |
| 58  | MG   | 23SB  | 3278 | 1/1   | 0.90 | 0.16 | 45,45,45,45                 | 0     |
| 59  | OHX  | 23SA  | 3355 | 7/7   | 0.90 | 0.08 | 117,125,148,217             | 0     |
| 60  | K    | 23SB  | 3468 | 1/1   | 0.90 | 0.06 | 97,97,97,97                 | 0     |
| 58  | MG   | 23SB  | 3236 | 1/1   | 0.90 | 0.28 | 58,58,58,58                 | 0     |
| 60  | K    | 23SB  | 3473 | 1/1   | 0.90 | 0.11 | 108,108,108,108             | 0     |
| 59  | OHX  | 23SA  | 3360 | 7/7   | 0.90 | 0.10 | 90,94,110,208               | 0     |
| 59  | OHX  | 16SA  | 2323 | 7/7   | 0.90 | 0.08 | 162,167,181,233             | 0     |
| 58  | MG   | 16SB  | 2293 | 1/1   | 0.90 | 0.22 | 48,48,48,48                 | 0     |
| 58  | MG   | 16SA  | 2214 | 1/1   | 0.90 | 0.16 | 76,76,76,76                 | 0     |
| 58  | MG   | 23SA  | 3044 | 1/1   | 0.90 | 0.12 | 65,65,65,65                 | 0     |
| 59  | OHX  | 23SB  | 3168 | 7/7   | 0.90 | 0.10 | 123,133,154,222             | 0     |
| 60  | K    | 23SB  | 3490 | 1/1   | 0.90 | 0.07 | 84,84,84,84                 | 0     |
| 59  | OHX  | 23SA  | 3368 | 7/7   | 0.90 | 0.10 | 115,130,133,209             | 0     |
| 59  | OHX  | 23SB  | 3171 | 7/7   | 0.90 | 0.09 | 129,131,134,212             | 0     |
| 58  | MG   | 23SA  | 3141 | 1/1   | 0.90 | 0.24 | 60,60,60,60                 | 0     |
| 58  | MG   | 23SA  | 3123 | 1/1   | 0.90 | 0.12 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 58  | MG   | 23SB  | 3202 | 1/1   | 0.90 | 0.28 | 51,51,51,51                | 0     |
| 60  | K    | 23SB  | 3500 | 1/1   | 0.90 | 0.06 | 80,80,80,80                | 0     |
| 60  | K    | 23SA  | 3556 | 1/1   | 0.90 | 0.07 | 60,60,60,60                | 0     |
| 58  | MG   | 23SA  | 3007 | 1/1   | 0.90 | 0.24 | 61,61,61,61                | 0     |
| 60  | K    | 23SB  | 3507 | 1/1   | 0.90 | 0.10 | 72,72,72,72                | 0     |
| 58  | MG   | 23SB  | 3292 | 1/1   | 0.90 | 0.17 | 57,57,57,57                | 0     |
| 59  | OHX  | 23SA  | 3252 | 7/7   | 0.90 | 0.16 | 83,84,115,187              | 0     |
| 58  | MG   | 23SB  | 3346 | 1/1   | 0.90 | 0.11 | 56,56,56,56                | 0     |
| 58  | MG   | 23SA  | 3165 | 1/1   | 0.90 | 0.29 | 62,62,62,62                | 0     |
| 59  | OHX  | 23SB  | 3183 | 7/7   | 0.90 | 0.08 | 148,155,160,237            | 0     |
| 59  | OHX  | 5SA   | 208  | 7/7   | 0.90 | 0.08 | 98,106,114,218             | 0     |
| 60  | K    | 23SB  | 3516 | 1/1   | 0.90 | 0.14 | 77,77,77,77                | 0     |
| 58  | MG   | 23SA  | 3073 | 1/1   | 0.90 | 0.11 | 42,42,42,42                | 0     |
| 60  | K    | 23SB  | 3518 | 1/1   | 0.90 | 0.11 | 86,86,86,86                | 0     |
| 58  | MG   | 23SB  | 3296 | 1/1   | 0.90 | 0.42 | 72,72,72,72                | 0     |
| 59  | OHX  | 23SA  | 3284 | 7/7   | 0.90 | 0.17 | 84,87,97,215               | 0     |
| 58  | MG   | 23SA  | 3078 | 1/1   | 0.90 | 0.23 | 50,50,50,50                | 0     |
| 59  | OHX  | 23SB  | 3191 | 7/7   | 0.90 | 0.09 | 112,116,127,213            | 0     |
| 59  | OHX  | 16SB  | 2217 | 7/7   | 0.90 | 0.10 | 95,102,111,201             | 0     |
| 58  | MG   | 16SB  | 2306 | 1/1   | 0.90 | 0.19 | 56,56,56,56                | 0     |
| 59  | OHX  | 23SA  | 3377 | 7/7   | 0.91 | 0.08 | 145,154,161,239            | 0     |
| 59  | OHX  | 23SB  | 3150 | 7/7   | 0.91 | 0.08 | 134,143,159,230            | 0     |
| 58  | MG   | L34A  | 101  | 1/1   | 0.91 | 0.22 | 50,50,50,50                | 0     |
| 60  | K    | 16SA  | 2406 | 1/1   | 0.91 | 0.07 | 87,87,87,87                | 0     |
| 59  | OHX  | 23SB  | 3153 | 7/7   | 0.91 | 0.08 | 123,135,155,235            | 0     |
| 60  | K    | 16SB  | 2380 | 1/1   | 0.91 | 0.07 | 91,91,91,91                | 0     |
| 60  | K    | 16SA  | 2409 | 1/1   | 0.91 | 0.11 | 81,81,81,81                | 0     |
| 59  | OHX  | 23SB  | 3155 | 7/7   | 0.91 | 0.08 | 136,149,154,230            | 0     |
| 60  | K    | 16SA  | 2412 | 1/1   | 0.91 | 0.14 | 92,92,92,92                | 0     |
| 58  | MG   | 23SA  | 3061 | 1/1   | 0.91 | 0.10 | 83,83,83,83                | 0     |
| 58  | MG   | 23SA  | 3157 | 1/1   | 0.91 | 0.20 | 39,39,39,39                | 0     |
| 58  | MG   | 16SA  | 2240 | 1/1   | 0.91 | 0.32 | 70,70,70,70                | 0     |
| 58  | MG   | 23SA  | 3483 | 1/1   | 0.91 | 0.07 | 92,92,92,92                | 0     |
| 58  | MG   | L3B   | 301  | 1/1   | 0.91 | 0.17 | 40,40,40,40                | 0     |
| 58  | MG   | 16SB  | 2286 | 1/1   | 0.91 | 0.17 | 77,77,77,77                | 0     |
| 60  | K    | S6A   | 201  | 1/1   | 0.91 | 0.11 | 82,82,82,82                | 0     |
| 58  | MG   | 23SA  | 3082 | 1/1   | 0.91 | 0.16 | 50,50,50,50                | 0     |
| 58  | MG   | 23SA  | 3018 | 1/1   | 0.91 | 0.23 | 30,30,30,30                | 0     |
| 59  | OHX  | 16SB  | 2222 | 7/7   | 0.91 | 0.10 | 108,112,124,190            | 0     |
| 59  | OHX  | 16SB  | 2227 | 7/7   | 0.91 | 0.07 | 115,116,122,221            | 0     |
| 58  | MG   | 23SA  | 3084 | 1/1   | 0.91 | 0.05 | 64,64,64,64                | 0     |
| 59  | OHX  | 16SA  | 2286 | 7/7   | 0.91 | 0.24 | 75,88,94,169               | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 60  | K    | 23SA  | 3541 | 1/1   | 0.91 | 0.09 | 102,102,102,102            | 0     |
| 58  | MG   | 16SB  | 2320 | 1/1   | 0.91 | 0.21 | 62,62,62,62                | 0     |
| 59  | OHX  | 23SA  | 3324 | 7/7   | 0.91 | 0.09 | 85,91,107,225              | 0     |
| 58  | MG   | 16SA  | 2231 | 1/1   | 0.91 | 0.20 | 57,57,57,57                | 0     |
| 58  | MG   | 23SA  | 3164 | 1/1   | 0.91 | 0.27 | 61,61,61,61                | 0     |
| 58  | MG   | 16SA  | 2203 | 1/1   | 0.91 | 0.33 | 60,60,60,60                | 0     |
| 58  | MG   | 16SA  | 2225 | 1/1   | 0.91 | 0.22 | 50,50,50,50                | 0     |
| 59  | OHX  | 16SB  | 2263 | 7/7   | 0.91 | 0.08 | 157,159,167,234            | 0     |
| 58  | MG   | 23SA  | 3091 | 1/1   | 0.91 | 0.15 | 66,66,66,66                | 0     |
| 60  | K    | 23SA  | 3552 | 1/1   | 0.91 | 0.14 | 83,83,83,83                | 0     |
| 58  | MG   | 23SA  | 3111 | 1/1   | 0.91 | 0.17 | 56,56,56,56                | 0     |
| 58  | MG   | 23SB  | 3275 | 1/1   | 0.91 | 0.23 | 65,65,65,65                | 0     |
| 60  | K    | 23SA  | 3555 | 1/1   | 0.91 | 0.17 | 71,71,71,71                | 0     |
| 58  | MG   | 23SA  | 3112 | 1/1   | 0.91 | 0.06 | 60,60,60,60                | 0     |
| 60  | K    | 23SB  | 3474 | 1/1   | 0.91 | 0.09 | 63,63,63,63                | 0     |
| 59  | OHX  | 23SA  | 3348 | 7/7   | 0.91 | 0.09 | 138,148,158,224            | 0     |
| 59  | OHX  | 16SA  | 2319 | 7/7   | 0.91 | 0.07 | 131,143,148,232            | 0     |
| 59  | OHX  | PSIB  | 102  | 7/7   | 0.91 | 0.08 | 143,157,164,248            | 0     |
| 58  | MG   | 23SB  | 3227 | 1/1   | 0.91 | 0.09 | 76,76,76,76                | 0     |
| 58  | MG   | 23SA  | 3115 | 1/1   | 0.91 | 0.21 | 91,91,91,91                | 0     |
| 58  | MG   | 16SB  | 2299 | 1/1   | 0.91 | 0.20 | 50,50,50,50                | 0     |
| 60  | K    | 23SB  | 3485 | 1/1   | 0.91 | 0.10 | 72,72,72,72                | 0     |
| 60  | K    | 23SB  | 3487 | 1/1   | 0.91 | 0.06 | 65,65,65,65                | 0     |
| 59  | OHX  | 23SB  | 3087 | 7/7   | 0.91 | 0.17 | 86,94,99,175               | 0     |
| 60  | K    | 23SA  | 3587 | 1/1   | 0.91 | 0.07 | 91,91,91,91                | 0     |
| 59  | OHX  | 23SB  | 3089 | 7/7   | 0.91 | 0.07 | 106,112,116,216            | 0     |
| 59  | OHX  | 5SB   | 207  | 7/7   | 0.91 | 0.08 | 115,121,127,222            | 0     |
| 58  | MG   | 16SA  | 2244 | 1/1   | 0.91 | 0.28 | 62,62,62,62                | 0     |
| 58  | MG   | 23SA  | 3033 | 1/1   | 0.91 | 0.18 | 74,74,74,74                | 0     |
| 59  | OHX  | 23SA  | 3356 | 7/7   | 0.91 | 0.08 | 111,129,143,223            | 0     |
| 59  | OHX  | 23SA  | 3357 | 7/7   | 0.91 | 0.09 | 156,158,169,238            | 0     |
| 58  | MG   | L15A  | 202  | 1/1   | 0.91 | 0.15 | 59,59,59,59                | 0     |
| 59  | OHX  | 23SA  | 3359 | 7/7   | 0.91 | 0.08 | 128,136,163,233            | 0     |
| 58  | MG   | PSIA  | 101  | 1/1   | 0.91 | 0.30 | 54,54,54,54                | 0     |
| 58  | MG   | 23SB  | 3336 | 1/1   | 0.91 | 0.08 | 64,64,64,64                | 0     |
| 58  | MG   | 23SA  | 3120 | 1/1   | 0.91 | 0.09 | 67,67,67,67                | 0     |
| 59  | OHX  | 23SA  | 3221 | 7/7   | 0.91 | 0.10 | 73,86,105,162              | 0     |
| 60  | K    | 23SA  | 3631 | 1/1   | 0.91 | 0.10 | 78,78,78,78                | 0     |
| 60  | K    | 23SB  | 3514 | 1/1   | 0.91 | 0.23 | 95,95,95,95                | 0     |
| 58  | MG   | 16SA  | 2215 | 1/1   | 0.91 | 0.40 | 58,58,58,58                | 0     |
| 59  | OHX  | 23SA  | 3367 | 7/7   | 0.91 | 0.08 | 122,139,164,218            | 0     |
| 58  | MG   | 23SB  | 3288 | 1/1   | 0.91 | 0.14 | 72,72,72,72                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 59  | OHX  | 23SB  | 3136 | 7/7   | 0.91 | 0.09 | 97,102,117,216             | 0     |
| 59  | OHX  | 23SB  | 3138 | 7/7   | 0.91 | 0.09 | 150,164,170,228            | 0     |
| 58  | MG   | 23SB  | 3291 | 1/1   | 0.91 | 0.14 | 79,79,79,79                | 0     |
| 58  | MG   | 23SA  | 3079 | 1/1   | 0.91 | 0.11 | 76,76,76,76                | 0     |
| 58  | MG   | 23SB  | 3389 | 1/1   | 0.91 | 0.09 | 54,54,54,54                | 0     |
| 58  | MG   | 23SB  | 3248 | 1/1   | 0.91 | 0.35 | 44,44,44,44                | 0     |
| 58  | MG   | 23SB  | 3252 | 1/1   | 0.91 | 0.08 | 68,68,68,68                | 0     |
| 60  | K    | 5SA   | 219  | 1/1   | 0.92 | 0.05 | 72,72,72,72                | 0     |
| 59  | OHX  | 23SB  | 3130 | 7/7   | 0.92 | 0.08 | 106,117,124,209            | 0     |
| 58  | MG   | 23SB  | 3203 | 1/1   | 0.92 | 0.29 | 40,40,40,40                | 0     |
| 58  | MG   | 23SA  | 3424 | 1/1   | 0.92 | 0.11 | 36,36,36,36                | 0     |
| 58  | MG   | 16SB  | 2319 | 1/1   | 0.92 | 0.33 | 57,57,57,57                | 0     |
| 58  | MG   | 23SA  | 3167 | 1/1   | 0.92 | 0.20 | 77,77,77,77                | 0     |
| 58  | MG   | 23SA  | 3040 | 1/1   | 0.92 | 0.21 | 55,55,55,55                | 0     |
| 59  | OHX  | 23SB  | 3139 | 7/7   | 0.92 | 0.08 | 90,97,109,222              | 0     |
| 59  | OHX  | 23SA  | 3378 | 7/7   | 0.92 | 0.23 | 81,87,102,184              | 0     |
| 58  | MG   | 23SB  | 3429 | 1/1   | 0.92 | 0.16 | 93,93,93,93                | 0     |
| 59  | OHX  | 23SB  | 3142 | 7/7   | 0.92 | 0.08 | 136,146,149,236            | 0     |
| 58  | MG   | 23SA  | 3461 | 1/1   | 0.92 | 0.11 | 44,44,44,44                | 0     |
| 58  | MG   | 23SA  | 3482 | 1/1   | 0.92 | 0.11 | 66,66,66,66                | 0     |
| 59  | OHX  | 5SA   | 206  | 7/7   | 0.92 | 0.15 | 91,97,113,184              | 0     |
| 58  | MG   | 23SB  | 3214 | 1/1   | 0.92 | 0.19 | 48,48,48,48                | 0     |
| 58  | MG   | L27A  | 101  | 1/1   | 0.92 | 0.17 | 35,35,35,35                | 0     |
| 58  | MG   | 16SA  | 2216 | 1/1   | 0.92 | 0.28 | 46,46,46,46                | 0     |
| 60  | K    | 16SA  | 2414 | 1/1   | 0.92 | 0.07 | 100,100,100,100            | 0     |
| 58  | MG   | L3B   | 302  | 1/1   | 0.92 | 0.11 | 50,50,50,50                | 0     |
| 60  | K    | 16SB  | 2391 | 1/1   | 0.92 | 0.07 | 87,87,87,87                | 0     |
| 59  | OHX  | L15A  | 201  | 7/7   | 0.92 | 0.19 | 84,91,102,193              | 0     |
| 59  | OHX  | L27A  | 103  | 7/7   | 0.92 | 0.08 | 108,119,145,199            | 0     |
| 60  | K    | 16SB  | 2394 | 1/1   | 0.92 | 0.09 | 92,92,92,92                | 0     |
| 58  | MG   | 23SB  | 3264 | 1/1   | 0.92 | 0.08 | 55,55,55,55                | 0     |
| 58  | MG   | 23SA  | 3031 | 1/1   | 0.92 | 0.13 | 58,58,58,58                | 0     |
| 59  | OHX  | 23SB  | 3162 | 7/7   | 0.92 | 0.07 | 129,137,145,231            | 0     |
| 58  | MG   | 23SA  | 3487 | 1/1   | 0.92 | 0.11 | 40,40,40,40                | 0     |
| 59  | OHX  | 23SB  | 3164 | 7/7   | 0.92 | 0.08 | 124,135,157,228            | 0     |
| 58  | MG   | 23SA  | 3046 | 1/1   | 0.92 | 0.19 | 52,52,52,52                | 0     |
| 59  | OHX  | 16SB  | 2228 | 7/7   | 0.92 | 0.08 | 99,100,112,192             | 0     |
| 59  | OHX  | 16SB  | 2244 | 7/7   | 0.92 | 0.07 | 99,108,114,225             | 0     |
| 58  | MG   | 23SB  | 3269 | 1/1   | 0.92 | 0.25 | 50,50,50,50                | 0     |
| 58  | MG   | 23SA  | 3047 | 1/1   | 0.92 | 0.11 | 52,52,52,52                | 0     |
| 59  | OHX  | 23SA  | 3333 | 7/7   | 0.92 | 0.08 | 101,104,130,208            | 0     |
| 58  | MG   | 23SB  | 3226 | 1/1   | 0.92 | 0.16 | 60,60,60,60                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 59  | OHX  | 16SA  | 2295 | 7/7   | 0.92 | 0.08 | 97,101,119,212             | 0     |
| 59  | OHX  | 16SA  | 2299 | 7/7   | 0.92 | 0.08 | 107,114,116,211            | 0     |
| 58  | MG   | 23SA  | 3497 | 1/1   | 0.92 | 0.07 | 81,81,81,81                | 0     |
