



# wwPDB X-ray Structure Validation Summary Report

Oct 9, 2014 – 10:08 PM BST

PDB ID : 4U4U  
Title : Crystal structure of Lycorine bound to the yeast 80S ribosome  
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.  
Deposited on : 2014-07-24  
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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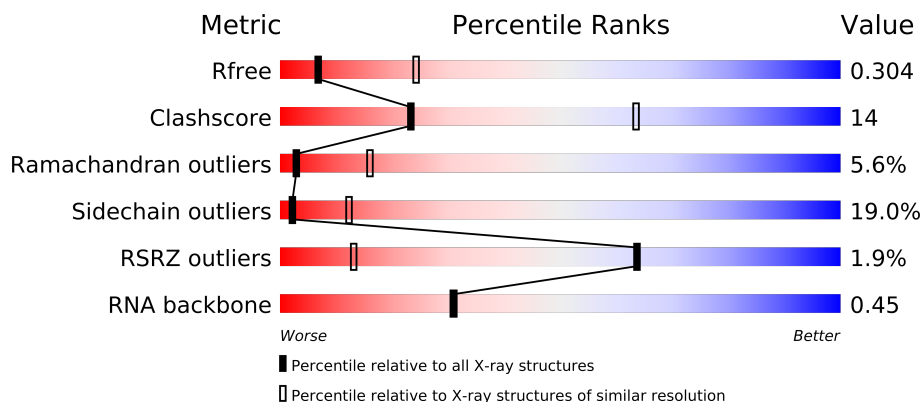
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable24037  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24037

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 66092                       | 1216 (3.00-3.00)                                      |
| Clashscore            | 79885                       | 1594 (3.00-3.00)                                      |
| Ramachandran outliers | 78287                       | 1537 (3.00-3.00)                                      |
| Sidechain outliers    | 78261                       | 1540 (3.00-3.00)                                      |
| RSRZ outliers         | 66119                       | 1217 (3.00-3.00)                                      |
| RNA backbone          | 1838                        | 1070 (3.50-2.50)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 2     | 1800   |                  |
| 1   | 6     | 1800   |                  |
| 2   | S0    | 251    |                  |
| 2   | s0    | 251    |                  |
| 3   | S1    | 254    |                  |
| 3   | s1    | 254    |                  |
| 4   | S2    | 253    |                  |
| 4   | s2    | 253    |                  |
| 5   | S3    | 239    |                  |
| 5   | s3    | 239    |                  |
| 6   | S4    | 260    |                  |
| 6   | s4    | 260    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 7   | S5    | 224    |                  |
| 7   | s5    | 224    |                  |
| 8   | S6    | 236    |                  |
| 8   | s6    | 236    |                  |
| 9   | S7    | 189    |                  |
| 9   | s7    | 189    |                  |
| 10  | S8    | 200    |                  |
| 10  | s8    | 200    |                  |
| 11  | S9    | 196    |                  |
| 11  | s9    | 196    |                  |
| 12  | C0    | 105    |                  |
| 12  | c0    | 105    |                  |
| 13  | C1    | 155    |                  |
| 13  | c1    | 155    |                  |
| 14  | C2    | 142    |                  |
| 14  | c2    | 142    |                  |
| 15  | C3    | 150    |                  |
| 15  | c3    | 150    |                  |
| 16  | C4    | 136    |                  |
| 16  | c4    | 136    |                  |
| 17  | C5    | 141    |                  |
| 17  | c5    | 141    |                  |
| 18  | C6    | 142    |                  |
| 18  | c6    | 142    |                  |
| 19  | C7    | 136    |                  |
| 19  | c7    | 136    |                  |
| 20  | C8    | 145    |                  |
| 20  | c8    | 145    |                  |
| 21  | C9    | 143    |                  |
| 21  | c9    | 143    |                  |
| 22  | D0    | 120    |                  |
| 22  | d0    | 120    |                  |
| 23  | D1    | 87     |                  |
| 23  | d1    | 87     |                  |
| 24  | D2    | 129    |                  |
| 24  | d2    | 129    |                  |
| 25  | D3    | 144    |                  |
| 25  | d3    | 144    |                  |
| 26  | D4    | 134    |                  |
| 26  | d4    | 134    |                  |
| 27  | D5    | 107    |                  |
| 27  | d5    | 107    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28  | D6    | 97     |                  |
| 28  | d6    | 97     |                  |
| 29  | D7    | 81     |                  |
| 29  | d7    | 81     |                  |
| 30  | D8    | 66     |                  |
| 30  | d8    | 66     |                  |
| 31  | D9    | 55     |                  |
| 31  | d9    | 55     |                  |
| 32  | E0    | 60     |                  |
| 33  | E1    | 76     |                  |
| 33  | e1    | 76     |                  |
| 34  | SR    | 318    |                  |
| 34  | sR    | 318    |                  |
| 35  | SM    | 273    |                  |
| 36  | 1     | 3396   |                  |
| 36  | 5     | 3396   |                  |
| 37  | 3     | 121    |                  |
| 37  | 7     | 121    |                  |
| 38  | 4     | 158    |                  |
| 38  | 8     | 158    |                  |
| 39  | L2    | 253    |                  |
| 39  | l2    | 253    |                  |
| 40  | L3    | 386    |                  |
| 40  | l3    | 386    |                  |
| 41  | L4    | 361    |                  |
| 41  | l4    | 361    |                  |
| 42  | L5    | 296    |                  |
| 42  | l5    | 296    |                  |
| 43  | L6    | 175    |                  |
| 43  | l6    | 175    |                  |
| 44  | L7    | 243    |                  |
| 44  | l7    | 243    |                  |
| 45  | L8    | 255    |                  |
| 45  | l8    | 255    |                  |
| 46  | L9    | 191    |                  |
| 46  | l9    | 191    |                  |
| 47  | M0    | 220    |                  |
| 47  | m0    | 220    |                  |
| 48  | M1    | 173    |                  |
| 48  | m1    | 173    |                  |
| 49  | M3    | 198    |                  |
| 49  | m3    | 198    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 50  | M4    | 137    |                  |
| 50  | m4    | 137    |                  |
| 51  | M5    | 203    |                  |
| 51  | m5    | 203    |                  |
| 52  | M6    | 198    |                  |
| 52  | m6    | 198    |                  |
| 53  | M7    | 183    |                  |
| 53  | m7    | 183    |                  |
| 54  | M8    | 185    |                  |
| 54  | m8    | 185    |                  |
| 55  | M9    | 188    |                  |
| 55  | m9    | 188    |                  |
| 56  | N0    | 172    |                  |
| 56  | n0    | 172    |                  |
| 57  | N1    | 159    |                  |
| 57  | n1    | 159    |                  |
| 58  | N2    | 120    |                  |
| 58  | n2    | 120    |                  |
| 59  | N3    | 136    |                  |
| 59  | n3    | 136    |                  |
| 60  | N4    | 155    |                  |
| 60  | n4    | 155    |                  |
| 61  | N5    | 141    |                  |