| 58  | MG   | 16SB  | 2339 | 1/1   | 0.92 | 0.06 | 124,124,124,124            | 0     |
| 58  | MG   | 23SB  | 3277 | 1/1   | 0.92 | 0.12 | 41,41,41,41                | 0     |
| 59  | OHX  | 23SB  | 3182 | 7/7   | 0.92 | 0.08 | 190,192,204,241            | 0     |
| 59  | OHX  | 16SA  | 2312 | 7/7   | 0.92 | 0.23 | 92,98,105,188              | 0     |
| 59  | OHX  | 23SB  | 3184 | 7/7   | 0.92 | 0.08 | 116,132,141,221            | 0     |
| 59  | OHX  | 16SB  | 2267 | 7/7   | 0.92 | 0.08 | 109,115,145,208            | 0     |
| 58  | MG   | 23SA  | 3032 | 1/1   | 0.92 | 0.16 | 49,49,49,49                | 0     |
| 58  | MG   | 16SB  | 2283 | 1/1   | 0.92 | 0.18 | 48,48,48,48                | 0     |
| 58  | MG   | 23SA  | 3500 | 1/1   | 0.92 | 0.12 | 49,49,49,49                | 0     |
| 60  | K    | 23SA  | 3559 | 1/1   | 0.92 | 0.19 | 82,82,82,82                | 0     |
| 58  | MG   | 16SB  | 2310 | 1/1   | 0.92 | 0.39 | 75,75,75,75                | 0     |
| 58  | MG   | 16SB  | 2285 | 1/1   | 0.92 | 0.14 | 65,65,65,65                | 0     |
| 58  | MG   | 16SA  | 2212 | 1/1   | 0.92 | 0.18 | 55,55,55,55                | 0     |
| 60  | K    | 23SA  | 3568 | 1/1   | 0.92 | 0.05 | 58,58,58,58                | 0     |
| 59  | OHX  | 16SA  | 2324 | 7/7   | 0.92 | 0.08 | 131,145,160,226            | 0     |
| 58  | MG   | 23SB  | 3329 | 1/1   | 0.92 | 0.24 | 64,64,64,64                | 0     |
| 58  | MG   | 23SA  | 3014 | 1/1   | 0.92 | 0.28 | 70,70,70,70                | 0     |
| 58  | MG   | 23SA  | 3384 | 1/1   | 0.92 | 0.11 | 43,43,43,43                | 0     |
| 58  | MG   | 23SB  | 3246 | 1/1   | 0.92 | 0.34 | 57,57,57,57                | 0     |
| 59  | OHX  | 23SB  | 3093 | 7/7   | 0.92 | 0.08 | 93,100,110,208             | 0     |
| 58  | MG   | 16SA  | 2208 | 1/1   | 0.92 | 0.17 | 77,77,77,77                | 0     |
| 59  | OHX  | 5SB   | 206  | 7/7   | 0.92 | 0.08 | 120,123,129,223            | 0     |
| 58  | MG   | 23SB  | 3361 | 1/1   | 0.92 | 0.11 | 51,51,51,51                | 0     |
| 59  | OHX  | 23SB  | 3104 | 7/7   | 0.92 | 0.08 | 111,116,130,225            | 0     |
| 60  | K    | 23SB  | 3505 | 1/1   | 0.92 | 0.12 | 75,75,75,75                | 0     |
| 59  | OHX  | 16SA  | 2340 | 7/7   | 0.92 | 0.08 | 102,105,115,209            | 0     |
| 59  | OHX  | 5SB   | 211  | 7/7   | 0.92 | 0.08 | 134,145,159,239            | 0     |
| 60  | K    | 23SA  | 3603 | 1/1   | 0.92 | 0.09 | 83,83,83,83                | 0     |
| 60  | K    | 23SA  | 3604 | 1/1   | 0.92 | 0.08 | 58,58,58,58                | 0     |
| 59  | OHX  | L20B  | 201  | 7/7   | 0.92 | 0.16 | 88,95,110,186              | 0     |
| 58  | MG   | 23SB  | 3364 | 1/1   | 0.92 | 0.08 | 65,65,65,65                | 0     |
| 58  | MG   | 23SA  | 3134 | 1/1   | 0.92 | 0.11 | 74,74,74,74                | 0     |
| 60  | K    | 23SA  | 3614 | 1/1   | 0.92 | 0.09 | 65,65,65,65                | 0     |
| 59  | OHX  | 23SA  | 3364 | 7/7   | 0.92 | 0.08 | 96,103,122,203             | 0     |
| 58  | MG   | 16SA  | 2233 | 1/1   | 0.92 | 0.10 | 71,71,71,71                | 0     |
| 60  | K    | 23SA  | 3626 | 1/1   | 0.92 | 0.06 | 69,69,69,69                | 0     |
| 59  | OHX  | 23SB  | 3120 | 7/7   | 0.92 | 0.07 | 94,104,115,226             | 0     |
| 59  | OHX  | 23SB  | 3121 | 7/7   | 0.92 | 0.08 | 95,102,110,221             | 0     |
| 59  | OHX  | 23SA  | 3239 | 7/7   | 0.92 | 0.08 | 95,99,109,191              | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 60  | K    | L4B   | 303  | 1/1   | 0.92 | 0.07 | 98,98,98,98                 | 0     |
| 58  | MG   | 23SB  | 3378 | 1/1   | 0.92 | 0.09 | 70,70,70,70                 | 0     |
| 58  | MG   | 23SB  | 3384 | 1/1   | 0.92 | 0.09 | 70,70,70,70                 | 0     |
| 59  | OHX  | 23SB  | 3129 | 7/7   | 0.92 | 0.07 | 103,109,115,227             | 0     |
| 58  | MG   | 23SA  | 3087 | 1/1   | 0.93 | 0.19 | 61,61,61,61                 | 0     |
| 59  | OHX  | 23SB  | 3158 | 7/7   | 0.93 | 0.08 | 105,107,121,203             | 0     |
| 60  | K    | 23SA  | 3578 | 1/1   | 0.93 | 0.05 | 54,54,54,54                 | 0     |
| 58  | MG   | 16SB  | 2336 | 1/1   | 0.93 | 0.07 | 105,105,105,105             | 0     |
| 58  | MG   | 23SA  | 3107 | 1/1   | 0.93 | 0.17 | 37,37,37,37                 | 0     |
| 58  | MG   | 23SB  | 3330 | 1/1   | 0.93 | 0.26 | 54,54,54,54                 | 0     |
| 59  | OHX  | 16SA  | 2327 | 7/7   | 0.93 | 0.07 | 134,143,149,217             | 0     |
| 58  | MG   | 23SA  | 3072 | 1/1   | 0.93 | 0.12 | 68,68,68,68                 | 0     |
| 59  | OHX  | 16SA  | 2331 | 7/7   | 0.93 | 0.07 | 155,162,169,236             | 0     |
| 59  | OHX  | 23SB  | 3167 | 7/7   | 0.93 | 0.08 | 121,136,143,203             | 0     |
| 60  | K    | 23SA  | 3593 | 1/1   | 0.93 | 0.05 | 69,69,69,69                 | 0     |
| 58  | MG   | 23SB  | 3333 | 1/1   | 0.93 | 0.10 | 42,42,42,42                 | 0     |
| 58  | MG   | 16SA  | 2253 | 1/1   | 0.93 | 0.27 | 50,50,50,50                 | 0     |
| 58  | MG   | 16SB  | 2348 | 1/1   | 0.93 | 0.07 | 56,56,56,56                 | 0     |
| 58  | MG   | 16SB  | 2305 | 1/1   | 0.93 | 0.27 | 67,67,67,67                 | 0     |
| 59  | OHX  | 23SB  | 3173 | 7/7   | 0.93 | 0.07 | 97,115,128,200              | 0     |
| 59  | OHX  | S4A   | 301  | 7/7   | 0.93 | 0.09 | 118,122,140,210             | 0     |
| 58  | MG   | 23SB  | 3241 | 1/1   | 0.93 | 0.13 | 50,50,50,50                 | 0     |
| 58  | MG   | 23SB  | 3243 | 1/1   | 0.93 | 0.23 | 30,30,30,30                 | 0     |
| 58  | MG   | 23SA  | 3437 | 1/1   | 0.93 | 0.23 | 67,67,67,67                 | 0     |
| 59  | OHX  | 23SA  | 3224 | 7/7   | 0.93 | 0.17 | 86,94,104,168               | 0     |
| 59  | OHX  | 5SA   | 212  | 7/7   | 0.93 | 0.07 | 89,95,109,210               | 0     |
| 60  | K    | 23SA  | 3618 | 1/1   | 0.93 | 0.05 | 62,62,62,62                 | 0     |
| 60  | K    | 23SA  | 3620 | 1/1   | 0.93 | 0.08 | 70,70,70,70                 | 0     |
| 60  | K    | 23SA  | 3623 | 1/1   | 0.93 | 0.06 | 80,80,80,80                 | 0     |
| 58  | MG   | 23SB  | 3287 | 1/1   | 0.93 | 0.16 | 61,61,61,61                 | 0     |
| 58  | MG   | 23SA  | 3075 | 1/1   | 0.93 | 0.30 | 61,61,61,61                 | 0     |
| 60  | K    | 23SA  | 3627 | 1/1   | 0.93 | 0.06 | 67,67,67,67                 | 0     |
| 58  | MG   | 23SB  | 3381 | 1/1   | 0.93 | 0.10 | 49,49,49,49                 | 0     |
| 58  | MG   | 23SB  | 3289 | 1/1   | 0.93 | 0.18 | 72,72,72,72                 | 0     |
| 59  | OHX  | 23SA  | 3261 | 7/7   | 0.93 | 0.18 | 78,81,93,181                | 0     |
| 59  | OHX  | 23SA  | 3262 | 7/7   | 0.93 | 0.17 | 81,85,101,178               | 0     |
| 59  | OHX  | 23SA  | 3266 | 7/7   | 0.93 | 0.23 | 81,85,97,177                | 0     |
| 59  | OHX  | 23SA  | 3270 | 7/7   | 0.93 | 0.08 | 109,117,127,194             | 0     |
| 60  | K    | 23SA  | 3639 | 1/1   | 0.93 | 0.07 | 80,80,80,80                 | 0     |
| 58  | MG   | 23SB  | 3386 | 1/1   | 0.93 | 0.07 | 91,91,91,91                 | 0     |
| 59  | OHX  | 16SB  | 2234 | 7/7   | 0.93 | 0.07 | 117,118,120,196             | 0     |
| 59  | OHX  | 16SB  | 2242 | 7/7   | 0.93 | 0.09 | 140,145,168,211             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 58  | MG   | 23SA  | 3452 | 1/1   | 0.93 | 0.11 | 40,40,40,40                | 0     |
| 58  | MG   | 23SA  | 3135 | 1/1   | 0.93 | 0.10 | 55,55,55,55                | 0     |
| 59  | OHX  | 23SA  | 3285 | 7/7   | 0.93 | 0.07 | 90,99,105,205              | 0     |
| 58  | MG   | 23SB  | 3391 | 1/1   | 0.93 | 0.07 | 71,71,71,71                | 0     |
| 59  | OHX  | 16SB  | 2252 | 7/7   | 0.93 | 0.08 | 109,120,138,208            | 0     |
| 58  | MG   | 23SB  | 3396 | 1/1   | 0.93 | 0.07 | 55,55,55,55                | 0     |
| 59  | OHX  | 23SA  | 3293 | 7/7   | 0.93 | 0.20 | 70,76,97,195               | 0     |
| 59  | OHX  | 5SB   | 205  | 7/7   | 0.93 | 0.07 | 120,123,130,211            | 0     |
| 58  | MG   | 23SB  | 3250 | 1/1   | 0.93 | 0.25 | 41,41,41,41                | 0     |
| 59  | OHX  | 16SB  | 2259 | 7/7   | 0.93 | 0.07 | 145,150,156,224            | 0     |
| 58  | MG   | 23SB  | 3294 | 1/1   | 0.93 | 0.07 | 55,55,55,55                | 0     |
| 59  | OHX  | 5SB   | 209  | 7/7   | 0.93 | 0.08 | 121,127,134,216            | 0     |
| 59  | OHX  | 23SA  | 3301 | 7/7   | 0.93 | 0.07 | 121,123,127,230            | 0     |
| 58  | MG   | L35A  | 101  | 1/1   | 0.93 | 0.16 | 51,51,51,51                | 0     |
| 58  | MG   | 23SB  | 3428 | 1/1   | 0.93 | 0.08 | 84,84,84,84                | 0     |
| 60  | K    | 16SA  | 2375 | 1/1   | 0.93 | 0.07 | 101,101,101,101            | 0     |
| 59  | OHX  | 23SA  | 3306 | 7/7   | 0.93 | 0.07 | 100,113,126,199            | 0     |
| 59  | OHX  | 16SB  | 2268 | 7/7   | 0.93 | 0.07 | 123,133,154,220            | 0     |
| 59  | OHX  | 16SB  | 2271 | 7/7   | 0.93 | 0.07 | 156,167,170,247            | 0     |
| 58  | MG   | 23SA  | 3467 | 1/1   | 0.93 | 0.08 | 41,41,41,41                | 0     |
| 58  | MG   | 23SA  | 3472 | 1/1   | 0.93 | 0.14 | 39,39,39,39                | 0     |
| 59  | OHX  | 23SA  | 3309 | 7/7   | 0.93 | 0.14 | 85,88,102,183              | 0     |
| 59  | OHX  | 16SB  | 2276 | 7/7   | 0.93 | 0.07 | 131,137,146,224            | 0     |
| 58  | MG   | 23SB  | 3437 | 1/1   | 0.93 | 0.29 | 86,86,86,86                | 0     |
| 58  | MG   | 23SA  | 3077 | 1/1   | 0.93 | 0.18 | 48,48,48,48                | 0     |
| 58  | MG   | 23SA  | 3003 | 1/1   | 0.93 | 0.15 | 60,60,60,60                | 0     |
| 59  | OHX  | 23SA  | 3314 | 7/7   | 0.93 | 0.07 | 95,99,111,204              | 0     |
| 58  | MG   | 23SA  | 3138 | 1/1   | 0.93 | 0.08 | 46,46,46,46                | 0     |
| 60  | K    | 23SB  | 3440 | 1/1   | 0.93 | 0.07 | 94,94,94,94                | 0     |
| 60  | K    | 16SA  | 2388 | 1/1   | 0.93 | 0.25 | 79,79,79,79                | 0     |
| 59  | OHX  | 23SB  | 3051 | 7/7   | 0.93 | 0.15 | 94,102,104,171             | 0     |
| 59  | OHX  | 23SB  | 3052 | 7/7   | 0.93 | 0.21 | 91,95,101,175              | 0     |
| 58  | MG   | 23SA  | 3114 | 1/1   | 0.93 | 0.08 | 55,55,55,55                | 0     |
| 59  | OHX  | 23SB  | 3067 | 7/7   | 0.93 | 0.09 | 79,95,108,174              | 0     |
| 59  | OHX  | 23SA  | 3319 | 7/7   | 0.93 | 0.19 | 82,85,93,207               | 0     |
| 59  | OHX  | 23SA  | 3320 | 7/7   | 0.93 | 0.07 | 94,95,109,191              | 0     |
| 59  | OHX  | 23SA  | 3323 | 7/7   | 0.93 | 0.12 | 84,89,105,197              | 0     |
| 58  | MG   | 16SA  | 2228 | 1/1   | 0.93 | 0.29 | 64,64,64,64                | 0     |
| 59  | OHX  | 23SA  | 3331 | 7/7   | 0.93 | 0.07 | 91,98,108,201              | 0     |
| 58  | MG   | 16SA  | 2217 | 1/1   | 0.93 | 0.14 | 40,40,40,40                | 0     |
| 60  | K    | 23SB  | 3470 | 1/1   | 0.93 | 0.14 | 78,78,78,78                | 0     |
| 59  | OHX  | 23SA  | 3334 | 7/7   | 0.93 | 0.07 | 99,115,137,214             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 60  | K    | 23SB  | 3472 | 1/1   | 0.93 | 0.16 | 77,77,77,77                | 0     |
| 59  | OHX  | 23SB  | 3111 | 7/7   | 0.93 | 0.08 | 103,108,114,205            | 0     |
| 59  | OHX  | 23SB  | 3112 | 7/7   | 0.93 | 0.07 | 104,112,119,206            | 0     |
| 59  | OHX  | 23SB  | 3113 | 7/7   | 0.93 | 0.07 | 112,115,125,216            | 0     |
| 58  | MG   | 16SA  | 2363 | 1/1   | 0.93 | 0.07 | 72,72,72,72                | 0     |
| 59  | OHX  | 23SA  | 3337 | 7/7   | 0.93 | 0.07 | 109,123,134,204            | 0     |
| 59  | OHX  | 23SA  | 3338 | 7/7   | 0.93 | 0.07 | 138,150,158,232            | 0     |
| 58  | MG   | 23SA  | 3054 | 1/1   | 0.93 | 0.24 | 51,51,51,51                | 0     |
| 59  | OHX  | 23SA  | 3340 | 7/7   | 0.93 | 0.08 | 133,146,163,217            | 0     |
| 58  | MG   | L35B  | 103  | 1/1   | 0.93 | 0.19 | 82,82,82,82                | 0     |
| 60  | K    | 23SB  | 3486 | 1/1   | 0.93 | 0.09 | 73,73,73,73                | 0     |
| 58  | MG   | 23SB  | 3213 | 1/1   | 0.93 | 0.16 | 40,40,40,40                | 0     |
| 60  | K    | 23SB  | 3488 | 1/1   | 0.93 | 0.08 | 85,85,85,85                | 0     |
| 60  | K    | 23SB  | 3489 | 1/1   | 0.93 | 0.05 | 65,65,65,65                | 0     |
| 59  | OHX  | 23SB  | 3124 | 7/7   | 0.93 | 0.08 | 83,94,106,213              | 0     |
| 58  | MG   | 16SA  | 2367 | 1/1   | 0.93 | 0.16 | 83,83,83,83                | 0     |
| 59  | OHX  | 23SA  | 3344 | 7/7   | 0.93 | 0.07 | 95,121,141,216             | 0     |
| 58  | MG   | 23SA  | 3146 | 1/1   | 0.93 | 0.23 | 48,48,48,48                | 0     |
| 58  | MG   | 23SB  | 3313 | 1/1   | 0.93 | 0.05 | 48,48,48,48                | 0     |
| 58  | MG   | 23SB  | 3266 | 1/1   | 0.93 | 0.17 | 38,38,38,38                | 0     |
| 59  | OHX  | 16SA  | 2296 | 7/7   | 0.93 | 0.08 | 87,99,108,193              | 0     |
| 58  | MG   | 16SA  | 2374 | 1/1   | 0.93 | 0.14 | 73,73,73,73                | 0     |
| 58  | MG   | 23SA  | 3122 | 1/1   | 0.93 | 0.10 | 57,57,57,57                | 0     |
| 60  | K    | 23SB  | 3504 | 1/1   | 0.93 | 0.09 | 87,87,87,87                | 0     |
| 60  | K    | 23SA  | 3543 | 1/1   | 0.93 | 0.10 | 86,86,86,86                | 0     |
| 59  | OHX  | 16SA  | 2304 | 7/7   | 0.93 | 0.20 | 88,96,98,193               | 0     |
| 59  | OHX  | 16SA  | 2306 | 7/7   | 0.93 | 0.08 | 109,111,118,204            | 0     |
| 58  | MG   | 23SB  | 3317 | 1/1   | 0.93 | 0.11 | 78,78,78,78                | 0     |
| 59  | OHX  | 16SA  | 2309 | 7/7   | 0.93 | 0.08 | 132,139,149,214            | 0     |
| 58  | MG   | 23SA  | 3085 | 1/1   | 0.93 | 0.15 | 52,52,52,52                | 0     |
| 58  | MG   | 23SB  | 3270 | 1/1   | 0.93 | 0.22 | 43,43,43,43                | 0     |
| 58  | MG   | 16SA  | 2256 | 1/1   | 0.93 | 0.14 | 72,72,72,72                | 0     |
| 59  | OHX  | 23SB  | 3145 | 7/7   | 0.93 | 0.08 | 106,124,142,220            | 0     |
| 58  | MG   | 23SA  | 3393 | 1/1   | 0.93 | 0.09 | 54,54,54,54                | 0     |
| 58  | MG   | 23SA  | 3125 | 1/1   | 0.93 | 0.15 | 62,62,62,62                | 0     |
| 58  | MG   | 23SA  | 3411 | 1/1   | 0.93 | 0.10 | 43,43,43,43                | 0     |
| 58  | MG   | 23SB  | 3325 | 1/1   | 0.93 | 0.16 | 47,47,47,47                | 0     |
| 60  | K    | 23SA  | 3557 | 1/1   | 0.93 | 0.07 | 84,84,84,84                | 0     |
| 59  | OHX  | 23SB  | 3152 | 7/7   | 0.93 | 0.08 | 103,105,129,194            | 0     |
| 59  | OHX  | 16SA  | 2321 | 7/7   | 0.93 | 0.07 | 157,159,162,233            | 0     |
| 59  | OHX  | 16SA  | 2322 | 7/7   | 0.93 | 0.07 | 118,126,134,205            | 0     |
| 59  | OHX  | 23SB  | 3156 | 7/7   | 0.93 | 0.06 | 125,130,147,212            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 60  | K    | 23SA  | 3564 | 1/1   | 0.93 | 0.08 | 72,72,72,72                | 0     |
| 61  | SJE  | 23SB  | 3521 | 87/87 | 0.93 | 0.14 | 48,59,87,95                | 0     |
| 59  | OHX  | 16SA  | 2274 | 7/7   | 0.94 | 0.14 | 93,97,105,164              | 0     |
| 59  | OHX  | 16SB  | 2233 | 7/7   | 0.94 | 0.07 | 93,102,105,189             | 0     |
| 59  | OHX  | 16SA  | 2279 | 7/7   | 0.94 | 0.08 | 118,121,129,197            | 0     |
| 59  | OHX  | 16SB  | 2236 | 7/7   | 0.94 | 0.07 | 104,107,118,194            | 0     |
| 59  | OHX  | 23SB  | 3175 | 7/7   | 0.94 | 0.07 | 138,142,159,216            | 0     |
| 59  | OHX  | 16SB  | 2238 | 7/7   | 0.94 | 0.06 | 124,131,141,228            | 0     |
| 60  | K    | 23SA  | 3601 | 1/1   | 0.94 | 0.08 | 55,55,55,55                | 0     |
| 59  | OHX  | 16SB  | 2239 | 7/7   | 0.94 | 0.07 | 116,122,133,205            | 0     |
| 58  | MG   | 23SA  | 3155 | 1/1   | 0.94 | 0.17 | 55,55,55,55                | 0     |
| 60  | K    | 23SA  | 3606 | 1/1   | 0.94 | 0.05 | 57,57,57,57                | 0     |
| 59  | OHX  | 23SA  | 3299 | 7/7   | 0.94 | 0.11 | 69,80,102,183              | 0     |
| 60  | K    | 23SA  | 3609 | 1/1   | 0.94 | 0.06 | 71,71,71,71                | 0     |
| 60  | K    | 23SA  | 3610 | 1/1   | 0.94 | 0.08 | 62,62,62,62                | 0     |
| 59  | OHX  | 23SA  | 3300 | 7/7   | 0.94 | 0.06 | 99,105,112,220             | 0     |
| 60  | K    | 23SA  | 3612 | 1/1   | 0.94 | 0.04 | 73,73,73,73                | 0     |
| 59  | OHX  | 16SB  | 2247 | 7/7   | 0.94 | 0.08 | 100,103,110,200            | 0     |
| 58  | MG   | 16SB  | 2297 | 1/1   | 0.94 | 0.29 | 64,64,64,64                | 0     |
| 59  | OHX  | 16SA  | 2288 | 7/7   | 0.94 | 0.07 | 90,100,106,201             | 0     |
| 58  | MG   | 23SB  | 3251 | 1/1   | 0.94 | 0.28 | 54,54,54,54                | 0     |
| 60  | K    | 23SA  | 3619 | 1/1   | 0.94 | 0.04 | 81,81,81,81                | 0     |
| 58  | MG   | 23SB  | 3206 | 1/1   | 0.94 | 0.24 | 34,34,34,34                | 0     |
| 60  | K    | 23SA  | 3622 | 1/1   | 0.94 | 0.07 | 61,61,61,61                | 0     |
| 59  | OHX  | 16SA  | 2293 | 7/7   | 0.94 | 0.09 | 92,98,111,198              | 0     |
| 59  | OHX  | 23SB  | 3187 | 7/7   | 0.94 | 0.06 | 134,143,152,229            | 0     |
| 58  | MG   | 23SA  | 3173 | 1/1   | 0.94 | 0.06 | 59,59,59,59                | 0     |
| 58  | MG   | 23SA  | 3093 | 1/1   | 0.94 | 0.06 | 77,77,77,77                | 0     |
| 59  | OHX  | 16SA  | 2297 | 7/7   | 0.94 | 0.07 | 114,122,131,209            | 0     |
| 59  | OHX  | 16SA  | 2298 | 7/7   | 0.94 | 0.19 | 80,87,106,181              | 0     |
| 58  | MG   | 16SB  | 2300 | 1/1   | 0.94 | 0.31 | 48,48,48,48                | 0     |
| 58  | MG   | 23SB  | 3256 | 1/1   | 0.94 | 0.16 | 47,47,47,47                | 0     |
| 59  | OHX  | 16SB  | 2266 | 7/7   | 0.94 | 0.07 | 135,142,152,217            | 0     |
| 59  | OHX  | 23SA  | 3315 | 7/7   | 0.94 | 0.07 | 98,100,118,232             | 0     |
| 59  | OHX  | 16SA  | 2301 | 7/7   | 0.94 | 0.07 | 107,112,121,213            | 0     |
| 59  | OHX  | 16SB  | 2270 | 7/7   | 0.94 | 0.08 | 116,127,150,209            | 0     |
| 58  | MG   | 16SA  | 2251 | 1/1   | 0.94 | 0.28 | 60,60,60,60                | 0     |
| 59  | OHX  | 16SA  | 2305 | 7/7   | 0.94 | 0.07 | 133,141,150,228            | 0     |
| 59  | OHX  | 5SB   | 204  | 7/7   | 0.94 | 0.07 | 98,106,120,191             | 0     |
| 58  | MG   | 23SB  | 3356 | 1/1   | 0.94 | 0.07 | 39,39,39,39                | 0     |
| 59  | OHX  | 16SB  | 2274 | 7/7   | 0.94 | 0.07 | 131,136,142,211            | 0     |
| 58  | MG   | 23SA  | 3056 | 1/1   | 0.94 | 0.14 | 48,48,48,48                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 23SA  | 3001 | 1/1   | 0.94 | 0.30 | 34,34,34,34                 | 0     |
| 59  | OHX  | 23SA  | 3325 | 7/7   | 0.94 | 0.06 | 89,95,103,220               | 0     |
| 59  | OHX  | 16SB  | 2278 | 7/7   | 0.94 | 0.07 | 112,116,120,223             | 0     |
| 60  | K    | 16SB  | 2376 | 1/1   | 0.94 | 0.05 | 75,75,75,75                 | 0     |
| 60  | K    | 16SB  | 2377 | 1/1   | 0.94 | 0.06 | 82,82,82,82                 | 0     |
| 59  | OHX  | 23SA  | 3327 | 7/7   | 0.94 | 0.07 | 88,96,114,211               | 0     |
| 58  | MG   | 23SB  | 3216 | 1/1   | 0.94 | 0.12 | 42,42,42,42                 | 0     |
| 58  | MG   | 16SB  | 2331 | 1/1   | 0.94 | 0.28 | 55,55,55,55                 | 0     |
| 59  | OHX  | 16SA  | 2313 | 7/7   | 0.94 | 0.07 | 110,116,122,207             | 0     |
| 58  | MG   | 23SB  | 3370 | 1/1   | 0.94 | 0.08 | 49,49,49,49                 | 0     |
| 58  | MG   | 23SA  | 3160 | 1/1   | 0.94 | 0.13 | 55,55,55,55                 | 0     |
| 59  | OHX  | 23SB  | 3054 | 7/7   | 0.94 | 0.18 | 89,95,100,168               | 0     |
| 59  | OHX  | 23SB  | 3058 | 7/7   | 0.94 | 0.15 | 80,87,94,165                | 0     |
| 59  | OHX  | 23SB  | 3059 | 7/7   | 0.94 | 0.12 | 91,101,107,175              | 0     |
| 58  | MG   | 23SB  | 3377 | 1/1   | 0.94 | 0.07 | 47,47,47,47                 | 0     |
| 59  | OHX  | 16SA  | 2317 | 7/7   | 0.94 | 0.09 | 112,120,138,202             | 0     |
| 59  | OHX  | 23SB  | 3074 | 7/7   | 0.94 | 0.21 | 82,94,96,173                | 0     |
| 59  | OHX  | 23SB  | 3079 | 7/7   | 0.94 | 0.12 | 94,98,106,173               | 0     |
| 59  | OHX  | 23SB  | 3081 | 7/7   | 0.94 | 0.07 | 100,106,119,201             | 0     |
| 58  | MG   | 16SA  | 2359 | 1/1   | 0.94 | 0.11 | 62,62,62,62                 | 0     |
| 58  | MG   | 23SA  | 3010 | 1/1   | 0.94 | 0.17 | 39,39,39,39                 | 0     |
| 58  | MG   | 23SB  | 3383 | 1/1   | 0.94 | 0.07 | 77,77,77,77                 | 0     |
| 58  | MG   | 23SB  | 3302 | 1/1   | 0.94 | 0.17 | 49,49,49,49                 | 0     |
| 58  | MG   | 23SB  | 3385 | 1/1   | 0.94 | 0.07 | 82,82,82,82                 | 0     |
| 59  | OHX  | 23SB  | 3103 | 7/7   | 0.94 | 0.18 | 67,90,98,176                | 0     |
| 58  | MG   | 23SA  | 3420 | 1/1   | 0.94 | 0.09 | 57,57,57,57                 | 0     |
| 59  | OHX  | 23SB  | 3105 | 7/7   | 0.94 | 0.17 | 88,96,107,174               | 0     |
| 59  | OHX  | 23SB  | 3107 | 7/7   | 0.94 | 0.07 | 102,114,119,205             | 0     |
| 58  | MG   | 16SB  | 2341 | 1/1   | 0.94 | 0.07 | 130,130,130,130             | 0     |
| 58  | MG   | 23SB  | 3305 | 1/1   | 0.94 | 0.10 | 65,65,65,65                 | 0     |
| 58  | MG   | 23SB  | 3390 | 1/1   | 0.94 | 0.10 | 44,44,44,44                 | 0     |
| 60  | K    | 16SA  | 2407 | 1/1   | 0.94 | 0.05 | 75,75,75,75                 | 0     |
| 58  | MG   | 23SB  | 3306 | 1/1   | 0.94 | 0.17 | 65,65,65,65                 | 0     |
| 59  | OHX  | 16SA  | 2330 | 7/7   | 0.94 | 0.07 | 153,156,163,230             | 0     |
| 60  | K    | 23SB  | 3450 | 1/1   | 0.94 | 0.07 | 72,72,72,72                 | 0     |
| 60  | K    | 23SB  | 3451 | 1/1   | 0.94 | 0.06 | 67,67,67,67                 | 0     |
| 59  | OHX  | 23SA  | 3351 | 7/7   | 0.94 | 0.07 | 116,125,140,218             | 0     |
| 58  | MG   | 23SB  | 3393 | 1/1   | 0.94 | 0.08 | 70,70,70,70                 | 0     |
| 60  | K    | 23SB  | 3464 | 1/1   | 0.94 | 0.07 | 53,53,53,53                 | 0     |
| 60  | K    | 23SB  | 3465 | 1/1   | 0.94 | 0.12 | 75,75,75,75                 | 0     |
| 60  | K    | 16SA  | 2413 | 1/1   | 0.94 | 0.07 | 84,84,84,84                 | 0     |
| 58  | MG   | 23SA  | 3505 | 1/1   | 0.94 | 0.11 | 40,40,40,40                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 23SA  | 3513 | 1/1   | 0.94 | 0.08 | 84,84,84,84                 | 0     |
| 58  | MG   | 23SB  | 3417 | 1/1   | 0.94 | 0.06 | 84,84,84,84                 | 0     |
| 58  | MG   | 23SB  | 3228 | 1/1   | 0.94 | 0.26 | 43,43,43,43                 | 0     |
| 59  | OHX  | 16SA  | 2341 | 7/7   | 0.94 | 0.07 | 135,136,149,239             | 0     |
| 58  | MG   | 23SA  | 3011 | 1/1   | 0.94 | 0.19 | 42,42,42,42                 | 0     |
| 59  | OHX  | S10A  | 201  | 7/7   | 0.94 | 0.08 | 106,108,115,206             | 0     |
| 58  | MG   | 23SB  | 3231 | 1/1   | 0.94 | 0.12 | 51,51,51,51                 | 0     |
| 58  | MG   | 23SB  | 3271 | 1/1   | 0.94 | 0.20 | 46,46,46,46                 | 0     |
| 59  | OHX  | 23SA  | 3195 | 7/7   | 0.94 | 0.11 | 71,86,93,123                | 0     |
| 59  | OHX  | 23SA  | 3212 | 7/7   | 0.94 | 0.11 | 51,57,86,140                | 0     |
| 58  | MG   | 23SB  | 3430 | 1/1   | 0.94 | 0.09 | 70,70,70,70                 | 0     |
| 58  | MG   | 16SB  | 2354 | 1/1   | 0.94 | 0.06 | 102,102,102,102             | 0     |
| 59  | OHX  | 23SA  | 3366 | 7/7   | 0.94 | 0.07 | 99,105,125,207              | 0     |
| 58  | MG   | 23SB  | 3434 | 1/1   | 0.94 | 0.06 | 96,96,96,96                 | 0     |
| 58  | MG   | 23SB  | 3436 | 1/1   | 0.94 | 0.10 | 94,94,94,94                 | 0     |
| 59  | OHX  | 23SA  | 3255 | 7/7   | 0.94 | 0.08 | 131,151,160,208             | 0     |
| 59  | OHX  | 23SA  | 3256 | 7/7   | 0.94 | 0.21 | 72,85,91,147                | 0     |
| 58  | MG   | 23SA  | 3076 | 1/1   | 0.94 | 0.18 | 57,57,57,57                 | 0     |
| 59  | OHX  | 23SA  | 3372 | 7/7   | 0.94 | 0.08 | 103,116,140,217             | 0     |
| 58  | MG   | 23SB  | 3439 | 1/1   | 0.94 | 0.08 | 87,87,87,87                 | 0     |
| 60  | K    | 23SB  | 3496 | 1/1   | 0.94 | 0.08 | 85,85,85,85                 | 0     |
| 59  | OHX  | 23SB  | 3146 | 7/7   | 0.94 | 0.07 | 98,108,114,209              | 0     |
| 59  | OHX  | 23SA  | 3259 | 7/7   | 0.94 | 0.07 | 90,96,110,189               | 0     |
| 59  | OHX  | 23SA  | 3376 | 7/7   | 0.94 | 0.08 | 121,128,151,229             | 0     |
| 59  | OHX  | 23SA  | 3260 | 7/7   | 0.94 | 0.19 | 71,90,98,175                | 0     |
| 58  | MG   | 23SA  | 3133 | 1/1   | 0.94 | 0.11 | 48,48,48,48                 | 0     |
| 58  | MG   | 23SA  | 3035 | 1/1   | 0.94 | 0.13 | 52,52,52,52                 | 0     |
| 58  | MG   | 23SA  | 3149 | 1/1   | 0.94 | 0.25 | 66,66,66,66                 | 0     |
| 59  | OHX  | 23SB  | 3154 | 7/7   | 0.94 | 0.09 | 165,172,176,225             | 0     |
| 59  | OHX  | 23SA  | 3267 | 7/7   | 0.94 | 0.18 | 91,99,103,186               | 0     |
| 60  | K    | 23SA  | 3558 | 1/1   | 0.94 | 0.10 | 55,55,55,55                 | 0     |
| 59  | OHX  | 23SA  | 3269 | 7/7   | 0.94 | 0.22 | 86,89,103,177               | 0     |
| 58  | MG   | 23SA  | 3443 | 1/1   | 0.94 | 0.16 | 32,32,32,32                 | 0     |
| 58  | MG   | 23SA  | 3050 | 1/1   | 0.94 | 0.16 | 58,58,58,58                 | 0     |
| 58  | MG   | 5SA   | 216  | 1/1   | 0.94 | 0.07 | 67,67,67,67                 | 0     |
| 59  | OHX  | 23SB  | 3160 | 7/7   | 0.94 | 0.07 | 120,142,146,214             | 0     |
| 59  | OHX  | 23SA  | 3275 | 7/7   | 0.94 | 0.07 | 100,110,119,213             | 0     |
| 59  | OHX  | 23SA  | 3277 | 7/7   | 0.94 | 0.19 | 76,84,101,204               | 0     |
| 59  | OHX  | 23SA  | 3278 | 7/7   | 0.94 | 0.07 | 85,98,101,210               | 0     |
| 60  | K    | 23SA  | 3580 | 1/1   | 0.94 | 0.11 | 39,39,39,39                 | 0     |
| 58  | MG   | 23SA  | 3151 | 1/1   | 0.94 | 0.12 | 59,59,59,59                 | 0     |