| 61  | n5    | 141    |                  |
| 62  | N6    | 126    |                  |
| 62  | n6    | 126    |                  |
| 63  | N7    | 135    |                  |
| 63  | n7    | 135    |                  |
| 64  | N8    | 148    |                  |
| 64  | n8    | 148    |                  |
| 65  | N9    | 58     |                  |
| 65  | n9    | 58     |                  |
| 66  | O0    | 104    |                  |
| 66  | o0    | 104    |                  |
| 67  | O1    | 112    |                  |
| 67  | o1    | 112    |                  |
| 68  | O2    | 129    |                  |
| 68  | o2    | 129    |                  |
| 69  | O3    | 106    |                  |
| 69  | o3    | 106    |                  |
| 70  | O4    | 119    |                  |
| 70  | o4    | 119    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 71  | O5    | 119    |                  |
| 71  | o5    | 119    |                  |
| 72  | O6    | 99     |                  |
| 72  | o6    | 99     |                  |
| 73  | O7    | 87     |                  |
| 73  | o7    | 87     |                  |
| 74  | O8    | 77     |                  |
| 74  | o8    | 77     |                  |
| 75  | O9    | 50     |                  |
| 75  | o9    | 50     |                  |
| 76  | Q0    | 52     |                  |
| 76  | q0    | 52     |                  |
| 77  | Q1    | 25     |                  |
| 77  | q1    | 25     |                  |
| 78  | Q2    | 105    |                  |
| 78  | q2    | 105    |                  |
| 79  | Q3    | 91     |                  |
| 79  | q3    | 91     |                  |
| 80  | e0    | 62     |                  |
| 81  | sM    | 273    |                  |
| 82  | m2    | 160    |                  |
| 83  | p0    | 311    |                  |
| 84  | p1    | 47     |                  |
| 85  | p2    | 46     |                  |

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 1     | 3401 | -        | X                |
| 86  | MG   | 1     | 3402 | -        | X                |
| 86  | MG   | 1     | 3403 | -        | X                |
| 86  | MG   | 1     | 3405 | -        | X                |
| 86  | MG   | 1     | 3406 | -        | X                |
| 86  | MG   | 1     | 3407 | -        | X                |
| 86  | MG   | 1     | 3408 | -        | X                |
| 86  | MG   | 1     | 3409 | -        | X                |
| 86  | MG   | 1     | 3410 | -        | X                |
| 86  | MG   | 1     | 3411 | -        | X                |
| 86  | MG   | 1     | 3412 | -        | X                |
| 86  | MG   | 1     | 3413 | -        | X                |
| 86  | MG   | 1     | 3414 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 1     | 3417 | -        | X                |
| 86  | MG   | 1     | 3418 | -        | X                |
| 86  | MG   | 1     | 3419 | -        | X                |
| 86  | MG   | 1     | 3421 | -        | X                |
| 86  | MG   | 1     | 3422 | -        | X                |
| 86  | MG   | 1     | 3423 | -        | X                |
| 86  | MG   | 1     | 3427 | -        | X                |
| 86  | MG   | 1     | 3429 | -        | X                |
| 86  | MG   | 1     | 3430 | -        | X                |
| 86  | MG   | 1     | 3431 | -        | X                |
| 86  | MG   | 1     | 3432 | -        | X                |
| 86  | MG   | 1     | 3433 | -        | X                |
| 86  | MG   | 1     | 3435 | -        | X                |
| 86  | MG   | 1     | 3437 | -        | X                |
| 86  | MG   | 1     | 3438 | -        | X                |
| 86  | MG   | 1     | 3439 | -        | X                |
| 86  | MG   | 1     | 3440 | -        | X                |
| 86  | MG   | 1     | 3441 | -        | X                |
| 86  | MG   | 1     | 3442 | -        | X                |
| 86  | MG   | 1     | 3444 | -        | X                |
| 86  | MG   | 1     | 3445 | -        | X                |
| 86  | MG   | 1     | 3448 | -        | X                |
| 86  | MG   | 1     | 3450 | -        | X                |
| 86  | MG   | 1     | 3451 | -        | X                |
| 86  | MG   | 1     | 3452 | -        | X                |
| 86  | MG   | 1     | 3453 | -        | X                |
| 86  | MG   | 1     | 3454 | -        | X                |
| 86  | MG   | 1     | 3455 | -        | X                |
| 86  | MG   | 1     | 3456 | -        | X                |
| 86  | MG   | 1     | 3457 | -        | X                |
| 86  | MG   | 1     | 3458 | -        | X                |
| 86  | MG   | 1     | 3459 | -        | X                |
| 86  | MG   | 1     | 3460 | -        | X                |
| 86  | MG   | 1     | 3461 | -        | X                |
| 86  | MG   | 1     | 3462 | -        | X                |
| 86  | MG   | 1     | 3463 | -        | X                |
| 86  | MG   | 1     | 3465 | -        | X                |
| 86  | MG   | 1     | 3467 | -        | X                |
| 86  | MG   | 1     | 3468 | -        | X                |
| 86  | MG   | 1     | 3469 | -        | X                |
| 86  | MG   | 1     | 3470 | -        | X                |
| 86  | MG   | 1     | 3471 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 1     | 3472 | -        | X                |
| 86  | MG   | 1     | 3473 | -        | X                |
| 86  | MG   | 1     | 3474 | -        | X                |
| 86  | MG   | 1     | 3475 | -        | X                |
| 86  | MG   | 1     | 3476 | -        | X                |
| 86  | MG   | 1     | 3477 | -        | X                |
| 86  | MG   | 1     | 3478 | -        | X                |
| 86  | MG   | 1     | 3479 | -        | X                |
| 86  | MG   | 1     | 3480 | -        | X                |
| 86  | MG   | 1     | 3481 | -        | X                |
| 86  | MG   | 1     | 3483 | -        | X                |
| 86  | MG   | 1     | 3484 | -        | X                |
| 86  | MG   | 1     | 3485 | -        | X                |
| 86  | MG   | 1     | 3486 | -        | X                |
| 86  | MG   | 1     | 3487 | -        | X                |
| 86  | MG   | 1     | 3488 | -        | X                |
| 86  | MG   | 1     | 3489 | -        | X                |
| 86  | MG   | 1     | 3490 | -        | X                |
| 86  | MG   | 1     | 3492 | -        | X                |
| 86  | MG   | 1     | 3493 | -        | X                |
| 86  | MG   | 1     | 3495 | -        | X                |