| 58  | MG   | 16SA  | 2368 | 1/1   | 0.94 | 0.06 | 91,91,91,91                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 59  | OHX  | 23SB  | 3166 | 7/7   | 0.94 | 0.08 | 91,100,114,205             | 0     |
| 58  | MG   | 16SA  | 2360 | 1/1   | 0.94 | 0.10 | 72,72,72,72                | 0     |
| 59  | OHX  | 16SA  | 2271 | 7/7   | 0.94 | 0.10 | 80,94,97,147               | 0     |
| 60  | K    | 23SA  | 3589 | 1/1   | 0.94 | 0.10 | 85,85,85,85                | 0     |
| 59  | OHX  | 23SA  | 3292 | 7/7   | 0.94 | 0.11 | 68,81,98,170               | 0     |
| 58  | MG   | 16SA  | 2369 | 1/1   | 0.95 | 0.05 | 120,120,120,120            | 0     |
| 58  | MG   | 23SA  | 3174 | 1/1   | 0.95 | 0.11 | 53,53,53,53                | 0     |
| 58  | MG   | 23SB  | 3298 | 1/1   | 0.95 | 0.27 | 55,55,55,55                | 0     |
| 59  | OHX  | 16SA  | 2308 | 7/7   | 0.95 | 0.06 | 110,118,129,200            | 0     |
| 60  | K    | 23SA  | 3602 | 1/1   | 0.95 | 0.06 | 67,67,67,67                | 0     |
| 58  | MG   | 23SA  | 3477 | 1/1   | 0.95 | 0.11 | 90,90,90,90                | 0     |
| 58  | MG   | 23SA  | 3478 | 1/1   | 0.95 | 0.08 | 50,50,50,50                | 0     |
| 60  | K    | 23SA  | 3605 | 1/1   | 0.95 | 0.05 | 74,74,74,74                | 0     |
| 59  | OHX  | 16SA  | 2311 | 7/7   | 0.95 | 0.07 | 102,108,117,196            | 0     |
| 59  | OHX  | 16SB  | 2251 | 7/7   | 0.95 | 0.07 | 125,131,136,216            | 0     |
| 58  | MG   | 23SA  | 3479 | 1/1   | 0.95 | 0.11 | 76,76,76,76                | 0     |
| 58  | MG   | 23SA  | 3098 | 1/1   | 0.95 | 0.06 | 54,54,54,54                | 0     |
| 59  | OHX  | 16SB  | 2254 | 7/7   | 0.95 | 0.07 | 100,105,128,186            | 0     |
| 58  | MG   | 23SA  | 3027 | 1/1   | 0.95 | 0.14 | 45,45,45,45                | 0     |
| 58  | MG   | 16SA  | 2371 | 1/1   | 0.95 | 0.05 | 100,100,100,100            | 0     |
| 58  | MG   | 16SB  | 2280 | 1/1   | 0.95 | 0.12 | 59,59,59,59                | 0     |
| 59  | OHX  | 16SB  | 2260 | 7/7   | 0.95 | 0.07 | 145,153,160,239            | 0     |
| 59  | OHX  | 23SA  | 3316 | 7/7   | 0.95 | 0.06 | 90,97,113,204              | 0     |
| 58  | MG   | 23SA  | 3486 | 1/1   | 0.95 | 0.08 | 42,42,42,42                | 0     |
| 58  | MG   | 23SA  | 3048 | 1/1   | 0.95 | 0.14 | 33,33,33,33                | 0     |
| 58  | MG   | 23SA  | 3391 | 1/1   | 0.95 | 0.10 | 37,37,37,37                | 0     |
| 59  | OHX  | 16SB  | 2265 | 7/7   | 0.95 | 0.07 | 110,127,139,201            | 0     |
| 59  | OHX  | 16SA  | 2320 | 7/7   | 0.95 | 0.08 | 99,106,126,191             | 0     |
| 58  | MG   | 23SB  | 3398 | 1/1   | 0.95 | 0.11 | 46,46,46,46                | 0     |
| 58  | MG   | 16SA  | 2202 | 1/1   | 0.95 | 0.20 | 57,57,57,57                | 0     |
| 60  | K    | 23SA  | 3628 | 1/1   | 0.95 | 0.15 | 83,83,83,83                | 0     |
| 60  | K    | 23SA  | 3629 | 1/1   | 0.95 | 0.06 | 65,65,65,65                | 0     |
| 58  | MG   | 23SB  | 3406 | 1/1   | 0.95 | 0.16 | 68,68,68,68                | 0     |
| 59  | OHX  | 23SA  | 3326 | 7/7   | 0.95 | 0.07 | 138,143,162,229            | 0     |
| 58  | MG   | 23SB  | 3407 | 1/1   | 0.95 | 0.10 | 51,51,51,51                | 0     |
| 58  | MG   | 23SB  | 3408 | 1/1   | 0.95 | 0.13 | 51,51,51,51                | 0     |
| 58  | MG   | 23SB  | 3215 | 1/1   | 0.95 | 0.19 | 37,37,37,37                | 0     |
| 58  | MG   | 23SB  | 3418 | 1/1   | 0.95 | 0.07 | 51,51,51,51                | 0     |
| 58  | MG   | 16SA  | 2353 | 1/1   | 0.95 | 0.05 | 138,138,138,138            | 0     |
| 59  | OHX  | 16SA  | 2329 | 7/7   | 0.95 | 0.06 | 144,149,154,226            | 0     |
| 58  | MG   | 23SB  | 3217 | 1/1   | 0.95 | 0.10 | 48,48,48,48                | 0     |
| 60  | K    | L4A   | 304  | 1/1   | 0.95 | 0.07 | 77,77,77,77                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 59  | OHX  | 5SB   | 203  | 7/7   | 0.95 | 0.07 | 102,107,119,182            | 0     |
| 59  | OHX  | S4B   | 301  | 7/7   | 0.95 | 0.08 | 116,119,128,186            | 0     |
| 59  | OHX  | ASIB  | 102  | 7/7   | 0.95 | 0.07 | 152,174,187,224            | 0     |
| 58  | MG   | 23SB  | 3424 | 1/1   | 0.95 | 0.09 | 71,71,71,71                | 0     |
| 58  | MG   | PSIA  | 103  | 1/1   | 0.95 | 0.08 | 83,83,83,83                | 0     |
| 60  | K    | 16SB  | 2369 | 1/1   | 0.95 | 0.15 | 82,82,82,82                | 0     |
| 58  | MG   | 23SA  | 3414 | 1/1   | 0.95 | 0.06 | 50,50,50,50                | 0     |
| 59  | OHX  | 23SB  | 3032 | 7/7   | 0.95 | 0.11 | 86,101,105,158             | 0     |
| 58  | MG   | 23SA  | 3504 | 1/1   | 0.95 | 0.06 | 67,67,67,67                | 0     |
| 59  | OHX  | 23SB  | 3036 | 7/7   | 0.95 | 0.08 | 113,117,131,172            | 0     |
| 59  | OHX  | 23SB  | 3041 | 7/7   | 0.95 | 0.14 | 82,86,98,151               | 0     |
| 59  | OHX  | L35B  | 101  | 7/7   | 0.95 | 0.09 | 120,126,131,191            | 0     |
| 59  | OHX  | 23SB  | 3050 | 7/7   | 0.95 | 0.17 | 74,79,98,166               | 0     |
| 59  | OHX  | 16SA  | 2336 | 7/7   | 0.95 | 0.07 | 106,114,119,210            | 0     |
| 59  | OHX  | 16SA  | 2337 | 7/7   | 0.95 | 0.07 | 197,199,204,249            | 0     |
| 59  | OHX  | 16SA  | 2339 | 7/7   | 0.95 | 0.08 | 93,98,102,201              | 0     |
| 58  | MG   | 23SA  | 3053 | 1/1   | 0.95 | 0.19 | 33,33,33,33                | 0     |
| 58  | MG   | 23SA  | 3511 | 1/1   | 0.95 | 0.05 | 36,36,36,36                | 0     |
| 59  | OHX  | 23SB  | 3061 | 7/7   | 0.95 | 0.07 | 100,105,115,190            | 0     |
| 60  | K    | 16SB  | 2389 | 1/1   | 0.95 | 0.04 | 82,82,82,82                | 0     |
| 59  | OHX  | 23SB  | 3062 | 7/7   | 0.95 | 0.06 | 100,103,111,185            | 0     |
| 58  | MG   | 23SA  | 3512 | 1/1   | 0.95 | 0.13 | 45,45,45,45                | 0     |
| 59  | OHX  | 23SB  | 3066 | 7/7   | 0.95 | 0.08 | 94,102,114,188             | 0     |
| 58  | MG   | 23SA  | 3145 | 1/1   | 0.95 | 0.06 | 70,70,70,70                | 0     |
| 59  | OHX  | 23SB  | 3073 | 7/7   | 0.95 | 0.07 | 89,100,113,186             | 0     |
| 58  | MG   | 23SA  | 3515 | 1/1   | 0.95 | 0.06 | 101,101,101,101            | 0     |
| 59  | OHX  | 23SB  | 3075 | 7/7   | 0.95 | 0.13 | 84,93,98,173               | 0     |
| 59  | OHX  | 23SB  | 3076 | 7/7   | 0.95 | 0.06 | 109,111,118,213            | 0     |
| 59  | OHX  | MRNA  | 101  | 7/7   | 0.95 | 0.07 | 109,113,121,212            | 0     |
| 58  | MG   | 23SB  | 3321 | 1/1   | 0.95 | 0.14 | 39,39,39,39                | 0     |
| 58  | MG   | 23SA  | 3009 | 1/1   | 0.95 | 0.22 | 40,40,40,40                | 0     |
| 59  | OHX  | 23SB  | 3088 | 7/7   | 0.95 | 0.08 | 110,117,123,193            | 0     |
| 60  | K    | 16SA  | 2401 | 1/1   | 0.95 | 0.08 | 63,63,63,63                | 0     |
| 58  | MG   | 23SA  | 3519 | 1/1   | 0.95 | 0.08 | 94,94,94,94                | 0     |
| 59  | OHX  | 23SB  | 3092 | 7/7   | 0.95 | 0.16 | 78,84,94,180               | 0     |
| 58  | MG   | 16SA  | 2357 | 1/1   | 0.95 | 0.07 | 63,63,63,63                | 0     |
| 60  | K    | 23SB  | 3443 | 1/1   | 0.95 | 0.14 | 110,110,110,110            | 0     |
| 60  | K    | 23SB  | 3444 | 1/1   | 0.95 | 0.07 | 84,84,84,84                | 0     |
| 58  | MG   | 23SA  | 3528 | 1/1   | 0.95 | 0.08 | 42,42,42,42                | 0     |
| 59  | OHX  | 23SA  | 3226 | 7/7   | 0.95 | 0.18 | 71,76,95,148               | 0     |
| 59  | OHX  | 23SB  | 3102 | 7/7   | 0.95 | 0.06 | 108,115,119,215            | 0     |
| 59  | OHX  | 23SA  | 3227 | 7/7   | 0.95 | 0.17 | 77,84,88,170               | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 59  | OHX  | 23SA  | 3231 | 7/7   | 0.95 | 0.16 | 79,87,94,150               | 0     |
| 59  | OHX  | 23SA  | 3233 | 7/7   | 0.95 | 0.11 | 83,89,99,153               | 0     |
| 59  | OHX  | 23SB  | 3106 | 7/7   | 0.95 | 0.08 | 100,119,134,193            | 0     |
| 60  | K    | 23SB  | 3452 | 1/1   | 0.95 | 0.08 | 84,84,84,84                | 0     |
| 59  | OHX  | 23SA  | 3236 | 7/7   | 0.95 | 0.18 | 76,86,90,178               | 0     |
| 60  | K    | 23SB  | 3456 | 1/1   | 0.95 | 0.04 | 75,75,75,75                | 0     |
| 60  | K    | 23SB  | 3458 | 1/1   | 0.95 | 0.07 | 72,72,72,72                | 0     |
| 60  | K    | 23SB  | 3461 | 1/1   | 0.95 | 0.06 | 67,67,67,67                | 0     |
| 58  | MG   | 23SB  | 3326 | 1/1   | 0.95 | 0.08 | 58,58,58,58                | 0     |
| 60  | K    | 23SB  | 3463 | 1/1   | 0.95 | 0.06 | 83,83,83,83                | 0     |
| 59  | OHX  | 23SA  | 3241 | 7/7   | 0.95 | 0.15 | 65,85,97,158               | 0     |
| 59  | OHX  | 23SA  | 3247 | 7/7   | 0.95 | 0.18 | 85,87,97,160               | 0     |
| 60  | K    | 23SB  | 3466 | 1/1   | 0.95 | 0.07 | 68,68,68,68                | 0     |
| 58  | MG   | 23SB  | 3233 | 1/1   | 0.95 | 0.21 | 41,41,41,41                | 0     |
| 59  | OHX  | 23SA  | 3254 | 7/7   | 0.95 | 0.14 | 74,86,94,175               | 0     |
| 60  | K    | 23SB  | 3469 | 1/1   | 0.95 | 0.07 | 64,64,64,64                | 0     |
| 59  | OHX  | 23SB  | 3116 | 7/7   | 0.95 | 0.07 | 126,131,140,206            | 0     |
| 58  | MG   | 23SA  | 3531 | 1/1   | 0.95 | 0.11 | 69,69,69,69                | 0     |
| 58  | MG   | L35B  | 102  | 1/1   | 0.95 | 0.11 | 91,91,91,91                | 0     |
| 58  | MG   | 16SA  | 2207 | 1/1   | 0.95 | 0.17 | 42,42,42,42                | 0     |
| 58  | MG   | 23SA  | 3434 | 1/1   | 0.95 | 0.12 | 102,102,102,102            | 0     |
| 58  | MG   | 23SA  | 3012 | 1/1   | 0.95 | 0.06 | 91,91,91,91                | 0     |
| 59  | OHX  | 16SA  | 2276 | 7/7   | 0.95 | 0.12 | 93,96,108,169              | 0     |
| 59  | OHX  | 23SB  | 3123 | 7/7   | 0.95 | 0.06 | 105,108,120,206            | 0     |
| 58  | MG   | 16SB  | 2351 | 1/1   | 0.95 | 0.07 | 68,68,68,68                | 0     |
| 59  | OHX  | 16SA  | 2280 | 7/7   | 0.95 | 0.07 | 100,102,112,186            | 0     |
| 59  | OHX  | 23SA  | 3375 | 7/7   | 0.95 | 0.06 | 102,110,125,192            | 0     |
| 58  | MG   | 23SB  | 3335 | 1/1   | 0.95 | 0.07 | 51,51,51,51                | 0     |
| 59  | OHX  | 16SA  | 2283 | 7/7   | 0.95 | 0.06 | 101,107,114,179            | 0     |
| 59  | OHX  | 23SA  | 3268 | 7/7   | 0.95 | 0.18 | 80,89,92,148               | 0     |
| 59  | OHX  | 23SA  | 3379 | 7/7   | 0.95 | 0.06 | 102,114,136,186            | 0     |
| 59  | OHX  | 16SA  | 2284 | 7/7   | 0.95 | 0.07 | 132,148,162,222            | 0     |
| 58  | MG   | 23SA  | 3132 | 1/1   | 0.95 | 0.05 | 57,57,57,57                | 0     |
| 58  | MG   | 16SB  | 2360 | 1/1   | 0.95 | 0.05 | 95,95,95,95                | 0     |
| 59  | OHX  | 23SA  | 3273 | 7/7   | 0.95 | 0.16 | 85,96,99,180               | 0     |
| 59  | OHX  | 16SA  | 2289 | 7/7   | 0.95 | 0.11 | 89,94,104,178              | 0     |
| 60  | K    | 23SB  | 3495 | 1/1   | 0.95 | 0.05 | 73,73,73,73                | 0     |
| 58  | MG   | 23SB  | 3349 | 1/1   | 0.95 | 0.08 | 71,71,71,71                | 0     |
| 58  | MG   | 16SB  | 2303 | 1/1   | 0.95 | 0.17 | 61,61,61,61                | 0     |
| 58  | MG   | 23SB  | 3357 | 1/1   | 0.95 | 0.10 | 65,65,65,65                | 0     |
| 59  | OHX  | 23SA  | 3280 | 7/7   | 0.95 | 0.06 | 90,100,112,211             | 0     |
| 59  | OHX  | 16SA  | 2294 | 7/7   | 0.95 | 0.07 | 89,94,99,207               | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 59  | OHX  | L20A  | 201  | 7/7   | 0.95 | 0.10 | 80,91,102,185              | 0     |
| 59  | OHX  | L27A  | 102  | 7/7   | 0.95 | 0.18 | 86,89,102,190              | 0     |
| 58  | MG   | 23SA  | 3042 | 1/1   | 0.95 | 0.14 | 47,47,47,47                | 0     |
| 58  | MG   | 23SA  | 3043 | 1/1   | 0.95 | 0.18 | 57,57,57,57                | 0     |
| 59  | OHX  | L35A  | 102  | 7/7   | 0.95 | 0.09 | 94,106,113,166             | 0     |
| 59  | OHX  | 16SB  | 2215 | 7/7   | 0.95 | 0.10 | 92,100,110,164             | 0     |
| 60  | K    | 23SB  | 3510 | 1/1   | 0.95 | 0.04 | 75,75,75,75                | 0     |
| 60  | K    | 23SA  | 3565 | 1/1   | 0.95 | 0.07 | 46,46,46,46                | 0     |
| 59  | OHX  | 16SB  | 2216 | 7/7   | 0.95 | 0.12 | 98,101,113,179             | 0     |
| 60  | K    | 23SA  | 3570 | 1/1   | 0.95 | 0.07 | 51,51,51,51                | 0     |
| 58  | MG   | 23SA  | 3024 | 1/1   | 0.95 | 0.14 | 45,45,45,45                | 0     |
| 59  | OHX  | 16SB  | 2218 | 7/7   | 0.95 | 0.12 | 95,98,107,169              | 0     |
| 59  | OHX  | 16SB  | 2220 | 7/7   | 0.95 | 0.07 | 98,104,110,191             | 0     |
| 59  | OHX  | 23SA  | 3291 | 7/7   | 0.95 | 0.07 | 126,133,145,190            | 0     |
| 59  | OHX  | 16SB  | 2224 | 7/7   | 0.95 | 0.06 | 97,105,114,200             | 0     |
| 58  | MG   | 23SB  | 3249 | 1/1   | 0.95 | 0.14 | 56,56,56,56                | 0     |
| 58  | MG   | 23SB  | 3369 | 1/1   | 0.95 | 0.07 | 46,46,46,46                | 0     |
| 59  | OHX  | 16SB  | 2229 | 7/7   | 0.95 | 0.06 | 111,112,116,211            | 0     |
| 58  | MG   | 23SA  | 3463 | 1/1   | 0.95 | 0.07 | 60,60,60,60                | 0     |
| 58  | MG   | 23SA  | 3465 | 1/1   | 0.95 | 0.09 | 53,53,53,53                | 0     |
| 59  | OHX  | 16SB  | 2235 | 7/7   | 0.95 | 0.06 | 105,111,120,212            | 0     |
| 59  | OHX  | 16SA  | 2303 | 7/7   | 0.95 | 0.06 | 117,118,127,222            | 0     |
| 58  | MG   | 23SB  | 3373 | 1/1   | 0.95 | 0.08 | 48,48,48,48                | 0     |
| 58  | MG   | 23SA  | 3510 | 1/1   | 0.96 | 0.12 | 75,75,75,75                | 0     |
| 60  | K    | 23SA  | 3600 | 1/1   | 0.96 | 0.07 | 68,68,68,68                | 0     |
| 58  | MG   | 16SA  | 2344 | 1/1   | 0.96 | 0.06 | 82,82,82,82                | 0     |
| 58  | MG   | 23SB  | 3347 | 1/1   | 0.96 | 0.07 | 65,65,65,65                | 0     |
| 59  | OHX  | 16SB  | 2255 | 7/7   | 0.96 | 0.06 | 133,135,154,207            | 0     |
| 59  | OHX  | ESIA  | 101  | 7/7   | 0.96 | 0.07 | 144,159,173,194            | 0     |
| 59  | OHX  | 23SA  | 3328 | 7/7   | 0.96 | 0.12 | 93,96,104,189              | 0     |
| 59  | OHX  | 23SA  | 3329 | 7/7   | 0.96 | 0.14 | 90,93,105,166              | 0     |
| 58  | MG   | 23SA  | 3129 | 1/1   | 0.96 | 0.06 | 54,54,54,54                | 0     |
| 59  | OHX  | 23SB  | 3169 | 7/7   | 0.96 | 0.06 | 104,124,127,192            | 0     |
| 59  | OHX  | 23SA  | 3332 | 7/7   | 0.96 | 0.06 | 98,103,115,190             | 0     |
| 58  | MG   | 23SB  | 3355 | 1/1   | 0.96 | 0.07 | 65,65,65,65                | 0     |
| 59  | OHX  | 16SA  | 2275 | 7/7   | 0.96 | 0.09 | 80,83,104,161              | 0     |
| 59  | OHX  | 23SA  | 3335 | 7/7   | 0.96 | 0.13 | 83,87,102,172              | 0     |
| 59  | OHX  | 23SA  | 3205 | 7/7   | 0.96 | 0.12 | 38,59,83,130               | 0     |
| 59  | OHX  | 23SA  | 3208 | 7/7   | 0.96 | 0.12 | 72,79,94,145               | 0     |
| 58  | MG   | 16SA  | 2361 | 1/1   | 0.96 | 0.05 | 75,75,75,75                | 0     |
| 59  | OHX  | 16SA  | 2278 | 7/7   | 0.96 | 0.06 | 100,115,119,183            | 0     |
| 58  | MG   | 23SA  | 3104 | 1/1   | 0.96 | 0.07 | 63,63,63,63                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | OHX  | 23SA  | 3225 | 7/7   | 0.96 | 0.06 | 96,99,104,174               | 0     |
| 58  | MG   | 23SB  | 3358 | 1/1   | 0.96 | 0.06 | 47,47,47,47                 | 0     |
| 58  | MG   | 23SB  | 3238 | 1/1   | 0.96 | 0.17 | 46,46,46,46                 | 0     |
| 59  | OHX  | 23SA  | 3230 | 7/7   | 0.96 | 0.09 | 67,77,97,168                | 0     |
| 58  | MG   | 23SA  | 3105 | 1/1   | 0.96 | 0.19 | 59,59,59,59                 | 0     |
| 58  | MG   | 23SB  | 3362 | 1/1   | 0.96 | 0.06 | 49,49,49,49                 | 0     |
| 58  | MG   | 16SB  | 2347 | 1/1   | 0.96 | 0.09 | 92,92,92,92                 | 0     |
| 59  | OHX  | 23SA  | 3237 | 7/7   | 0.96 | 0.11 | 79,89,105,162               | 0     |
| 58  | MG   | 23SA  | 3431 | 1/1   | 0.96 | 0.05 | 79,79,79,79                 | 0     |
| 60  | K    | 23SA  | 3633 | 1/1   | 0.96 | 0.15 | 77,77,77,77                 | 0     |
| 59  | OHX  | 23SA  | 3240 | 7/7   | 0.96 | 0.11 | 69,78,93,170                | 0     |
| 58  | MG   | 23SB  | 3367 | 1/1   | 0.96 | 0.09 | 49,49,49,49                 | 0     |
| 59  | OHX  | 23SA  | 3243 | 7/7   | 0.96 | 0.10 | 79,89,95,159                | 0     |
| 60  | K    | 23SA  | 3637 | 1/1   | 0.96 | 0.13 | 60,60,60,60                 | 0     |
| 59  | OHX  | 23SA  | 3245 | 7/7   | 0.96 | 0.13 | 86,96,104,177               | 0     |
| 59  | OHX  | 23SB  | 3030 | 7/7   | 0.96 | 0.14 | 80,86,109,145               | 0     |
| 58  | MG   | 23SB  | 3242 | 1/1   | 0.96 | 0.19 | 39,39,39,39                 | 0     |
| 59  | OHX  | 23SB  | 3034 | 7/7   | 0.96 | 0.12 | 90,91,105,156               | 0     |
| 59  | OHX  | 23SA  | 3250 | 7/7   | 0.96 | 0.13 | 58,64,77,149                | 0     |
| 59  | OHX  | 16SA  | 2291 | 7/7   | 0.96 | 0.12 | 91,96,102,165               | 0     |
| 58  | MG   | 23SA  | 3523 | 1/1   | 0.96 | 0.09 | 70,70,70,70                 | 0     |
| 59  | OHX  | 23SB  | 3048 | 7/7   | 0.96 | 0.08 | 111,117,132,161             | 0     |
| 59  | OHX  | 23SB  | 3049 | 7/7   | 0.96 | 0.06 | 92,103,111,173              | 0     |
| 58  | MG   | 16SB  | 2352 | 1/1   | 0.96 | 0.07 | 73,73,73,73                 | 0     |
| 60  | K    | 16SB  | 2368 | 1/1   | 0.96 | 0.04 | 103,103,103,103             | 0     |
| 58  | MG   | 16SA  | 2362 | 1/1   | 0.96 | 0.12 | 93,93,93,93                 | 0     |
| 58  | MG   | 23SB  | 3375 | 1/1   | 0.96 | 0.07 | 66,66,66,66                 | 0     |
| 58  | MG   | 16SB  | 2357 | 1/1   | 0.96 | 0.06 | 96,96,96,96                 | 0     |
| 59  | OHX  | 23SB  | 3055 | 7/7   | 0.96 | 0.14 | 65,81,87,153                | 0     |
| 58  | MG   | 16SB  | 2358 | 1/1   | 0.96 | 0.06 | 105,105,105,105             | 0     |
| 58  | MG   | 23SA  | 3526 | 1/1   | 0.96 | 0.12 | 76,76,76,76                 | 0     |
| 60  | K    | 16SB  | 2378 | 1/1   | 0.96 | 0.07 | 94,94,94,94                 | 0     |
| 59  | OHX  | 23SB  | 3060 | 7/7   | 0.96 | 0.10 | 95,99,105,180               | 0     |
| 58  | MG   | 16SA  | 2345 | 1/1   | 0.96 | 0.06 | 89,89,89,89                 | 0     |
| 58  | MG   | 23SA  | 3529 | 1/1   | 0.96 | 0.09 | 42,42,42,42                 | 0     |
| 59  | OHX  | 23SA  | 3264 | 7/7   | 0.96 | 0.05 | 98,101,114,196              | 0     |
| 60  | K    | 16SB  | 2383 | 1/1   | 0.96 | 0.05 | 92,92,92,92                 | 0     |
| 59  | OHX  | 23SB  | 3064 | 7/7   | 0.96 | 0.18 | 77,82,98,167                | 0     |
| 59  | OHX  | 23SA  | 3265 | 7/7   | 0.96 | 0.07 | 83,93,109,192               | 0     |
| 58  | MG   | 23SA  | 3442 | 1/1   | 0.96 | 0.06 | 48,48,48,48                 | 0     |
| 59  | OHX  | 23SB  | 3068 | 7/7   | 0.96 | 0.17 | 87,92,101,181               | 0     |
| 59  | OHX  | 23SB  | 3069 | 7/7   | 0.96 | 0.07 | 98,105,118,189              | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 59  | OHX  | 23SB  | 3070 | 7/7   | 0.96 | 0.14 | 81,89,95,163               | 0     |
| 59  | OHX  | 23SB  | 3071 | 7/7   | 0.96 | 0.12 | 85,94,100,182              | 0     |
| 59  | OHX  | 16SA  | 2302 | 7/7   | 0.96 | 0.07 | 105,107,113,183            | 0     |
| 58  | MG   | 23SA  | 3038 | 1/1   | 0.96 | 0.15 | 45,45,45,45                | 0     |
| 58  | MG   | 23SA  | 3535 | 1/1   | 0.96 | 0.14 | 59,59,59,59                | 0     |
| 58  | MG   | 23SA  | 3004 | 1/1   | 0.96 | 0.24 | 35,35,35,35                | 0     |
| 58  | MG   | 16SA  | 2364 | 1/1   | 0.96 | 0.07 | 86,86,86,86                | 0     |
| 60  | K    | 16SB  | 2397 | 1/1   | 0.96 | 0.04 | 97,97,97,97                | 0     |
| 58  | MG   | 16SA  | 2365 | 1/1   | 0.96 | 0.09 | 53,53,53,53                | 0     |
| 59  | OHX  | 23SB  | 3082 | 7/7   | 0.96 | 0.12 | 79,84,97,168               | 0     |
| 59  | OHX  | 23SB  | 3084 | 7/7   | 0.96 | 0.09 | 94,97,110,191              | 0     |
| 59  | OHX  | 23SB  | 3085 | 7/7   | 0.96 | 0.06 | 105,109,112,199            | 0     |
| 58  | MG   | 23SB  | 3392 | 1/1   | 0.96 | 0.09 | 52,52,52,52                | 0     |
| 58  | MG   | 23SA  | 3462 | 1/1   | 0.96 | 0.07 | 51,51,51,51                | 0     |
| 59  | OHX  | 23SA  | 3276 | 7/7   | 0.96 | 0.06 | 87,98,104,204              | 0     |
| 59  | OHX  | 23SB  | 3091 | 7/7   | 0.96 | 0.12 | 81,89,94,189               | 0     |
| 58  | MG   | 23SA  | 3066 | 1/1   | 0.96 | 0.18 | 59,59,59,59                | 0     |
| 58  | MG   | 23SA  | 3113 | 1/1   | 0.96 | 0.21 | 52,52,52,52                | 0     |
| 59  | OHX  | 23SB  | 3094 | 7/7   | 0.96 | 0.06 | 107,111,129,187            | 0     |
| 59  | OHX  | 23SA  | 3279 | 7/7   | 0.96 | 0.06 | 92,97,106,198              | 0     |
| 59  | OHX  | 23SB  | 3096 | 7/7   | 0.96 | 0.06 | 128,134,148,208            | 0     |
| 59  | OHX  | 23SB  | 3097 | 7/7   | 0.96 | 0.16 | 82,88,95,172               | 0     |
| 59  | OHX  | 23SB  | 3098 | 7/7   | 0.96 | 0.10 | 97,101,109,177             | 0     |
| 58  | MG   | 23SA  | 3021 | 1/1   | 0.96 | 0.18 | 40,40,40,40                | 0     |
| 59  | OHX  | 23SB  | 3100 | 7/7   | 0.96 | 0.11 | 90,93,100,175              | 0     |
| 59  | OHX  | 23SB  | 3101 | 7/7   | 0.96 | 0.07 | 104,111,115,185            | 0     |
| 59  | OHX  | 23SA  | 3282 | 7/7   | 0.96 | 0.06 | 101,104,113,206            | 0     |
| 60  | K    | 23SB  | 3453 | 1/1   | 0.96 | 0.05 | 59,59,59,59                | 0     |
| 58  | MG   | 23SA  | 3022 | 1/1   | 0.96 | 0.22 | 40,40,40,40                | 0     |
| 59  | OHX  | 5SA   | 207  | 7/7   | 0.96 | 0.06 | 97,103,109,176             | 0     |
| 60  | K    | 23SB  | 3457 | 1/1   | 0.96 | 0.05 | 63,63,63,63                | 0     |
| 58  | MG   | 23SA  | 3474 | 1/1   | 0.96 | 0.07 | 59,59,59,59                | 0     |
| 60  | K    | 23SB  | 3460 | 1/1   | 0.96 | 0.06 | 61,61,61,61                | 0     |
| 58  | MG   | 23SA  | 3476 | 1/1   | 0.96 | 0.08 | 51,51,51,51                | 0     |
| 59  | OHX  | 5SA   | 210  | 7/7   | 0.96 | 0.17 | 81,88,100,168              | 0     |
| 59  | OHX  | 23SB  | 3108 | 7/7   | 0.96 | 0.06 | 95,101,104,191             | 0     |
| 59  | OHX  | 23SB  | 3109 | 7/7   | 0.96 | 0.05 | 118,119,125,207            | 0     |
| 59  | OHX  | 5SA   | 211  | 7/7   | 0.96 | 0.06 | 101,107,113,190            | 0     |
| 59  | OHX  | 23SA  | 3287 | 7/7   | 0.96 | 0.07 | 97,100,105,189             | 0     |
| 58  | MG   | 23SB  | 3413 | 1/1   | 0.96 | 0.07 | 42,42,42,42                | 0     |
| 58  | MG   | 23SB  | 3414 | 1/1   | 0.96 | 0.06 | 83,83,83,83                | 0     |
| 58  | MG   | L27A  | 104  | 1/1   | 0.96 | 0.09 | 65,65,65,65                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 59  | OHX  | 23SB  | 3115 | 7/7   | 0.96 | 0.05 | 98,104,112,200             | 0     |
| 58  | MG   | 16SA  | 2366 | 1/1   | 0.96 | 0.06 | 107,107,107,107            | 0     |
| 59  | OHX  | 23SA  | 3294 | 7/7   | 0.96 | 0.10 | 85,97,105,191              | 0     |
| 58  | MG   | 23SA  | 3070 | 1/1   | 0.96 | 0.24 | 58,58,58,58                | 0     |
| 59  | OHX  | 23SA  | 3296 | 7/7   | 0.96 | 0.06 | 94,97,113,192              | 0     |
| 58  | MG   | 16SA  | 2347 | 1/1   | 0.96 | 0.07 | 78,78,78,78                | 0     |
| 59  | OHX  | 16SB  | 2207 | 7/7   | 0.96 | 0.07 | 89,95,104,159              | 0     |
| 59  | OHX  | 16SB  | 2213 | 7/7   | 0.96 | 0.07 | 123,129,137,180            | 0     |
| 59  | OHX  | 16SB  | 2214 | 7/7   | 0.96 | 0.08 | 116,119,134,169            | 0     |
| 58  | MG   | 23SB  | 3422 | 1/1   | 0.96 | 0.07 | 72,72,72,72                | 0     |
| 59  | OHX  | 23SB  | 3125 | 7/7   | 0.96 | 0.07 | 90,93,105,217              | 0     |
| 60  | K    | 23SB  | 3482 | 1/1   | 0.96 | 0.04 | 66,66,66,66                | 0     |
| 58  | MG   | 23SA  | 3119 | 1/1   | 0.96 | 0.05 | 61,61,61,61                | 0     |
| 60  | K    | 23SA  | 3551 | 1/1   | 0.96 | 0.04 | 80,80,80,80                | 0     |
| 58  | MG   | 23SA  | 3025 | 1/1   | 0.96 | 0.29 | 64,64,64,64                | 0     |
| 58  | MG   | 16SA  | 2210 | 1/1   | 0.96 | 0.14 | 46,46,46,46                | 0     |
| 58  | MG   | 16SA  | 2355 | 1/1   | 0.96 | 0.08 | 51,51,51,51                | 0     |
| 59  | OHX  | 16SB  | 2221 | 7/7   | 0.96 | 0.05 | 108,115,121,190            | 0     |
| 59  | OHX  | 23SA  | 3305 | 7/7   | 0.96 | 0.05 | 97,104,122,196             | 0     |
| 58  | MG   | 23SA  | 3029 | 1/1   | 0.96 | 0.16 | 37,37,37,37                | 0     |
| 59  | OHX  | 16SB  | 2225 | 7/7   | 0.96 | 0.10 | 94,95,103,163              | 0     |
| 59  | OHX  | 23SB  | 3137 | 7/7   | 0.96 | 0.06 | 99,103,110,209             | 0     |
| 58  | MG   | 23SB  | 3433 | 1/1   | 0.96 | 0.06 | 106,106,106,106            | 0     |
| 58  | MG   | 16SA  | 2206 | 1/1   | 0.96 | 0.34 | 40,40,40,40                | 0     |
| 58  | MG   | 23SB  | 3274 | 1/1   | 0.96 | 0.30 | 57,57,57,57                | 0     |
| 59  | OHX  | 16SB  | 2231 | 7/7   | 0.96 | 0.06 | 94,98,110,186              | 0     |
| 59  | OHX  | 16SB  | 2232 | 7/7   | 0.96 | 0.05 | 126,132,138,218            | 0     |
| 60  | K    | 23SA  | 3566 | 1/1   | 0.96 | 0.04 | 51,51,51,51                | 0     |
| 60  | K    | 23SB  | 3503 | 1/1   | 0.96 | 0.12 | 72,72,72,72                | 0     |
| 58  | MG   | 23SA  | 3392 | 1/1   | 0.96 | 0.08 | 52,52,52,52                | 0     |
| 58  | MG   | 16SA  | 2358 | 1/1   | 0.96 | 0.10 | 48,48,48,48                | 0     |
| 60  | K    | 23SA  | 3574 | 1/1   | 0.96 | 0.04 | 52,52,52,52                | 0     |
| 58  | MG   | 23SA  | 3401 | 1/1   | 0.96 | 0.07 | 63,63,63,63                | 0     |
| 59  | OHX  | 16SA  | 2334 | 7/7   | 0.96 | 0.06 | 161,169,178,239            | 0     |
| 60  | K    | 23SA  | 3579 | 1/1   | 0.96 | 0.04 | 60,60,60,60                | 0     |
| 58  | MG   | 23SA  | 3153 | 1/1   | 0.96 | 0.12 | 51,51,51,51                | 0     |
| 58  | MG   | 16SB  | 2329 | 1/1   | 0.96 | 0.11 | 63,63,63,63                | 0     |
| 60  | K    | 23SA  | 3582 | 1/1   | 0.96 | 0.06 | 53,53,53,53                | 0     |
| 60  | K    | 23SA  | 3583 | 1/1   | 0.96 | 0.10 | 65,65,65,65                | 0     |