| 86  | MG   | 1     | 3496 | -        | X                |
| 86  | MG   | 1     | 3497 | -        | X                |
| 86  | MG   | 1     | 3498 | -        | X                |
| 86  | MG   | 1     | 3499 | -        | X                |
| 86  | MG   | 1     | 3500 | -        | X                |
| 86  | MG   | 1     | 3501 | -        | X                |
| 86  | MG   | 1     | 3502 | -        | X                |
| 86  | MG   | 1     | 3503 | -        | X                |
| 86  | MG   | 1     | 3504 | -        | X                |
| 86  | MG   | 1     | 3505 | -        | X                |
| 86  | MG   | 1     | 3506 | -        | X                |
| 86  | MG   | 1     | 3507 | -        | X                |
| 86  | MG   | 1     | 3509 | -        | X                |
| 86  | MG   | 1     | 3510 | -        | X                |
| 86  | MG   | 1     | 3511 | -        | X                |
| 86  | MG   | 1     | 3512 | -        | X                |
| 86  | MG   | 1     | 3513 | -        | X                |
| 86  | MG   | 1     | 3514 | -        | X                |
| 86  | MG   | 1     | 3515 | -        | X                |
| 86  | MG   | 1     | 3516 | -        | X                |
| 86  | MG   | 1     | 3517 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 1     | 3518 | -        | X                |
| 86  | MG   | 1     | 3519 | -        | X                |
| 86  | MG   | 1     | 3520 | -        | X                |
| 86  | MG   | 1     | 3521 | -        | X                |
| 86  | MG   | 1     | 3523 | -        | X                |
| 86  | MG   | 1     | 3524 | -        | X                |
| 86  | MG   | 1     | 3525 | -        | X                |
| 86  | MG   | 1     | 3526 | -        | X                |
| 86  | MG   | 1     | 3527 | -        | X                |
| 86  | MG   | 1     | 3528 | -        | X                |
| 86  | MG   | 1     | 3529 | -        | X                |
| 86  | MG   | 1     | 3530 | -        | X                |
| 86  | MG   | 1     | 3532 | -        | X                |
| 86  | MG   | 1     | 3533 | -        | X                |
| 86  | MG   | 1     | 3534 | -        | X                |
| 86  | MG   | 1     | 3535 | -        | X                |
| 86  | MG   | 1     | 3536 | -        | X                |
| 86  | MG   | 1     | 3537 | -        | X                |
| 86  | MG   | 1     | 3538 | -        | X                |
| 86  | MG   | 1     | 3539 | -        | X                |
| 86  | MG   | 1     | 3540 | -        | X                |
| 86  | MG   | 1     | 3542 | -        | X                |
| 86  | MG   | 1     | 3543 | -        | X                |
| 86  | MG   | 1     | 3544 | -        | X                |
| 86  | MG   | 1     | 3545 | -        | X                |
| 86  | MG   | 1     | 3546 | -        | X                |
| 86  | MG   | 1     | 3547 | -        | X                |
| 86  | MG   | 1     | 3548 | -        | X                |
| 86  | MG   | 1     | 3549 | -        | X                |
| 86  | MG   | 1     | 3550 | -        | X                |
| 86  | MG   | 1     | 3551 | -        | X                |
| 86  | MG   | 1     | 3552 | -        | X                |
| 86  | MG   | 1     | 3553 | -        | X                |
| 86  | MG   | 1     | 3554 | -        | X                |
| 86  | MG   | 1     | 3555 | -        | X                |
| 86  | MG   | 1     | 3556 | -        | X                |
| 86  | MG   | 1     | 3557 | -        | X                |
| 86  | MG   | 1     | 3559 | -        | X                |
| 86  | MG   | 1     | 3560 | -        | X                |
| 86  | MG   | 1     | 3561 | -        | X                |
| 86  | MG   | 1     | 3562 | -        | X                |
| 86  | MG   | 1     | 3563 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 1     | 3564 | -        | X                |
| 86  | MG   | 1     | 3565 | -        | X                |
| 86  | MG   | 1     | 3566 | -        | X                |
| 86  | MG   | 1     | 3567 | -        | X                |
| 86  | MG   | 1     | 3568 | -        | X                |
| 86  | MG   | 1     | 3569 | -        | X                |
| 86  | MG   | 1     | 3570 | -        | X                |
| 86  | MG   | 1     | 3571 | -        | X                |
| 86  | MG   | 1     | 3572 | -        | X                |
| 86  | MG   | 1     | 3573 | -        | X                |
| 86  | MG   | 1     | 3574 | -        | X                |
| 86  | MG   | 1     | 3575 | -        | X                |
| 86  | MG   | 1     | 3576 | -        | X                |
| 86  | MG   | 1     | 3577 | -        | X                |
| 86  | MG   | 1     | 3578 | -        | X                |
| 86  | MG   | 1     | 3579 | -        | X                |
| 86  | MG   | 1     | 3580 | -        | X                |
| 86  | MG   | 1     | 3581 | -        | X                |
| 86  | MG   | 1     | 3584 | -        | X                |
| 86  | MG   | 1     | 3585 | -        | X                |
| 86  | MG   | 1     | 3586 | -        | X                |
| 86  | MG   | 1     | 3587 | -        | X                |
| 86  | MG   | 1     | 3588 | -        | X                |
| 86  | MG   | 1     | 3589 | -        | X                |
| 86  | MG   | 1     | 3590 | -        | X                |
| 86  | MG   | 1     | 3591 | -        | X                |
| 86  | MG   | 1     | 3592 | -        | X                |
| 86  | MG   | 1     | 3593 | -        | X                |
| 86  | MG   | 1     | 3595 | -        | X                |
| 86  | MG   | 1     | 3596 | -        | X                |
| 86  | MG   | 1     | 3597 | -        | X                |
| 86  | MG   | 1     | 3598 | -        | X                |
| 86  | MG   | 1     | 3599 | -        | X                |
| 86  | MG   | 1     | 3600 | -        | X                |
| 86  | MG   | 1     | 3601 | -        | X                |
| 86  | MG   | 1     | 3602 | -        | X                |
| 86  | MG   | 1     | 3603 | -        | X                |
| 86  | MG   | 1     | 3604 | -        | X                |
| 86  | MG   | 1     | 3605 | -        | X                |
| 86  | MG   | 1     | 3608 | -        | X                |
| 86  | MG   | 1     | 3609 | -        | X                |
| 86  | MG   | 1     | 3610 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 1     | 3613 | -        | X                |
| 86  | MG   | 1     | 3614 | -        | X                |
| 86  | MG   | 1     | 3615 | -        | X                |
| 86  | MG   | 1     | 3616 | -        | X                |