| 59  | OHX  | 16SB  | 2240 | 7/7   | 0.96 | 0.06 | 120,126,130,218            | 0     |
| 58  | MG   | 23SB  | 3331 | 1/1   | 0.96 | 0.19 | 58,58,58,58                | 0     |
| 59  | OHX  | 16SB  | 2243 | 7/7   | 0.96 | 0.06 | 115,117,121,193            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 59  | OHX  | 16SA  | 2338 | 7/7   | 0.96 | 0.07 | 96,105,108,199             | 0     |
| 59  | OHX  | 16SB  | 2245 | 7/7   | 0.96 | 0.06 | 100,107,114,181            | 0     |
| 60  | K    | 23SA  | 3590 | 1/1   | 0.96 | 0.10 | 67,67,67,67                | 0     |
| 58  | MG   | 23SA  | 3501 | 1/1   | 0.96 | 0.08 | 66,66,66,66                | 0     |
| 58  | MG   | 23SA  | 3126 | 1/1   | 0.96 | 0.08 | 62,62,62,62                | 0     |
| 59  | OHX  | 16SB  | 2248 | 7/7   | 0.96 | 0.05 | 123,130,136,226            | 0     |
| 59  | OHX  | 23SA  | 3321 | 7/7   | 0.96 | 0.13 | 77,81,92,196               | 0     |
| 59  | OHX  | 23SA  | 3322 | 7/7   | 0.96 | 0.06 | 88,102,106,193             | 0     |
| 58  | MG   | 16SA  | 2342 | 1/1   | 0.96 | 0.07 | 85,85,85,85                | 0     |
| 59  | OHX  | 23SA  | 3246 | 7/7   | 0.97 | 0.08 | 88,94,111,180              | 0     |
| 58  | MG   | 23SA  | 3028 | 1/1   | 0.97 | 0.23 | 41,41,41,41                | 0     |
| 59  | OHX  | 23SA  | 3248 | 7/7   | 0.97 | 0.11 | 84,89,103,166              | 0     |
| 59  | OHX  | 16SB  | 2237 | 7/7   | 0.97 | 0.06 | 109,114,118,214            | 0     |
| 59  | OHX  | 23SA  | 3249 | 7/7   | 0.97 | 0.13 | 81,94,100,157              | 0     |
| 58  | MG   | 23SA  | 3433 | 1/1   | 0.97 | 0.05 | 77,77,77,77                | 0     |
| 58  | MG   | 16SA  | 2372 | 1/1   | 0.97 | 0.05 | 92,92,92,92                | 0     |
| 59  | OHX  | 16SB  | 2241 | 7/7   | 0.97 | 0.06 | 97,104,110,191             | 0     |
| 59  | OHX  | 23SA  | 3253 | 7/7   | 0.97 | 0.05 | 106,111,120,187            | 0     |
| 60  | K    | 5SA   | 218  | 1/1   | 0.97 | 0.04 | 79,79,79,79                | 0     |
| 58  | MG   | 16SB  | 2359 | 1/1   | 0.97 | 0.06 | 103,103,103,103            | 0     |
| 60  | K    | L2A   | 301  | 1/1   | 0.97 | 0.05 | 47,47,47,47                | 0     |
| 58  | MG   | 23SB  | 3229 | 1/1   | 0.97 | 0.29 | 44,44,44,44                | 0     |
| 58  | MG   | 23SA  | 3395 | 1/1   | 0.97 | 0.07 | 34,34,34,34                | 0     |
| 58  | MG   | 23SA  | 3438 | 1/1   | 0.97 | 0.05 | 88,88,88,88                | 0     |
| 58  | MG   | 16SB  | 2362 | 1/1   | 0.97 | 0.08 | 113,113,113,113            | 0     |
| 58  | MG   | 23SA  | 3441 | 1/1   | 0.97 | 0.05 | 43,43,43,43                | 0     |
| 58  | MG   | 23SA  | 3396 | 1/1   | 0.97 | 0.06 | 34,34,34,34                | 0     |
| 58  | MG   | 23SB  | 3235 | 1/1   | 0.97 | 0.20 | 59,59,59,59                | 0     |
| 60  | K    | 16SA  | 2397 | 1/1   | 0.97 | 0.07 | 62,62,62,62                | 0     |
| 58  | MG   | 23SA  | 3493 | 1/1   | 0.97 | 0.05 | 44,44,44,44                | 0     |
| 60  | K    | 16SA  | 2400 | 1/1   | 0.97 | 0.04 | 89,89,89,89                | 0     |
| 60  | K    | 16SB  | 2371 | 1/1   | 0.97 | 0.05 | 99,99,99,99                | 0     |
| 60  | K    | 16SB  | 2372 | 1/1   | 0.97 | 0.03 | 105,105,105,105            | 0     |
| 60  | K    | 16SB  | 2373 | 1/1   | 0.97 | 0.13 | 93,93,93,93                | 0     |
| 58  | MG   | 23SA  | 3399 | 1/1   | 0.97 | 0.05 | 37,37,37,37                | 0     |
| 58  | MG   | 23SB  | 3374 | 1/1   | 0.97 | 0.10 | 48,48,48,48                | 0     |
| 58  | MG   | 23SA  | 3444 | 1/1   | 0.97 | 0.10 | 29,29,29,29                | 0     |
| 58  | MG   | 5SA   | 217  | 1/1   | 0.97 | 0.13 | 85,85,85,85                | 0     |
| 58  | MG   | 23SA  | 3030 | 1/1   | 0.97 | 0.27 | 51,51,51,51                | 0     |
| 58  | MG   | 16SA  | 2370 | 1/1   | 0.97 | 0.05 | 102,102,102,102            | 0     |
| 59  | OHX  | 16SB  | 2258 | 7/7   | 0.97 | 0.05 | 144,147,157,204            | 0     |
| 58  | MG   | 23SA  | 3456 | 1/1   | 0.97 | 0.06 | 50,50,50,50                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | OHX  | 16SA  | 2265 | 7/7   | 0.97 | 0.07 | 104,105,123,150             | 0     |
| 60  | K    | 16SA  | 2410 | 1/1   | 0.97 | 0.03 | 77,77,77,77                 | 0     |
| 59  | OHX  | 16SA  | 2269 | 7/7   | 0.97 | 0.08 | 81,87,100,141               | 0     |
| 58  | MG   | L15A  | 203  | 1/1   | 0.97 | 0.11 | 65,65,65,65                 | 0     |
| 59  | OHX  | 16SA  | 2273 | 7/7   | 0.97 | 0.09 | 96,101,112,163              | 0     |
| 58  | MG   | 23SA  | 3458 | 1/1   | 0.97 | 0.07 | 55,55,55,55                 | 0     |
| 58  | MG   | 23SA  | 3460 | 1/1   | 0.97 | 0.09 | 38,38,38,38                 | 0     |
| 58  | MG   | 23SA  | 3507 | 1/1   | 0.97 | 0.06 | 55,55,55,55                 | 0     |
| 59  | OHX  | 23SB  | 3128 | 7/7   | 0.97 | 0.05 | 108,110,117,202             | 0     |
| 58  | MG   | 23SB  | 3247 | 1/1   | 0.97 | 0.06 | 45,45,45,45                 | 0     |
| 58  | MG   | 23SB  | 3208 | 1/1   | 0.97 | 0.28 | 52,52,52,52                 | 0     |
| 59  | OHX  | 23SA  | 3281 | 7/7   | 0.97 | 0.11 | 76,91,95,177                | 0     |
| 58  | MG   | S4A   | 302  | 1/1   | 0.97 | 0.06 | 98,98,98,98                 | 0     |
| 59  | OHX  | 23SB  | 3133 | 7/7   | 0.97 | 0.05 | 96,99,110,198               | 0     |
| 59  | OHX  | 23SA  | 3283 | 7/7   | 0.97 | 0.05 | 106,113,119,187             | 0     |
| 58  | MG   | 23SA  | 3413 | 1/1   | 0.97 | 0.07 | 55,55,55,55                 | 0     |
| 59  | OHX  | 16SA  | 2282 | 7/7   | 0.97 | 0.12 | 84,85,91,155                | 0     |
| 58  | MG   | 23SA  | 3039 | 1/1   | 0.97 | 0.15 | 30,30,30,30                 | 0     |
| 58  | MG   | 23SB  | 3395 | 1/1   | 0.97 | 0.11 | 43,43,43,43                 | 0     |
| 58  | MG   | 23SA  | 3415 | 1/1   | 0.97 | 0.05 | 67,67,67,67                 | 0     |
| 59  | OHX  | 23SA  | 3289 | 7/7   | 0.97 | 0.14 | 72,79,86,180                | 0     |
| 59  | OHX  | 23SA  | 3290 | 7/7   | 0.97 | 0.12 | 83,93,105,198               | 0     |
| 59  | OHX  | S19A  | 101  | 7/7   | 0.97 | 0.06 | 115,125,129,181             | 0     |
| 59  | OHX  | 16SA  | 2287 | 7/7   | 0.97 | 0.08 | 96,103,109,167              | 0     |
| 59  | OHX  | PSIB  | 101  | 7/7   | 0.97 | 0.08 | 104,107,121,137             | 0     |
| 59  | OHX  | ASIA  | 103  | 7/7   | 0.97 | 0.07 | 142,155,169,215             | 0     |
| 59  | OHX  | 23SB  | 3147 | 7/7   | 0.97 | 0.05 | 109,122,129,186             | 0     |
| 59  | OHX  | ESIB  | 101  | 7/7   | 0.97 | 0.06 | 150,166,173,207             | 0     |
| 58  | MG   | 23SB  | 3290 | 1/1   | 0.97 | 0.31 | 47,47,47,47                 | 0     |
| 59  | OHX  | 23SB  | 3020 | 7/7   | 0.97 | 0.07 | 89,94,103,130               | 0     |
| 59  | OHX  | 23SB  | 3022 | 7/7   | 0.97 | 0.08 | 92,97,106,138               | 0     |
| 59  | OHX  | 23SB  | 3023 | 7/7   | 0.97 | 0.08 | 75,79,88,131                | 0     |
| 59  | OHX  | 23SB  | 3025 | 7/7   | 0.97 | 0.11 | 87,93,101,135               | 0     |
| 59  | OHX  | 23SB  | 3026 | 7/7   | 0.97 | 0.12 | 83,92,104,131               | 0     |
| 58  | MG   | 23SA  | 3417 | 1/1   | 0.97 | 0.10 | 58,58,58,58                 | 0     |
| 59  | OHX  | TRNA  | 101  | 7/7   | 0.97 | 0.06 | 135,137,154,191             | 0     |
| 60  | K    | 23SB  | 3455 | 1/1   | 0.97 | 0.11 | 61,61,61,61                 | 0     |
| 59  | OHX  | 23SA  | 3297 | 7/7   | 0.97 | 0.09 | 97,99,109,183               | 0     |
| 58  | MG   | 23SB  | 3403 | 1/1   | 0.97 | 0.06 | 52,52,52,52                 | 0     |
| 59  | OHX  | 5SA   | 205  | 7/7   | 0.97 | 0.09 | 75,95,106,138               | 0     |
| 60  | K    | 23SA  | 3561 | 1/1   | 0.97 | 0.06 | 75,75,75,75                 | 0     |
| 59  | OHX  | 23SB  | 3038 | 7/7   | 0.97 | 0.09 | 82,91,105,153               | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 59  | OHX  | 23SB  | 3039 | 7/7   | 0.97 | 0.07 | 92,95,103,158              | 0     |
| 58  | MG   | 23SB  | 3404 | 1/1   | 0.97 | 0.08 | 37,37,37,37                | 0     |
| 59  | OHX  | 23SB  | 3043 | 7/7   | 0.97 | 0.08 | 81,88,108,166              | 0     |
| 59  | OHX  | 23SB  | 3044 | 7/7   | 0.97 | 0.15 | 69,77,95,151               | 0     |
| 60  | K    | 23SA  | 3567 | 1/1   | 0.97 | 0.05 | 46,46,46,46                | 0     |
| 59  | OHX  | 23SB  | 3045 | 7/7   | 0.97 | 0.08 | 84,95,110,160              | 0     |
| 59  | OHX  | 23SB  | 3046 | 7/7   | 0.97 | 0.09 | 64,76,84,147               | 0     |
| 60  | K    | 23SA  | 3572 | 1/1   | 0.97 | 0.05 | 51,51,51,51                | 0     |
| 59  | OHX  | 23SB  | 3047 | 7/7   | 0.97 | 0.11 | 74,90,94,149               | 0     |
| 59  | OHX  | 23SA  | 3200 | 7/7   | 0.97 | 0.11 | 62,89,92,138               | 0     |
| 58  | MG   | 16SA  | 2351 | 1/1   | 0.97 | 0.08 | 103,103,103,103            | 0     |
| 59  | OHX  | 23SA  | 3207 | 7/7   | 0.97 | 0.11 | 73,78,88,136               | 0     |
| 59  | OHX  | 23SA  | 3303 | 7/7   | 0.97 | 0.10 | 91,92,104,183              | 0     |
| 58  | MG   | 23SA  | 3518 | 1/1   | 0.97 | 0.14 | 61,61,61,61                | 0     |
| 59  | OHX  | 23SA  | 3209 | 7/7   | 0.97 | 0.08 | 76,90,103,134              | 0     |
| 60  | K    | 23SB  | 3477 | 1/1   | 0.97 | 0.03 | 60,60,60,60                | 0     |
| 59  | OHX  | 23SA  | 3210 | 7/7   | 0.97 | 0.11 | 57,67,87,122               | 0     |
| 59  | OHX  | 23SB  | 3057 | 7/7   | 0.97 | 0.10 | 96,99,115,167              | 0     |
| 59  | OHX  | 23SA  | 3211 | 7/7   | 0.97 | 0.11 | 61,66,83,132               | 0     |
| 58  | MG   | 23SA  | 3058 | 1/1   | 0.97 | 0.04 | 53,53,53,53                | 0     |
| 59  | OHX  | 23SA  | 3220 | 7/7   | 0.97 | 0.07 | 85,86,101,146              | 0     |
| 60  | K    | 23SB  | 3484 | 1/1   | 0.97 | 0.07 | 80,80,80,80                | 0     |
| 58  | MG   | 23SB  | 3411 | 1/1   | 0.97 | 0.06 | 41,41,41,41                | 0     |
| 59  | OHX  | 23SA  | 3222 | 7/7   | 0.97 | 0.06 | 99,103,115,175             | 0     |
| 58  | MG   | 23SB  | 3412 | 1/1   | 0.97 | 0.05 | 56,56,56,56                | 0     |
| 58  | MG   | 23SA  | 3387 | 1/1   | 0.97 | 0.05 | 55,55,55,55                | 0     |
| 59  | OHX  | 23SB  | 3065 | 7/7   | 0.97 | 0.10 | 86,93,109,147              | 0     |
| 58  | MG   | 16SB  | 2349 | 1/1   | 0.97 | 0.17 | 90,90,90,90                | 0     |
| 60  | K    | 23SB  | 3491 | 1/1   | 0.97 | 0.08 | 68,68,68,68                | 0     |
| 59  | OHX  | 16SB  | 2210 | 7/7   | 0.97 | 0.10 | 96,101,107,163             | 0     |
| 60  | K    | 23SA  | 3596 | 1/1   | 0.97 | 0.03 | 59,59,59,59                | 0     |
| 59  | OHX  | 16SB  | 2211 | 7/7   | 0.97 | 0.07 | 101,114,117,162            | 0     |
| 60  | K    | 23SA  | 3598 | 1/1   | 0.97 | 0.11 | 58,58,58,58                | 0     |
| 58  | MG   | 23SB  | 3415 | 1/1   | 0.97 | 0.07 | 46,46,46,46                | 0     |
| 60  | K    | 23SB  | 3497 | 1/1   | 0.97 | 0.06 | 48,48,48,48                | 0     |
| 59  | OHX  | 23SA  | 3228 | 7/7   | 0.97 | 0.09 | 70,82,89,143               | 0     |
| 58  | MG   | 23SB  | 3416 | 1/1   | 0.97 | 0.07 | 98,98,98,98                | 0     |
| 59  | OHX  | 23SB  | 3072 | 7/7   | 0.97 | 0.08 | 81,88,103,161              | 0     |
| 58  | MG   | 23SB  | 3337 | 1/1   | 0.97 | 0.06 | 48,48,48,48                | 0     |
| 59  | OHX  | 23SA  | 3232 | 7/7   | 0.97 | 0.07 | 78,84,95,161               | 0     |
| 58  | MG   | 23SB  | 3344 | 1/1   | 0.97 | 0.06 | 50,50,50,50                | 0     |
| 59  | OHX  | 23SA  | 3234 | 7/7   | 0.97 | 0.08 | 91,94,101,156              | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 60  | K    | 23SA  | 3607 | 1/1   | 0.97 | 0.04 | 59,59,59,59                | 0     |
| 60  | K    | 23SB  | 3506 | 1/1   | 0.97 | 0.06 | 75,75,75,75                | 0     |
| 59  | OHX  | 23SB  | 3077 | 7/7   | 0.97 | 0.10 | 87,95,105,161              | 0     |
| 59  | OHX  | 23SB  | 3078 | 7/7   | 0.97 | 0.05 | 115,122,131,189            | 0     |
| 58  | MG   | 16SB  | 2350 | 1/1   | 0.97 | 0.08 | 99,99,99,99                | 0     |
| 59  | OHX  | 23SB  | 3080 | 7/7   | 0.97 | 0.06 | 95,105,112,179             | 0     |
| 58  | MG   | 23SB  | 3221 | 1/1   | 0.97 | 0.14 | 47,47,47,47                | 0     |
| 59  | OHX  | 5SB   | 201  | 7/7   | 0.97 | 0.07 | 103,112,120,159            | 0     |
| 58  | MG   | 23SA  | 3389 | 1/1   | 0.97 | 0.06 | 41,41,41,41                | 0     |
| 60  | K    | 23SA  | 3616 | 1/1   | 0.97 | 0.05 | 42,42,42,42                | 0     |
| 59  | OHX  | 23SB  | 3083 | 7/7   | 0.97 | 0.05 | 110,114,121,181            | 0     |
| 58  | MG   | 23SB  | 3423 | 1/1   | 0.97 | 0.05 | 73,73,73,73                | 0     |
| 59  | OHX  | 16SB  | 2226 | 7/7   | 0.97 | 0.05 | 117,119,123,191            | 0     |
| 59  | OHX  | 23SB  | 3086 | 7/7   | 0.97 | 0.10 | 85,86,104,167              | 0     |
| 58  | MG   | 23SA  | 3041 | 1/1   | 0.97 | 0.07 | 32,32,32,32                | 0     |