| 86  | MG   | 1     | 3619 | -        | X                |
| 86  | MG   | 1     | 3620 | -        | X                |
| 86  | MG   | 1     | 3621 | -        | X                |
| 86  | MG   | 1     | 3622 | -        | X                |
| 86  | MG   | 1     | 3625 | -        | X                |
| 86  | MG   | 1     | 3626 | -        | X                |
| 86  | MG   | 1     | 3627 | -        | X                |
| 86  | MG   | 1     | 3628 | -        | X                |
| 86  | MG   | 1     | 3629 | -        | X                |
| 86  | MG   | 1     | 3631 | -        | X                |
| 86  | MG   | 1     | 3635 | -        | X                |
| 86  | MG   | 1     | 3637 | -        | X                |
| 86  | MG   | 1     | 3641 | -        | X                |
| 86  | MG   | 1     | 3643 | -        | X                |
| 86  | MG   | 1     | 3644 | -        | X                |
| 86  | MG   | 1     | 3647 | -        | X                |
| 86  | MG   | 1     | 3648 | -        | X                |
| 86  | MG   | 1     | 3649 | -        | X                |
| 86  | MG   | 1     | 3650 | -        | X                |
| 86  | MG   | 1     | 3651 | -        | X                |
| 86  | MG   | 1     | 3652 | -        | X                |
| 86  | MG   | 1     | 3653 | -        | X                |
| 86  | MG   | 1     | 3654 | -        | X                |
| 86  | MG   | 1     | 3655 | -        | X                |
| 86  | MG   | 1     | 3656 | -        | X                |
| 86  | MG   | 1     | 3657 | -        | X                |
| 86  | MG   | 1     | 3658 | -        | X                |
| 86  | MG   | 1     | 3659 | -        | X                |
| 86  | MG   | 1     | 3660 | -        | X                |
| 86  | MG   | 1     | 3661 | -        | X                |
| 86  | MG   | 1     | 3665 | -        | X                |
| 86  | MG   | 1     | 3666 | -        | X                |
| 86  | MG   | 1     | 3668 | -        | X                |
| 86  | MG   | 1     | 3670 | -        | X                |
| 86  | MG   | 1     | 3671 | -        | X                |
| 86  | MG   | 1     | 3673 | -        | X                |
| 86  | MG   | 1     | 3674 | -        | X                |
| 86  | MG   | 1     | 3675 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 1     | 3676 | -        | X                |
| 86  | MG   | 1     | 3678 | -        | X                |
| 86  | MG   | 1     | 3679 | -        | X                |
| 86  | MG   | 1     | 3680 | -        | X                |
| 86  | MG   | 1     | 3681 | -        | X                |
| 86  | MG   | 1     | 3682 | -        | X                |
| 86  | MG   | 1     | 3684 | -        | X                |
| 86  | MG   | 1     | 3685 | -        | X                |
| 86  | MG   | 1     | 3687 | -        | X                |
| 86  | MG   | 1     | 3688 | -        | X                |
| 86  | MG   | 1     | 3689 | -        | X                |
| 86  | MG   | 1     | 3690 | -        | X                |
| 86  | MG   | 1     | 3691 | -        | X                |
| 86  | MG   | 1     | 3692 | -        | X                |
| 86  | MG   | 1     | 3693 | -        | X                |
| 86  | MG   | 1     | 3694 | -        | X                |
| 86  | MG   | 1     | 3695 | -        | X                |
| 86  | MG   | 1     | 3696 | -        | X                |
| 86  | MG   | 1     | 3697 | -        | X                |
| 86  | MG   | 1     | 3698 | -        | X                |
| 86  | MG   | 1     | 3699 | -        | X                |
| 86  | MG   | 1     | 3700 | -        | X                |
| 86  | MG   | 1     | 3701 | -        | X                |
| 86  | MG   | 1     | 3702 | -        | X                |
| 86  | MG   | 1     | 3703 | -        | X                |
| 86  | MG   | 1     | 3704 | -        | X                |
| 86  | MG   | 1     | 3705 | -        | X                |
| 86  | MG   | 1     | 3706 | -        | X                |
| 86  | MG   | 1     | 3707 | -        | X                |
| 86  | MG   | 1     | 3708 | -        | X                |
| 86  | MG   | 1     | 3711 | -        | X                |
| 86  | MG   | 1     | 3712 | -        | X                |
| 86  | MG   | 1     | 3713 | -        | X                |
| 86  | MG   | 1     | 3715 | -        | X                |
| 86  | MG   | 1     | 3717 | -        | X                |
| 86  | MG   | 1     | 3720 | -        | X                |
| 86  | MG   | 1     | 3721 | -        | X                |
| 86  | MG   | 1     | 3723 | -        | X                |
| 86  | MG   | 1     | 3725 | -        | X                |
| 86  | MG   | 1     | 3726 | -        | X                |
| 86  | MG   | 1     | 3727 | -        | X                |
| 86  | MG   | 1     | 3729 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 1     | 3731 | -        | X                |
| 86  | MG   | 1     | 3732 | -        | X                |
| 86  | MG   | 1     | 3733 | -        | X                |
| 86  | MG   | 1     | 3735 | -        | X                |
| 86  | MG   | 1     | 3739 | -        | X                |
| 86  | MG   | 1     | 3740 | -        | X                |
| 86  | MG   | 1     | 3741 | -        | X                |
| 86  | MG   | 1     | 3744 | -        | X                |
| 86  | MG   | 1     | 3745 | -        | X                |
| 86  | MG   | 1     | 3748 | -        | X                |
| 86  | MG   | 1     | 3750 | -        | X                |
| 86  | MG   | 1     | 3755 | -        | X                |
| 86  | MG   | 1     | 3757 | -        | X                |
| 86  | MG   | 1     | 3758 | -        | X                |
| 86  | MG   | 1     | 3760 | -        | X                |
| 86  | MG   | 1     | 3761 | -        | X                |
| 86  | MG   | 1     | 3762 | -        | X                |
| 86  | MG   | 1     | 3763 | -        | X                |
| 86  | MG   | 1     | 3764 | -        | X                |
| 86  | MG   | 1     | 3765 | -        | X                |
| 86  | MG   | 1     | 3766 | -        | X                |
| 86  | MG   | 1     | 3768 | -        | X                |
| 86  | MG   | 1     | 3773 | -        | X                |
| 86  | MG   | 1     | 3775 | -        | X                |
| 86  | MG   | 1     | 3777 | -        | X                |
| 86  | MG   | 1     | 3780 | -        | X                |
| 86  | MG   | 1     | 3781 | -        | X                |
| 86  | MG   | 1     | 3782 | -        | X                |