| 59  | OHX  | 23SA  | 3242 | 7/7   | 0.97 | 0.17 | 54,62,72,135               | 0     |
| 60  | K    | 5SB   | 216  | 1/1   | 0.97 | 0.03 | 101,101,101,101            | 0     |
| 60  | K    | L2B   | 301  | 1/1   | 0.97 | 0.05 | 62,62,62,62                | 0     |
| 58  | MG   | 23SB  | 3425 | 1/1   | 0.97 | 0.18 | 84,84,84,84                | 0     |
| 59  | OHX  | 16SB  | 2230 | 7/7   | 0.97 | 0.04 | 126,136,146,203            | 0     |
| 59  | OHX  | 23SA  | 3330 | 7/7   | 0.97 | 0.06 | 112,118,131,203            | 0     |
| 59  | OHX  | 23SA  | 3244 | 7/7   | 0.97 | 0.10 | 76,82,89,144               | 0     |
| 58  | MG   | 23SB  | 3427 | 1/1   | 0.97 | 0.13 | 49,49,49,49                | 0     |
| 60  | K    | 23SA  | 3630 | 1/1   | 0.97 | 0.07 | 80,80,80,80                | 0     |
| 58  | MG   | 23SB  | 3343 | 1/1   | 0.98 | 0.08 | 65,65,65,65                | 0     |
| 58  | MG   | 23SA  | 3490 | 1/1   | 0.98 | 0.07 | 42,42,42,42                | 0     |
| 60  | K    | 16SA  | 2392 | 1/1   | 0.98 | 0.04 | 88,88,88,88                | 0     |
| 60  | K    | 16SA  | 2393 | 1/1   | 0.98 | 0.07 | 80,80,80,80                | 0     |
| 60  | K    | 16SA  | 2394 | 1/1   | 0.98 | 0.03 | 75,75,75,75                | 0     |
| 58  | MG   | 23SB  | 3345 | 1/1   | 0.98 | 0.05 | 65,65,65,65                | 0     |
| 58  | MG   | L4A   | 301  | 1/1   | 0.98 | 0.12 | 48,48,48,48                | 0     |
| 58  | MG   | L4A   | 303  | 1/1   | 0.98 | 0.08 | 73,73,73,73                | 0     |
| 58  | MG   | 23SA  | 3492 | 1/1   | 0.98 | 0.04 | 52,52,52,52                | 0     |
| 60  | K    | 16SA  | 2399 | 1/1   | 0.98 | 0.04 | 65,65,65,65                | 0     |
| 58  | MG   | 23SB  | 3426 | 1/1   | 0.98 | 0.05 | 70,70,70,70                | 0     |
| 59  | OHX  | 23SA  | 3251 | 7/7   | 0.98 | 0.04 | 99,104,112,176             | 0     |
| 58  | MG   | 23SB  | 3350 | 1/1   | 0.98 | 0.07 | 37,37,37,37                | 0     |
| 58  | MG   | 23SB  | 3351 | 1/1   | 0.98 | 0.04 | 53,53,53,53                | 0     |
| 58  | MG   | 23SB  | 3352 | 1/1   | 0.98 | 0.06 | 47,47,47,47                | 0     |
| 58  | MG   | 23SB  | 3353 | 1/1   | 0.98 | 0.05 | 57,57,57,57                | 0     |
| 58  | MG   | 23SA  | 3448 | 1/1   | 0.98 | 0.05 | 40,40,40,40                | 0     |
| 58  | MG   | 23SA  | 3494 | 1/1   | 0.98 | 0.05 | 48,48,48,48                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 23SA  | 3449 | 1/1   | 0.98 | 0.04 | 44,44,44,44                 | 0     |
| 58  | MG   | 23SB  | 3435 | 1/1   | 0.98 | 0.10 | 94,94,94,94                 | 0     |
| 58  | MG   | 23SA  | 3419 | 1/1   | 0.98 | 0.05 | 64,64,64,64                 | 0     |
| 58  | MG   | 23SA  | 3498 | 1/1   | 0.98 | 0.06 | 38,38,38,38                 | 0     |
| 59  | OHX  | 16SB  | 2269 | 7/7   | 0.98 | 0.06 | 146,151,156,215             | 0     |
| 58  | MG   | 23SA  | 3453 | 1/1   | 0.98 | 0.05 | 34,34,34,34                 | 0     |
| 59  | OHX  | 23SA  | 3263 | 7/7   | 0.98 | 0.08 | 64,70,95,142                | 0     |
| 58  | MG   | 16SA  | 2348 | 1/1   | 0.98 | 0.03 | 58,58,58,58                 | 0     |
| 58  | MG   | 23SA  | 3457 | 1/1   | 0.98 | 0.09 | 37,37,37,37                 | 0     |
| 58  | MG   | 23SB  | 3365 | 1/1   | 0.98 | 0.03 | 45,45,45,45                 | 0     |
| 60  | K    | 16SB  | 2385 | 1/1   | 0.98 | 0.04 | 92,92,92,92                 | 0     |
| 58  | MG   | 5SB   | 215  | 1/1   | 0.98 | 0.05 | 88,88,88,88                 | 0     |
| 58  | MG   | 23SA  | 3394 | 1/1   | 0.98 | 0.08 | 71,71,71,71                 | 0     |
| 58  | MG   | 23SA  | 3074 | 1/1   | 0.98 | 0.04 | 72,72,72,72                 | 0     |
| 58  | MG   | 23SA  | 3062 | 1/1   | 0.98 | 0.09 | 61,61,61,61                 | 0     |
| 59  | OHX  | 23SA  | 3271 | 7/7   | 0.98 | 0.09 | 70,73,91,159                | 0     |
| 59  | OHX  | ASIB  | 101  | 7/7   | 0.98 | 0.04 | 114,126,131,187             | 0     |
| 59  | OHX  | 23SB  | 3134 | 7/7   | 0.98 | 0.10 | 82,85,92,165                | 0     |
| 58  | MG   | 23SA  | 3508 | 1/1   | 0.98 | 0.05 | 38,38,38,38                 | 0     |
| 60  | K    | 23SA  | 3538 | 1/1   | 0.98 | 0.06 | 63,63,63,63                 | 0     |
| 58  | MG   | 23SA  | 3509 | 1/1   | 0.98 | 0.05 | 52,52,52,52                 | 0     |
| 58  | MG   | 23SB  | 3211 | 1/1   | 0.98 | 0.05 | 52,52,52,52                 | 0     |
| 58  | MG   | 23SA  | 3425 | 1/1   | 0.98 | 0.09 | 61,61,61,61                 | 0     |
| 58  | MG   | 23SA  | 3383 | 1/1   | 0.98 | 0.05 | 39,39,39,39                 | 0     |
| 59  | OHX  | 16SA  | 2266 | 7/7   | 0.98 | 0.07 | 89,99,109,141               | 0     |
| 59  | OHX  | 23SB  | 3008 | 7/7   | 0.98 | 0.07 | 89,94,103,131               | 0     |
| 59  | OHX  | 23SB  | 3012 | 7/7   | 0.98 | 0.08 | 71,76,93,139                | 0     |
| 59  | OHX  | 23SB  | 3016 | 7/7   | 0.98 | 0.06 | 91,93,102,122               | 0     |
| 59  | OHX  | 23SB  | 3018 | 7/7   | 0.98 | 0.07 | 53,69,86,133                | 0     |
| 58  | MG   | 23SA  | 3428 | 1/1   | 0.98 | 0.07 | 78,78,78,78                 | 0     |
| 59  | OHX  | 23SB  | 3021 | 7/7   | 0.98 | 0.08 | 68,77,87,136                | 0     |
| 59  | OHX  | 16SA  | 2270 | 7/7   | 0.98 | 0.06 | 108,118,121,150             | 0     |
| 58  | MG   | 23SA  | 3430 | 1/1   | 0.98 | 0.05 | 74,74,74,74                 | 0     |
| 59  | OHX  | 23SB  | 3024 | 7/7   | 0.98 | 0.10 | 69,75,81,158                | 0     |
| 59  | OHX  | 16SA  | 2272 | 7/7   | 0.98 | 0.07 | 96,111,118,140              | 0     |
| 58  | MG   | 23SB  | 3379 | 1/1   | 0.98 | 0.05 | 41,41,41,41                 | 0     |
| 59  | OHX  | 23SB  | 3028 | 7/7   | 0.98 | 0.07 | 85,85,101,143               | 0     |
| 59  | OHX  | ASIA  | 101  | 7/7   | 0.98 | 0.06 | 100,111,125,168             | 0     |
| 59  | OHX  | 23SB  | 3031 | 7/7   | 0.98 | 0.07 | 88,95,98,151                | 0     |
| 58  | MG   | 16SB  | 2328 | 1/1   | 0.98 | 0.08 | 58,58,58,58                 | 0     |
| 58  | MG   | 23SA  | 3514 | 1/1   | 0.98 | 0.13 | 51,51,51,51                 | 0     |
| 59  | OHX  | 5SA   | 204  | 7/7   | 0.98 | 0.06 | 79,82,94,113                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 58  | MG   | 23SA  | 3468 | 1/1   | 0.98 | 0.07 | 36,36,36,36                | 0     |
| 59  | OHX  | 23SB  | 3037 | 7/7   | 0.98 | 0.08 | 97,101,106,155             | 0     |
| 59  | OHX  | 16SA  | 2277 | 7/7   | 0.98 | 0.07 | 94,95,103,165              | 0     |
| 58  | MG   | 23SA  | 3469 | 1/1   | 0.98 | 0.06 | 40,40,40,40                | 0     |
| 59  | OHX  | 23SB  | 3040 | 7/7   | 0.98 | 0.07 | 68,76,88,142               | 0     |
| 58  | MG   | 23SA  | 3090 | 1/1   | 0.98 | 0.13 | 49,49,49,49                | 0     |
| 60  | K    | 23SB  | 3459 | 1/1   | 0.98 | 0.07 | 56,56,56,56                | 0     |
| 59  | OHX  | 23SB  | 3042 | 7/7   | 0.98 | 0.05 | 101,107,110,164            | 0     |
| 59  | OHX  | 23SA  | 3191 | 7/7   | 0.98 | 0.06 | 79,89,101,127              | 0     |
| 59  | OHX  | 23SA  | 3193 | 7/7   | 0.98 | 0.08 | 66,70,81,129               | 0     |
| 59  | OHX  | 23SA  | 3194 | 7/7   | 0.98 | 0.08 | 71,75,90,126               | 0     |
| 60  | K    | 23SA  | 3573 | 1/1   | 0.98 | 0.06 | 63,63,63,63                | 0     |
| 58  | MG   | 23SA  | 3473 | 1/1   | 0.98 | 0.05 | 67,67,67,67                | 0     |
| 59  | OHX  | 23SA  | 3196 | 7/7   | 0.98 | 0.10 | 70,74,94,114               | 0     |
| 60  | K    | 23SA  | 3576 | 1/1   | 0.98 | 0.07 | 39,39,39,39                | 0     |
| 59  | OHX  | 23SA  | 3197 | 7/7   | 0.98 | 0.07 | 73,80,93,129               | 0     |
| 59  | OHX  | 23SA  | 3198 | 7/7   | 0.98 | 0.07 | 58,71,88,129               | 0     |
| 59  | OHX  | L17A  | 201  | 7/7   | 0.98 | 0.12 | 63,68,78,121               | 0     |
| 59  | OHX  | 23SA  | 3199 | 7/7   | 0.98 | 0.06 | 65,73,83,129               | 0     |
| 58  | MG   | 23SA  | 3521 | 1/1   | 0.98 | 0.04 | 58,58,58,58                | 0     |
| 59  | OHX  | 23SB  | 3053 | 7/7   | 0.98 | 0.06 | 92,97,113,157              | 0     |
| 59  | OHX  | 23SA  | 3201 | 7/7   | 0.98 | 0.07 | 79,87,98,127               | 0     |
| 60  | K    | 23SA  | 3585 | 1/1   | 0.98 | 0.08 | 54,54,54,54                | 0     |
| 59  | OHX  | 23SA  | 3202 | 7/7   | 0.98 | 0.08 | 55,70,77,136               | 0     |
| 59  | OHX  | 23SB  | 3056 | 7/7   | 0.98 | 0.06 | 95,102,108,155             | 0     |
| 59  | OHX  | 23SA  | 3203 | 7/7   | 0.98 | 0.06 | 77,78,101,130              | 0     |
| 59  | OHX  | 16SB  | 2202 | 7/7   | 0.98 | 0.08 | 86,91,97,124               | 0     |
| 59  | OHX  | 16SB  | 2204 | 7/7   | 0.98 | 0.07 | 86,96,104,143              | 0     |
| 59  | OHX  | 23SA  | 3204 | 7/7   | 0.98 | 0.06 | 66,71,91,123               | 0     |
| 59  | OHX  | 16SB  | 2209 | 7/7   | 0.98 | 0.06 | 90,99,108,137              | 0     |
| 60  | K    | 23SB  | 3483 | 1/1   | 0.98 | 0.05 | 69,69,69,69                | 0     |
| 58  | MG   | 23SA  | 3432 | 1/1   | 0.98 | 0.03 | 67,67,67,67                | 0     |
| 59  | OHX  | 23SA  | 3206 | 7/7   | 0.98 | 0.10 | 74,75,95,140               | 0     |
| 59  | OHX  | 16SB  | 2212 | 7/7   | 0.98 | 0.07 | 96,100,102,148             | 0     |
| 58  | MG   | 23SA  | 3385 | 1/1   | 0.98 | 0.05 | 41,41,41,41                | 0     |
| 58  | MG   | 23SB  | 3225 | 1/1   | 0.98 | 0.08 | 39,39,39,39                | 0     |
| 59  | OHX  | 16SA  | 2285 | 7/7   | 0.98 | 0.04 | 123,129,131,218            | 0     |
| 58  | MG   | 23SA  | 3407 | 1/1   | 0.98 | 0.05 | 48,48,48,48                | 0     |
| 58  | MG   | 23SA  | 3527 | 1/1   | 0.98 | 0.06 | 42,42,42,42                | 0     |
| 58  | MG   | 16SB  | 2345 | 1/1   | 0.98 | 0.08 | 64,64,64,64                | 0     |
| 59  | OHX  | 16SB  | 2219 | 7/7   | 0.98 | 0.05 | 103,105,116,174            | 0     |
| 59  | OHX  | 23SA  | 3213 | 7/7   | 0.98 | 0.07 | 74,78,90,126               | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 59  | OHX  | 23SA  | 3216 | 7/7   | 0.98 | 0.08 | 85,94,99,152               | 0     |
| 59  | OHX  | 23SA  | 3313 | 7/7   | 0.98 | 0.10 | 67,73,83,167               | 0     |
| 59  | OHX  | 16SB  | 2223 | 7/7   | 0.98 | 0.04 | 110,112,122,172            | 0     |
| 59  | OHX  | 23SA  | 3217 | 7/7   | 0.98 | 0.05 | 80,82,89,137               | 0     |
| 59  | OHX  | 23SA  | 3218 | 7/7   | 0.98 | 0.09 | 78,86,101,146              | 0     |
| 59  | OHX  | 23SA  | 3219 | 7/7   | 0.98 | 0.08 | 82,94,104,144              | 0     |
| 58  | MG   | 23SB  | 3397 | 1/1   | 0.98 | 0.06 | 59,59,59,59                | 0     |
| 58  | MG   | 23SA  | 3409 | 1/1   | 0.98 | 0.05 | 42,42,42,42                | 0     |
| 58  | MG   | 23SA  | 3052 | 1/1   | 0.98 | 0.22 | 40,40,40,40                | 0     |
| 59  | OHX  | 23SA  | 3223 | 7/7   | 0.98 | 0.06 | 81,87,101,144              | 0     |
| 58  | MG   | 23SB  | 3401 | 1/1   | 0.98 | 0.09 | 70,70,70,70                | 0     |
| 60  | K    | 23SA  | 3615 | 1/1   | 0.98 | 0.08 | 69,69,69,69                | 0     |
| 58  | MG   | 23SB  | 3402 | 1/1   | 0.98 | 0.05 | 45,45,45,45                | 0     |
| 58  | MG   | 23SA  | 3481 | 1/1   | 0.98 | 0.10 | 55,55,55,55                | 0     |
| 58  | MG   | 16SA  | 2373 | 1/1   | 0.98 | 0.12 | 98,98,98,98                | 0     |
| 58  | MG   | 23SA  | 3533 | 1/1   | 0.98 | 0.05 | 49,49,49,49                | 0     |
| 59  | OHX  | L17B  | 201  | 7/7   | 0.98 | 0.10 | 72,77,87,116               | 0     |
| 60  | K    | 23SA  | 3621 | 1/1   | 0.98 | 0.08 | 77,77,77,77                | 0     |
| 59  | OHX  | 23SA  | 3229 | 7/7   | 0.98 | 0.07 | 81,96,99,154               | 0     |
| 58  | MG   | 23SA  | 3390 | 1/1   | 0.98 | 0.05 | 38,38,38,38                | 0     |
| 59  | OHX  | 23SB  | 3090 | 7/7   | 0.98 | 0.05 | 110,117,123,191            | 0     |
| 58  | MG   | 16SA  | 2343 | 1/1   | 0.98 | 0.09 | 73,73,73,73                | 0     |
| 58  | MG   | 23SB  | 3409 | 1/1   | 0.98 | 0.04 | 58,58,58,58                | 0     |
| 58  | MG   | 23SB  | 3410 | 1/1   | 0.98 | 0.03 | 75,75,75,75                | 0     |
| 58  | MG   | 16SB  | 2355 | 1/1   | 0.98 | 0.05 | 90,90,90,90                | 0     |
| 59  | OHX  | 23SA  | 3235 | 7/7   | 0.98 | 0.06 | 75,87,106,150              | 0     |
| 58  | MG   | 23SA  | 3485 | 1/1   | 0.98 | 0.04 | 51,51,51,51                | 0     |
| 58  | MG   | 16SA  | 2356 | 1/1   | 0.98 | 0.10 | 67,67,67,67                | 0     |
| 59  | OHX  | 23SA  | 3238 | 7/7   | 0.98 | 0.11 | 64,65,76,149               | 0     |
| 58  | MG   | 23SA  | 3418 | 1/1   | 0.98 | 0.08 | 36,36,36,36                | 0     |
| 58  | MG   | 23SA  | 3488 | 1/1   | 0.98 | 0.06 | 49,49,49,49                | 0     |
| 58  | MG   | 23SA  | 3447 | 1/1   | 0.98 | 0.05 | 34,34,34,34                | 0     |
| 60  | K    | L16B  | 201  | 1/1   | 0.98 | 0.04 | 92,92,92,92                | 0     |
| 58  | MG   | 23SB  | 3340 | 1/1   | 0.98 | 0.08 | 45,45,45,45                | 0     |
| 58  | MG   | 23SB  | 3341 | 1/1   | 0.98 | 0.06 | 53,53,53,53                | 0     |
| 59  | OHX  | 23SB  | 3029 | 7/7   | 0.99 | 0.05 | 91,95,103,141              | 0     |
| 58  | MG   | 16SA  | 2352 | 1/1   | 0.99 | 0.05 | 62,62,62,62                | 0     |
| 59  | OHX  | 16SB  | 2203 | 7/7   | 0.99 | 0.06 | 91,94,102,133              | 0     |
| 58  | MG   | 23SA  | 3475 | 1/1   | 0.99 | 0.05 | 64,64,64,64                | 0     |
| 59  | OHX  | 23SB  | 3033 | 7/7   | 0.99 | 0.08 | 79,88,93,147               | 0     |
| 59  | OHX  | 16SB  | 2205 | 7/7   | 0.99 | 0.04 | 105,111,117,152            | 0     |
| 59  | OHX  | 16SB  | 2206 | 7/7   | 0.99 | 0.06 | 95,98,106,125              | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 23SA  | 3405 | 1/1   | 0.99 | 0.09 | 46,46,46,46                 | 0     |
| 59  | OHX  | 16SB  | 2208 | 7/7   | 0.99 | 0.05 | 79,80,93,120                | 0     |
| 58  | MG   | 23SA  | 3406 | 1/1   | 0.99 | 0.04 | 63,63,63,63                 | 0     |
| 58  | MG   | 23SB  | 3359 | 1/1   | 0.99 | 0.11 | 66,66,66,66                 | 0     |
| 58  | MG   | 23SA  | 3446 | 1/1   | 0.99 | 0.05 | 43,43,43,43                 | 0     |
| 58  | MG   | 23SA  | 3386 | 1/1   | 0.99 | 0.04 | 47,47,47,47                 | 0     |
| 58  | MG   | 23SA  | 3480 | 1/1   | 0.99 | 0.04 | 82,82,82,82                 | 0     |
| 58  | MG   | 23SB  | 3363 | 1/1   | 0.99 | 0.08 | 47,47,47,47                 | 0     |
| 58  | MG   | 23SA  | 3408 | 1/1   | 0.99 | 0.03 | 45,45,45,45                 | 0     |
| 58  | MG   | 23SB  | 3432 | 1/1   | 0.99 | 0.04 | 46,46,46,46                 | 0     |
| 58  | MG   | 23SA  | 3426 | 1/1   | 0.99 | 0.04 | 42,42,42,42                 | 0     |
| 58  | MG   | 23SA  | 3517 | 1/1   | 0.99 | 0.08 | 82,82,82,82                 | 0     |
| 58  | MG   | 23SA  | 3450 | 1/1   | 0.99 | 0.03 | 56,56,56,56                 | 0     |
| 58  | MG   | 23SB  | 3368 | 1/1   | 0.99 | 0.03 | 47,47,47,47                 | 0     |
| 58  | MG   | 23SA  | 3451 | 1/1   | 0.99 | 0.04 | 33,33,33,33                 | 0     |
| 58  | MG   | 23SB  | 3438 | 1/1   | 0.99 | 0.05 | 45,45,45,45                 | 0     |
| 58  | MG   | 23SA  | 3520 | 1/1   | 0.99 | 0.13 | 79,79,79,79                 | 0     |
| 58  | MG   | 23SB  | 3371 | 1/1   | 0.99 | 0.04 | 39,39,39,39                 | 0     |
| 58  | MG   | 16SA  | 2349 | 1/1   | 0.99 | 0.03 | 82,82,82,82                 | 0     |
| 58  | MG   | 23SA  | 3522 | 1/1   | 0.99 | 0.03 | 73,73,73,73                 | 0     |
| 58  | MG   | 23SA  | 3410 | 1/1   | 0.99 | 0.03 | 57,57,57,57                 | 0     |
| 58  | MG   | 23SA  | 3454 | 1/1   | 0.99 | 0.03 | 54,54,54,54                 | 0     |
| 58  | MG   | 23SB  | 3376 | 1/1   | 0.99 | 0.03 | 50,50,50,50                 | 0     |
| 58  | MG   | 23SA  | 3525 | 1/1   | 0.99 | 0.10 | 40,40,40,40                 | 0     |
| 58  | MG   | 23SA  | 3429 | 1/1   | 0.99 | 0.07 | 60,60,60,60                 | 0     |
| 58  | MG   | 23SA  | 3388 | 1/1   | 0.99 | 0.04 | 33,33,33,33                 | 0     |
| 58  | MG   | 23SA  | 3412 | 1/1   | 0.99 | 0.04 | 40,40,40,40                 | 0     |
| 58  | MG   | 23SB  | 3382 | 1/1   | 0.99 | 0.04 | 61,61,61,61                 | 0     |
| 60  | K    | 23SA  | 3569 | 1/1   | 0.99 | 0.03 | 46,46,46,46                 | 0     |
| 59  | OHX  | 16SA  | 2260 | 7/7   | 0.99 | 0.06 | 68,70,81,89                 | 0     |
| 60  | K    | 23SA  | 3571 | 1/1   | 0.99 | 0.04 | 38,38,38,38                 | 0     |
| 59  | OHX  | 16SA  | 2261 | 7/7   | 0.99 | 0.07 | 71,82,87,97                 | 0     |
| 59  | OHX  | 16SA  | 2262 | 7/7   | 0.99 | 0.06 | 62,71,88,103                | 0     |
| 59  | OHX  | 16SA  | 2263 | 7/7   | 0.99 | 0.07 | 80,83,92,128                | 0     |
| 59  | OHX  | 16SA  | 2264 | 7/7   | 0.99 | 0.05 | 96,101,107,133              | 0     |
| 58  | MG   | 16SB  | 2334 | 1/1   | 0.99 | 0.06 | 68,68,68,68                 | 0     |
| 60  | K    | 23SA  | 3577 | 1/1   | 0.99 | 0.03 | 45,45,45,45                 | 0     |
| 58  | MG   | 16SB  | 2335 | 1/1   | 0.99 | 0.07 | 74,74,74,74                 | 0     |
| 59  | OHX  | 16SA  | 2267 | 7/7   | 0.99 | 0.05 | 85,94,97,129                | 0     |
| 59  | OHX  | 16SA  | 2268 | 7/7   | 0.99 | 0.06 | 96,97,109,142               | 0     |
| 58  | MG   | 23SA  | 3491 | 1/1   | 0.99 | 0.05 | 43,43,43,43                 | 0     |
| 58  | MG   | 16SB  | 2337 | 1/1   | 0.99 | 0.08 | 100,100,100,100             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 23SB  | 3387 | 1/1   | 0.99 | 0.08 | 53,53,53,53                 | 0     |
| 58  | MG   | 16SB  | 2338 | 1/1   | 0.99 | 0.05 | 86,86,86,86                 | 0     |
| 58  | MG   | 23SA  | 3530 | 1/1   | 0.99 | 0.05 | 57,57,57,57                 | 0     |
| 59  | OHX  | PSIA  | 102  | 7/7   | 0.99 | 0.09 | 94,95,102,131               | 0     |
| 58  | MG   | 23SA  | 3459 | 1/1   | 0.99 | 0.04 | 66,66,66,66                 | 0     |
| 58  | MG   | 16SB  | 2342 | 1/1   | 0.99 | 0.09 | 98,98,98,98                 | 0     |
| 58  | MG   | 16SA  | 2354 | 1/1   | 0.99 | 0.03 | 68,68,68,68                 | 0     |
| 58  | MG   | 23SA  | 3397 | 1/1   | 0.99 | 0.04 | 46,46,46,46                 | 0     |
| 59  | OHX  | 23SA  | 3178 | 7/7   | 0.99 | 0.10 | 43,55,71,95                 | 0     |
| 59  | OHX  | 23SA  | 3179 | 7/7   | 0.99 | 0.12 | 41,50,60,111                | 0     |
| 59  | OHX  | 23SA  | 3180 | 7/7   | 0.99 | 0.10 | 70,70,90,126                | 0     |
| 59  | OHX  | 5SB   | 202  | 7/7   | 0.99 | 0.05 | 96,105,116,131              | 0     |
| 59  | OHX  | 23SA  | 3181 | 7/7   | 0.99 | 0.06 | 55,67,74,94                 | 0     |
| 59  | OHX  | 23SA  | 3182 | 7/7   | 0.99 | 0.06 | 81,85,100,104               | 0     |
| 59  | OHX  | 23SA  | 3183 | 7/7   | 0.99 | 0.05 | 63,65,71,97                 | 0     |
| 59  | OHX  | 23SA  | 3185 | 7/7   | 0.99 | 0.05 | 69,73,78,116                | 0     |
| 59  | OHX  | 23SA  | 3186 | 7/7   | 0.99 | 0.04 | 62,68,77,96                 | 0     |
| 59  | OHX  | 23SA  | 3187 | 7/7   | 0.99 | 0.06 | 61,66,83,110                | 0     |
| 59  | OHX  | 23SA  | 3188 | 7/7   | 0.99 | 0.06 | 58,67,76,91                 | 0     |
| 59  | OHX  | 23SA  | 3189 | 7/7   | 0.99 | 0.07 | 60,72,78,115                | 0     |
| 59  | OHX  | 23SA  | 3190 | 7/7   | 0.99 | 0.06 | 79,85,92,109                | 0     |
| 58  | MG   | 23SB  | 3394 | 1/1   | 0.99 | 0.05 | 73,73,73,73                 | 0     |
| 59  | OHX  | 23SA  | 3192 | 7/7   | 0.99 | 0.07 | 68,74,81,100                | 0     |
| 58  | MG   | 23SA  | 3534 | 1/1   | 0.99 | 0.10 | 55,55,55,55                 | 0     |
| 58  | MG   | 16SB  | 2346 | 1/1   | 0.99 | 0.04 | 84,84,84,84                 | 0     |
| 58  | MG   | 23SA  | 3398 | 1/1   | 0.99 | 0.04 | 35,35,35,35                 | 0     |
| 58  | MG   | 23SA  | 3536 | 1/1   | 0.99 | 0.09 | 36,36,36,36                 | 0     |
| 58  | MG   | 23SA  | 3496 | 1/1   | 0.99 | 0.06 | 63,63,63,63                 | 0     |
| 58  | MG   | 23SB  | 3334 | 1/1   | 0.99 | 0.05 | 58,58,58,58                 | 0     |
| 58  | MG   | 23SA  | 3436 | 1/1   | 0.99 | 0.10 | 80,80,80,80                 | 0     |
| 58  | MG   | 23SA  | 3416 | 1/1   | 0.99 | 0.04 | 63,63,63,63                 | 0     |
| 58  | MG   | 16SA  | 2350 | 1/1   | 0.99 | 0.06 | 89,89,89,89                 | 0     |
| 58  | MG   | 23SB  | 3405 | 1/1   | 0.99 | 0.07 | 53,53,53,53                 | 0     |
| 58  | MG   | 23SB  | 3338 | 1/1   | 0.99 | 0.04 | 48,48,48,48                 | 0     |
| 58  | MG   | 23SB  | 3339 | 1/1   | 0.99 | 0.04 | 47,47,47,47                 | 0     |
| 59  | OHX  | S14B  | 101  | 7/7   | 0.99 | 0.04 | 121,125,132,169             | 0     |
| 58  | MG   | 16SB  | 2353 | 1/1   | 0.99 | 0.11 | 76,76,76,76                 | 0     |
| 58  | MG   | 5SA   | 215  | 1/1   | 0.99 | 0.04 | 64,64,64,64                 | 0     |
| 58  | MG   | 23SA  | 3439 | 1/1   | 0.99 | 0.07 | 38,38,38,38                 | 0     |
| 60  | K    | 16SA  | 2390 | 1/1   | 0.99 | 0.10 | 67,67,67,67                 | 0     |
| 58  | MG   | 16SB  | 2356 | 1/1   | 0.99 | 0.11 | 78,78,78,78                 | 0     |
| 60  | K    | 23SA  | 3624 | 1/1   | 0.99 | 0.03 | 60,60,60,60                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 23SA  | 3440 | 1/1   | 0.99 | 0.11 | 88,88,88,88                 | 0     |
| 58  | MG   | 23SA  | 3502 | 1/1   | 0.99 | 0.07 | 32,32,32,32                 | 0     |
| 58  | MG   | L3A   | 302  | 1/1   | 0.99 | 0.04 | 39,39,39,39                 | 0     |
| 59  | OHX  | 23SB  | 3001 | 7/7   | 0.99 | 0.10 | 59,64,68,112                | 0     |
| 59  | OHX  | 23SB  | 3002 | 7/7   | 0.99 | 0.08 | 66,72,95,109                | 0     |
| 59  | OHX  | 23SB  | 3004 | 7/7   | 0.99 | 0.04 | 64,70,79,95                 | 0     |
| 59  | OHX  | 23SB  | 3005 | 7/7   | 0.99 | 0.06 | 74,76,93,97                 | 0     |
| 59  | OHX  | 23SB  | 3006 | 7/7   | 0.99 | 0.06 | 70,76,84,116                | 0     |
| 59  | OHX  | 23SB  | 3007 | 7/7   | 0.99 | 0.06 | 85,90,107,121               | 0     |
| 58  | MG   | 23SB  | 3348 | 1/1   | 0.99 | 0.12 | 75,75,75,75                 | 0     |
| 59  | OHX  | 23SB  | 3009 | 7/7   | 0.99 | 0.07 | 75,77,79,117                | 0     |
| 59  | OHX  | 23SB  | 3010 | 7/7   | 0.99 | 0.08 | 79,84,90,126                | 0     |
| 59  | OHX  | 23SB  | 3011 | 7/7   | 0.99 | 0.07 | 74,84,94,103                | 0     |
| 58  | MG   | 23SA  | 3503 | 1/1   | 0.99 | 0.10 | 70,70,70,70                 | 0     |
| 59  | OHX  | 23SB  | 3013 | 7/7   | 0.99 | 0.05 | 86,91,94,110                | 0     |
| 59  | OHX  | 23SB  | 3014 | 7/7   | 0.99 | 0.04 | 74,88,94,117                | 0     |
| 59  | OHX  | 23SB  | 3015 | 7/7   | 0.99 | 0.07 | 103,106,113,117             | 0     |
| 59  | OHX  | L4A   | 302  | 7/7   | 0.99 | 0.17 | 37,47,53,146                | 0     |
| 59  | OHX  | 23SB  | 3017 | 7/7   | 0.99 | 0.06 | 83,87,98,124                | 0     |
| 59  | OHX  | 23SA  | 3214 | 7/7   | 0.99 | 0.05 | 62,70,75,153                | 0     |
| 59  | OHX  | 23SB  | 3019 | 7/7   | 0.99 | 0.06 | 68,75,83,123                | 0     |
| 59  | OHX  | 23SA  | 3215 | 7/7   | 0.99 | 0.05 | 81,87,93,144                | 0     |
| 59  | OHX  | L19A  | 201  | 7/7   | 0.99 | 0.05 | 85,89,97,137                | 0     |
| 58  | MG   | 23SA  | 3470 | 1/1   | 0.99 | 0.05 | 53,53,53,53                 | 0     |
| 58  | MG   | 23SA  | 3400 | 1/1   | 0.99 | 0.07 | 69,69,69,69                 | 0     |
| 58  | MG   | 23SA  | 3506 | 1/1   | 0.99 | 0.03 | 39,39,39,39                 | 0     |
| 58  | MG   | 16SA  | 2346 | 1/1   | 0.99 | 0.07 | 70,70,70,70                 | 0     |
| 58  | MG   | 23SB  | 3421 | 1/1   | 0.99 | 0.02 | 96,96,96,96                 | 0     |
| 59  | OHX  | 23SB  | 3027 | 7/7   | 0.99 | 0.07 | 78,82,92,125                | 0     |
| 59  | OHX  | 16SB  | 2201 | 7/7   | 0.99 | 0.05 | 81,88,90,106                | 0     |
| 58  | MG   | 23SA  | 3404 | 1/1   | 1.00 | 0.06 | 45,45,45,45                 | 0     |
| 58  | MG   | 23SA  | 3466 | 1/1   | 1.00 | 0.06 | 57,57,57,57                 | 0     |
| 58  | MG   | 23SA  | 3455 | 1/1   | 1.00 | 0.11 | 51,51,51,51                 | 0     |
| 58  | MG   | 23SA  | 3435 | 1/1   | 1.00 | 0.07 | 75,75,75,75                 | 0     |
| 58  | MG   | 23SB  | 3342 | 1/1   | 1.00 | 0.09 | 46,46,46,46                 | 0     |
| 58  | MG   | 16SB  | 2340 | 1/1   | 1.00 | 0.09 | 64,64,64,64                 | 0     |
| 58  | MG   | 23SB  | 3400 | 1/1   | 1.00 | 0.04 | 84,84,84,84                 | 0     |
| 58  | MG   | 23SB  | 3354 | 1/1   | 1.00 | 0.03 | 77,77,77,77                 | 0     |
| 58  | MG   | 23SA  | 3423 | 1/1   | 1.00 | 0.02 | 50,50,50,50                 | 0     |
| 58  | MG   | 23SA  | 3403 | 1/1   | 1.00 | 0.03 | 33,33,33,33                 | 0     |
| 58  | MG   | 23SA  | 3471 | 1/1   | 1.00 | 0.02 | 53,53,53,53                 | 0     |
| 59  | OHX  | L4B   | 301  | 7/7   | 1.00 | 0.09 | 48,52,62,94                 | 0     |

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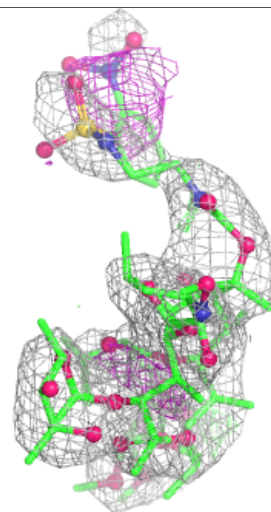
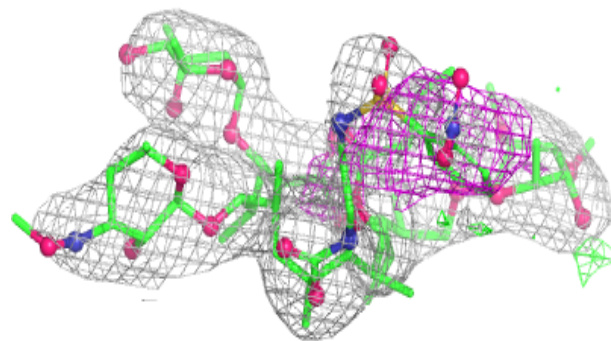
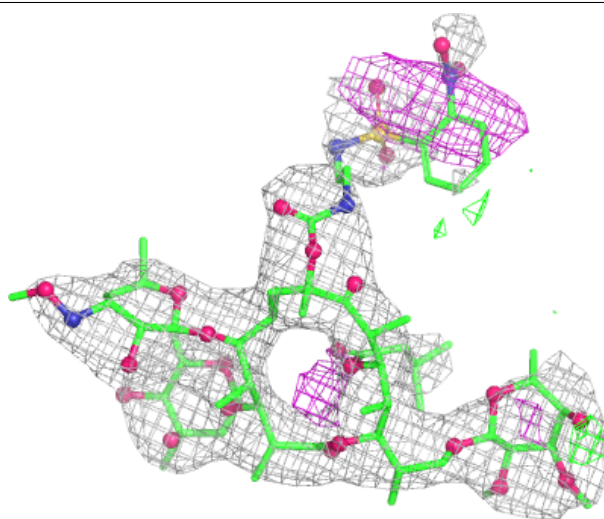
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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 23SB  | 3380 | 1/1   | 1.00 | 0.03 | 39,39,39,39                 | 0     |
| 58  | MG   | 23SA  | 3464 | 1/1   | 1.00 | 0.02 | 37,37,37,37                 | 0     |
| 59  | OHX  | 23SB  | 3003 | 7/7   | 1.00 | 0.05 | 75,81,93,98                 | 0     |
| 59  | OHX  | 23SA  | 3184 | 7/7   | 1.00 | 0.03 | 57,62,65,92                 | 0     |

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

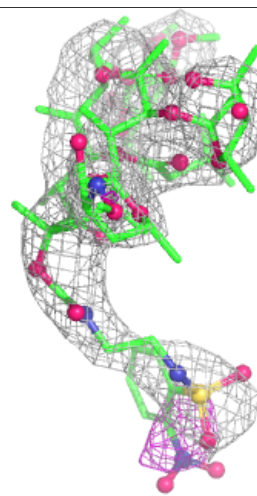
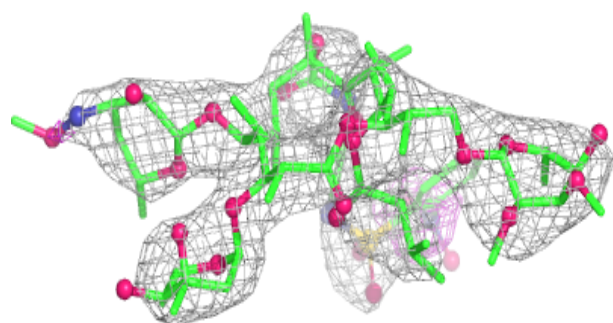
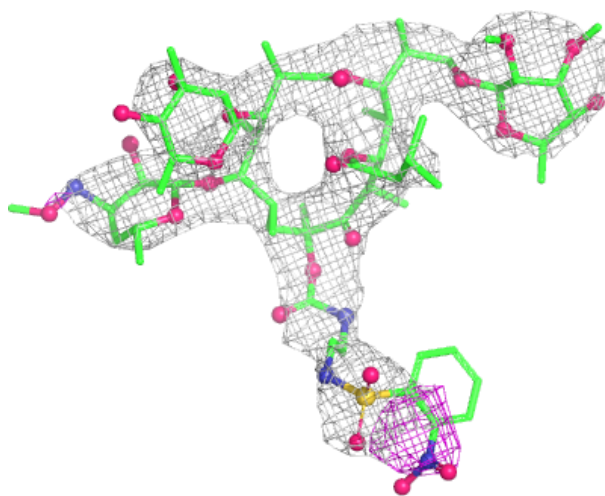
**Electron density around SJE 23SA 3640:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SJE 23SB 3521:**

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



## 5.5 Other polymers [i](#)

There are no such residues in this entry.