| 86  | MG   | 1     | 3783 | -        | X                |
| 86  | MG   | 1     | 3784 | -        | X                |
| 86  | MG   | 1     | 3785 | -        | X                |
| 86  | MG   | 1     | 3787 | -        | X                |
| 86  | MG   | 1     | 3789 | -        | X                |
| 86  | MG   | 1     | 3790 | -        | X                |
| 86  | MG   | 1     | 3791 | -        | X                |
| 86  | MG   | 1     | 3795 | -        | X                |
| 86  | MG   | 1     | 3797 | -        | X                |
| 86  | MG   | 1     | 3798 | -        | X                |
| 86  | MG   | 1     | 3799 | -        | X                |
| 86  | MG   | 1     | 3800 | -        | X                |
| 86  | MG   | 1     | 3801 | -        | X                |
| 86  | MG   | 1     | 3802 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 1     | 3805 | -        | X                |
| 86  | MG   | 1     | 3807 | -        | X                |
| 86  | MG   | 1     | 3808 | -        | X                |
| 86  | MG   | 1     | 3809 | -        | X                |
| 86  | MG   | 1     | 3812 | -        | X                |
| 86  | MG   | 1     | 3815 | -        | X                |
| 86  | MG   | 1     | 3818 | -        | X                |
| 86  | MG   | 1     | 3819 | -        | X                |
| 86  | MG   | 1     | 3820 | -        | X                |
| 86  | MG   | 1     | 3823 | -        | X                |
| 86  | MG   | 1     | 3825 | -        | X                |
| 86  | MG   | 1     | 3826 | -        | X                |
| 86  | MG   | 1     | 3831 | -        | X                |
| 86  | MG   | 1     | 3833 | -        | X                |
| 86  | MG   | 1     | 3834 | -        | X                |
| 86  | MG   | 1     | 3835 | -        | X                |
| 86  | MG   | 1     | 3836 | -        | X                |
| 86  | MG   | 1     | 3837 | -        | X                |
| 86  | MG   | 1     | 3838 | -        | X                |
| 86  | MG   | 1     | 3841 | -        | X                |
| 86  | MG   | 1     | 3843 | -        | X                |
| 86  | MG   | 1     | 3844 | -        | X                |
| 86  | MG   | 1     | 3845 | -        | X                |
| 86  | MG   | 1     | 3846 | -        | X                |
| 86  | MG   | 1     | 3847 | -        | X                |
| 86  | MG   | 1     | 3848 | -        | X                |
| 86  | MG   | 1     | 3849 | -        | X                |
| 86  | MG   | 1     | 3850 | -        | X                |
| 86  | MG   | 1     | 3851 | -        | X                |
| 86  | MG   | 1     | 3852 | -        | X                |
| 86  | MG   | 1     | 3854 | -        | X                |
| 86  | MG   | 1     | 3855 | -        | X                |
| 86  | MG   | 1     | 3856 | -        | X                |
| 86  | MG   | 1     | 3857 | -        | X                |
| 86  | MG   | 1     | 3858 | -        | X                |
| 86  | MG   | 1     | 3859 | -        | X                |
| 86  | MG   | 1     | 3860 | -        | X                |
| 86  | MG   | 1     | 3862 | -        | X                |
| 86  | MG   | 1     | 3863 | -        | X                |
| 86  | MG   | 1     | 3865 | -        | X                |
| 86  | MG   | 1     | 3866 | -        | X                |
| 86  | MG   | 1     | 3867 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 1     | 3868 | -        | X                |
| 86  | MG   | 1     | 3869 | -        | X                |
| 86  | MG   | 1     | 4221 | -        | X                |
| 86  | MG   | 2     | 1901 | -        | X                |
| 86  | MG   | 2     | 1902 | -        | X                |
| 86  | MG   | 2     | 1903 | -        | X                |
| 86  | MG   | 2     | 1905 | -        | X                |
| 86  | MG   | 2     | 1906 | -        | X                |
| 86  | MG   | 2     | 1907 | -        | X                |
| 86  | MG   | 2     | 1908 | -        | X                |
| 86  | MG   | 2     | 1909 | -        | X                |
| 86  | MG   | 2     | 1910 | -        | X                |
| 86  | MG   | 2     | 1911 | -        | X                |
| 86  | MG   | 2     | 1912 | -        | X                |
| 86  | MG   | 2     | 1913 | -        | X                |
| 86  | MG   | 2     | 1914 | -        | X                |
| 86  | MG   | 2     | 1915 | -        | X                |
| 86  | MG   | 2     | 1916 | -        | X                |
| 86  | MG   | 2     | 1917 | -        | X                |
| 86  | MG   | 2     | 1918 | -        | X                |
| 86  | MG   | 2     | 1919 | -        | X                |
| 86  | MG   | 2     | 1920 | -        | X                |
| 86  | MG   | 2     | 1921 | -        | X                |
| 86  | MG   | 2     | 1922 | -        | X                |
| 86  | MG   | 2     | 1923 | -        | X                |
| 86  | MG   | 2     | 1924 | -        | X                |
| 86  | MG   | 2     | 1925 | -        | X                |
| 86  | MG   | 2     | 1926 | -        | X                |
| 86  | MG   | 2     | 1927 | -        | X                |
| 86  | MG   | 2     | 1928 | -        | X                |
| 86  | MG   | 2     | 1929 | -        | X                |
| 86  | MG   | 2     | 1930 | -        | X                |
| 86  | MG   | 2     | 1931 | -        | X                |
| 86  | MG   | 2     | 1932 | -        | X                |
| 86  | MG   | 2     | 1933 | -        | X                |
| 86  | MG   | 2     | 1934 | -        | X                |
| 86  | MG   | 2     | 1935 | -        | X                |
| 86  | MG   | 2     | 1936 | -        | X                |
| 86  | MG   | 2     | 1937 | -        | X                |
| 86  | MG   | 2     | 1938 | -        | X                |
| 86  | MG   | 2     | 1939 | -        | X                |
| 86  | MG   | 2     | 1940 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 2     | 1941 | -        | X                |
| 86  | MG   | 2     | 1942 | -        | X                |
| 86  | MG   | 2     | 1943 | -        | X                |
| 86  | MG   | 2     | 1944 | -        | X                |
| 86  | MG   | 2     | 1945 | -        | X                |
| 86  | MG   | 2     | 1947 | -        | X                |
| 86  | MG   | 2     | 1948 | -        | X                |
| 86  | MG   | 2     | 1949 | -        | X                |
| 86  | MG   | 2     | 1950 | -        | X                |
| 86  | MG   | 2     | 1951 | -        | X                |
| 86  | MG   | 2     | 1952 | -        | X                |
| 86  | MG   | 2     | 1954 | -        | X                |
| 86  | MG   | 2     | 1955 | -        | X                |
| 86  | MG   | 2     | 1956 | -        | X                |
| 86  | MG   | 2     | 1957 | -        | X                |
| 86  | MG   | 2     | 1958 | -        | X                |
| 86  | MG   | 2     | 1959 | -        | X                |
| 86  | MG   | 2     | 1960 | -        | X                |
| 86  | MG   | 2     | 1961 | -        | X                |
| 86  | MG   | 2     | 1962 | -        | X                |
| 86  | MG   | 2     | 1964 | -        | X                |
| 86  | MG   | 2     | 1965 | -        | X                |
| 86  | MG   | 2     | 1966 | -        | X                |
| 86  | MG   | 2     | 1967 | -        | X                |
| 86  | MG   | 2     | 1968 | -        | X                |
| 86  | MG   | 2     | 1970 | -        | X                |
| 86  | MG   | 2     | 1971 | -        | X                |
| 86  | MG   | 2     | 1972 | -        | X                |
| 86  | MG   | 2     | 1973 | -        | X                |
| 86  | MG   | 2     | 1974 | -        | X                |
| 86  | MG   | 2     | 1975 | -        | X                |
| 86  | MG   | 2     | 1976 | -        | X                |
| 86  | MG   | 2     | 1977 | -        | X                |
| 86  | MG   | 2     | 1978 | -        | X                |
| 86  | MG   | 2     | 1979 | -        | X                |
| 86  | MG   | 2     | 1980 | -        | X                |
| 86  | MG   | 2     | 1981 | -        | X                |
| 86  | MG   | 2     | 1982 | -        | X                |
| 86  | MG   | 2     | 1983 | -        | X                |
| 86  | MG   | 2     | 1984 | -        | X                |
| 86  | MG   | 2     | 1987 | -        | X                |
| 86  | MG   | 2     | 1988 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 2     | 1989 | -        | X                |
| 86  | MG   | 2     | 1990 | -        | X                |
| 86  | MG   | 2     | 1991 | -        | X                |
| 86  | MG   | 2     | 1992 | -        | X                |
| 86  | MG   | 2     | 1994 | -        | X                |
| 86  | MG   | 2     | 1996 | -        | X                |
| 86  | MG   | 2     | 1998 | -        | X                |
| 86  | MG   | 2     | 1999 | -        | X                |
| 86  | MG   | 2     | 2000 | -        | X                |
| 86  | MG   | 2     | 2003 | -        | X                |
| 86  | MG   | 2     | 2004 | -        | X                |
| 86  | MG   | 2     | 2005 | -        | X                |
| 86  | MG   | 2     | 2006 | -        | X                |
| 86  | MG   | 2     | 2007 | -        | X                |
| 86  | MG   | 2     | 2008 | -        | X                |
| 86  | MG   | 2     | 2009 | -        | X                |
| 86  | MG   | 2     | 2010 | -        | X                |
| 86  | MG   | 2     | 2011 | -        | X                |
| 86  | MG   | 2     | 2012 | -        | X                |
| 86  | MG   | 2     | 2013 | -        | X                |
| 86  | MG   | 2     | 2014 | -        | X                |
| 86  | MG   | 2     | 2015 | -        | X                |
| 86  | MG   | 2     | 2016 | -        | X                |
| 86  | MG   | 2     | 2017 | -        | X                |
| 86  | MG   | 2     | 2020 | -        | X                |
| 86  | MG   | 3     | 201  | -        | X                |
| 86  | MG   | 3     | 202  | -        | X                |
| 86  | MG   | 3     | 203  | -        | X                |
| 86  | MG   | 3     | 204  | -        | X                |
| 86  | MG   | 3     | 205  | -        | X                |
| 86  | MG   | 3     | 206  | -        | X                |
| 86  | MG   | 3     | 207  | -        | X                |
| 86  | MG   | 3     | 209  | -        | X                |
| 86  | MG   | 3     | 210  | -        | X                |
| 86  | MG   | 3     | 212  | -        | X                |
| 86  | MG   | 3     | 213  | -        | X                |
| 86  | MG   | 3     | 214  | -        | X                |
| 86  | MG   | 4     | 202  | -        | X                |
| 86  | MG   | 4     | 203  | -        | X                |
| 86  | MG   | 4     | 204  | -        | X                |
| 86  | MG   | 4     | 205  | -        | X                |
| 86  | MG   | 4     | 206  | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 4     | 207  | -        | X                |
| 86  | MG   | 4     | 208  | -        | X                |
| 86  | MG   | 4     | 210  | -        | X                |
| 86  | MG   | 4     | 211  | -        | X                |
| 86  | MG   | 4     | 213  | -        | X                |
| 86  | MG   | 4     | 214  | -        | X                |
| 86  | MG   | 4     | 215  | -        | X                |
| 86  | MG   | 4     | 217  | -        | X                |
| 86  | MG   | 4     | 218  | -        | X                |
| 86  | MG   | 4     | 219  | -        | X                |
| 86  | MG   | 5     | 3402 | -        | X                |
| 86  | MG   | 5     | 3403 | -        | X                |
| 86  | MG   | 5     | 3405 | -        | X                |
| 86  | MG   | 5     | 3406 | -        | X                |
| 86  | MG   | 5     | 3409 | -        | X                |
| 86  | MG   | 5     | 3410 | -        | X                |
| 86  | MG   | 5     | 3411 | -        | X                |
| 86  | MG   | 5     | 3414 | -        | X                |
| 86  | MG   | 5     | 3416 | -        | X                |
| 86  | MG   | 5     | 3417 | -        | X                |
| 86  | MG   | 5     | 3418 | -        | X                |
| 86  | MG   | 5     | 3421 | -        | X                |
| 86  | MG   | 5     | 3422 | -        | X                |
| 86  | MG   | 5     | 3423 | -        | X                |
| 86  | MG   | 5     | 3424 | -        | X                |
| 86  | MG   | 5     | 3425 | -        | X                |
| 86  | MG   | 5     | 3426 | -        | X                |
| 86  | MG   | 5     | 3427 | -        | X                |
| 86  | MG   | 5     | 3428 | -        | X                |
| 86  | MG   | 5     | 3430 | -        | X                |
| 86  | MG   | 5     | 3431 | -        | X                |
| 86  | MG   | 5     | 3432 | -        | X                |
| 86  | MG   | 5     | 3433 | -        | X                |
| 86  | MG   | 5     | 3435 | -        | X                |
| 86  | MG   | 5     | 3436 | -        | X                |
| 86  | MG   | 5     | 3437 | -        | X                |
| 86  | MG   | 5     | 3438 | -        | X                |
| 86  | MG   | 5     | 3439 | -        | X                |
| 86  | MG   | 5     | 3440 | -        | X                |
| 86  | MG   | 5     | 3441 | -        | X                |
| 86  | MG   | 5     | 3442 | -        | X                |
| 86  | MG   | 5     | 3443 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 5     | 3444 | -        | X                |
| 86  | MG   | 5     | 3445 | -        | X                |
| 86  | MG   | 5     | 3446 | -        | X                |
| 86  | MG   | 5     | 3447 | -        | X                |
| 86  | MG   | 5     | 3448 | -        | X                |
| 86  | MG   | 5     | 3449 | -        | X                |
| 86  | MG   | 5     | 3450 | -        | X                |
| 86  | MG   | 5     | 3452 | -        | X                |
| 86  | MG   | 5     | 3453 | -        | X                |
| 86  | MG   | 5     | 3456 | -        | X                |
| 86  | MG   | 5     | 3457 | -        | X                |
| 86  | MG   | 5     | 3458 | -        | X                |
| 86  | MG   | 5     | 3459 | -        | X                |
| 86  | MG   | 5     | 3461 | -        | X                |
| 86  | MG   | 5     | 3462 | -        | X                |
| 86  | MG   | 5     | 3463 | -        | X                |
| 86  | MG   | 5     | 3464 | -        | X                |
| 86  | MG   | 5     | 3465 | -        | X                |
| 86  | MG   | 5     | 3466 | -        | X                |
| 86  | MG   | 5     | 3467 | -        | X                |
| 86  | MG   | 5     | 3468 | -        | X                |
| 86  | MG   | 5     | 3470 | -        | X                |
| 86  | MG   | 5     | 3472 | -        | X                |
| 86  | MG   | 5     | 3475 | -        | X                |
| 86  | MG   | 5     | 3476 | -        | X                |
| 86  | MG   | 5     | 3478 | -        | X                |
| 86  | MG   | 5     | 3479 | -        | X                |
| 86  | MG   | 5     | 3480 | -        | X                |
| 86  | MG   | 5     | 3481 | -        | X                |
| 86  | MG   | 5     | 3482 | -        | X                |
| 86  | MG   | 5     | 3483 | -        | X                |
| 86  | MG   | 5     | 3485 | -        | X                |
| 86  | MG   | 5     | 3486 | -        | X                |
| 86  | MG   | 5     | 3487 | -        | X                |
| 86  | MG   | 5     | 3488 | -        | X                |
| 86  | MG   | 5     | 3489 | -        | X                |
| 86  | MG   | 5     | 3490 | -        | X                |
| 86  | MG   | 5     | 3491 | -        | X                |
| 86  | MG   | 5     | 3492 | -        | X                |
| 86  | MG   | 5     | 3493 | -        | X                |
| 86  | MG   | 5     | 3495 | -        | X                |
| 86  | MG   | 5     | 3496 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 5     | 3497 | -        | X                |
| 86  | MG   | 5     | 3498 | -        | X                |
| 86  | MG   | 5     | 3499 | -        | X                |
| 86  | MG   | 5     | 3500 | -        | X                |
| 86  | MG   | 5     | 3501 | -        | X                |
| 86  | MG   | 5     | 3502 | -        | X                |
| 86  | MG   | 5     | 3503 | -        | X                |
| 86  | MG   | 5     | 3504 | -        | X                |
| 86  | MG   | 5     | 3505 | -        | X                |
| 86  | MG   | 5     | 3506 | -        | X                |
| 86  | MG   | 5     | 3507 | -        | X                |
| 86  | MG   | 5     | 3508 | -        | X                |
| 86  | MG   | 5     | 3509 | -        | X                |
| 86  | MG   | 5     | 3510 | -        | X                |
| 86  | MG   | 5     | 3511 | -        | X                |
| 86  | MG   | 5     | 3512 | -        | X                |
| 86  | MG   | 5     | 3513 | -        | X                |
| 86  | MG   | 5     | 3514 | -        | X                |
| 86  | MG   | 5     | 3515 | -        | X                |
| 86  | MG   | 5     | 3516 | -        | X                |
| 86  | MG   | 5     | 3517 | -        | X                |
| 86  | MG   | 5     | 3518 | -        | X                |
| 86  | MG   | 5     | 3519 | -        | X                |
| 86  | MG   | 5     | 3520 | -        | X                |
| 86  | MG   | 5     | 3521 | -        | X                |
| 86  | MG   | 5     | 3522 | -        | X                |
| 86  | MG   | 5     | 3523 | -        | X                |
| 86  | MG   | 5     | 3524 | -        | X                |
| 86  | MG   | 5     | 3525 | -        | X                |
| 86  | MG   | 5     | 3526 | -        | X                |
| 86  | MG   | 5     | 3527 | -        | X                |
| 86  | MG   | 5     | 3529 | -        | X                |
| 86  | MG   | 5     | 3530 | -        | X                |
| 86  | MG   | 5     | 3531 | -        | X                |
| 86  | MG   | 5     | 3532 | -        | X                |
| 86  | MG   | 5     | 3533 | -        | X                |
| 86  | MG   | 5     | 3534 | -        | X                |
| 86  | MG   | 5     | 3535 | -        | X                |
| 86  | MG   | 5     | 3536 | -        | X                |
| 86  | MG   | 5     | 3537 | -        | X                |
| 86  | MG   | 5     | 3538 | -        | X                |
| 86  | MG   | 5     | 3539 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 5     | 3540 | -        | X                |
| 86  | MG   | 5     | 3541 | -        | X                |
| 86  | MG   | 5     | 3542 | -        | X                |
| 86  | MG   | 5     | 3544 | -        | X                |
| 86  | MG   | 5     | 3545 | -        | X                |
| 86  | MG   | 5     | 3546 | -        | X                |
| 86  | MG   | 5     | 3547 | -        | X                |
| 86  | MG   | 5     | 3548 | -        | X                |
| 86  | MG   | 5     | 3549 | -        | X                |
| 86  | MG   | 5     | 3550 | -        | X                |
| 86  | MG   | 5     | 3551 | -        | X                |
| 86  | MG   | 5     | 3552 | -        | X                |
| 86  | MG   | 5     | 3553 | -        | X                |
| 86  | MG   | 5     | 3554 | -        | X                |
| 86  | MG   | 5     | 3555 | -        | X                |
| 86  | MG   | 5     | 3556 | -        | X                |
| 86  | MG   | 5     | 3557 | -        | X                |
| 86  | MG   | 5     | 3558 | -        | X                |
| 86  | MG   | 5     | 3559 | -        | X                |
| 86  | MG   | 5     | 3560 | -        | X                |
| 86  | MG   | 5     | 3561 | -        | X                |
| 86  | MG   | 5     | 3562 | -        | X                |
| 86  | MG   | 5     | 3563 | -        | X                |
| 86  | MG   | 5     | 3564 | -        | X                |
| 86  | MG   | 5     | 3566 | -        | X                |
| 86  | MG   | 5     | 3567 | -        | X                |
| 86  | MG   | 5     | 3568 | -        | X                |
| 86  | MG   | 5     | 3569 | -        | X                |
| 86  | MG   | 5     | 3570 | -        | X                |
| 86  | MG   | 5     | 3571 | -        | X                |
| 86  | MG   | 5     | 3572 | -        | X                |
| 86  | MG   | 5     | 3573 | -        | X                |
| 86  | MG   | 5     | 3574 | -        | X                |
| 86  | MG   | 5     | 3575 | -        | X                |
| 86  | MG   | 5     | 3576 | -        | X                |
| 86  | MG   | 5     | 3577 | -        | X                |
| 86  | MG   | 5     | 3578 | -        | X                |
| 86  | MG   | 5     | 3579 | -        | X                |
| 86  | MG   | 5     | 3580 | -        | X                |
| 86  | MG   | 5     | 3581 | -        | X                |
| 86  | MG   | 5     | 3582 | -        | X                |
| 86  | MG   | 5     | 3583 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 5     | 3584 | -        | X                |
| 86  | MG   | 5     | 3585 | -        | X                |
| 86  | MG   | 5     | 3586 | -        | X                |
| 86  | MG   | 5     | 3587 | -        | X                |
| 86  | MG   | 5     | 3588 | -        | X                |
| 86  | MG   | 5     | 3589 | -        | X                |
| 86  | MG   | 5     | 3590 | -        | X                |
| 86  | MG   | 5     | 3591 | -        | X                |
| 86  | MG   | 5     | 3592 | -        | X                |
| 86  | MG   | 5     | 3593 | -        | X                |
| 86  | MG   | 5     | 3594 | -        | X                |
| 86  | MG   | 5     | 3595 | -        | X                |
| 86  | MG   | 5     | 3596 | -        | X                |
| 86  | MG   | 5     | 3597 | -        | X                |
| 86  | MG   | 5     | 3598 | -        | X                |
| 86  | MG   | 5     | 3603 | -        | X                |
| 86  | MG   | 5     | 3604 | -        | X                |
| 86  | MG   | 5     | 3605 | -        | X                |
| 86  | MG   | 5     | 3607 | -        | X                |
| 86  | MG   | 5     | 3608 | -        | X                |
| 86  | MG   | 5     | 3609 | -        | X                |
| 86  | MG   | 5     | 3610 | -        | X                |
| 86  | MG   | 5     | 3612 | -        | X                |
| 86  | MG   | 5     | 3614 | -        | X                |
| 86  | MG   | 5     | 3616 | -        | X                |
| 86  | MG   | 5     | 3618 | -        | X                |
| 86  | MG   | 5     | 3619 | -        | X                |
| 86  | MG   | 5     | 3621 | -        | X                |
| 86  | MG   | 5     | 3622 | -        | X                |
| 86  | MG   | 5     | 3623 | -        | X                |
| 86  | MG   | 5     | 3624 | -        | X                |
| 86  | MG   | 5     | 3625 | -        | X                |
| 86  | MG   | 5     | 3626 | -        | X                |
| 86  | MG   | 5     | 3627 | -        | X                |
| 86  | MG   | 5     | 3629 | -        | X                |
| 86  | MG   | 5     | 3630 | -        | X                |
| 86  | MG   | 5     | 3631 | -        | X                |
| 86  | MG   | 5     | 3632 | -        | X                |
| 86  | MG   | 5     | 3633 | -        | X                |
| 86  | MG   | 5     | 3634 | -        | X                |
| 86  | MG   | 5     | 3635 | -        | X                |
| 86  | MG   | 5     | 3636 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 5     | 3639 | -        | X                |
| 86  | MG   | 5     | 3640 | -        | X                |
| 86  | MG   | 5     | 3641 | -        | X                |
| 86  | MG   | 5     | 3644 | -        | X                |
| 86  | MG   | 5     | 3645 | -        | X                |
| 86  | MG   | 5     | 3646 | -        | X                |
| 86  | MG   | 5     | 3647 | -        | X                |
| 86  | MG   | 5     | 3648 | -        | X                |
| 86  | MG   | 5     | 3649 | -        | X                |
| 86  | MG   | 5     | 3650 | -        | X                |
| 86  | MG   | 5     | 3653 | -        | X                |
| 86  | MG   | 5     | 3654 | -        | X                |
| 86  | MG   | 5     | 3656 | -        | X                |
| 86  | MG   | 5     | 3657 | -        | X                |
| 86  | MG   | 5     | 3659 | -        | X                |
| 86  | MG   | 5     | 3661 | -        | X                |
| 86  | MG   | 5     | 3663 | -        | X                |
| 86  | MG   | 5     | 3664 | -        | X                |
| 86  | MG   | 5     | 3665 | -        | X                |
| 86  | MG   | 5     | 3667 | -        | X                |
| 86  | MG   | 5     | 3669 | -        | X                |
| 86  | MG   | 5     | 3670 | -        | X                |
| 86  | MG   | 5     | 3671 | -        | X                |
| 86  | MG   | 5     | 3673 | -        | X                |
| 86  | MG   | 5     | 3674 | -        | X                |
| 86  | MG   | 5     | 3675 | -        | X                |
| 86  | MG   | 5     | 3676 | -        | X                |
| 86  | MG   | 5     | 3677 | -        | X                |
| 86  | MG   | 5     | 3681 | -        | X                |
| 86  | MG   | 5     | 3682 | -        | X                |
| 86  | MG   | 5     | 3683 | -        | X                |
| 86  | MG   | 5     | 3685 | -        | X                |
| 86  | MG   | 5     | 3688 | -        | X                |
| 86  | MG   | 5     | 3689 | -        | X                |
| 86  | MG   | 5     | 3690 | -        | X                |
| 86  | MG   | 5     | 3691 | -        | X                |
| 86  | MG   | 5     | 3692 | -        | X                |
| 86  | MG   | 5     | 3694 | -        | X                |
| 86  | MG   | 5     | 3696 | -        | X                |
| 86  | MG   | 5     | 3698 | -        | X                |
| 86  | MG   | 5     | 3699 | -        | X                |
| 86  | MG   | 5     | 3702 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 5     | 3704 | -        | X                |
| 86  | MG   | 5     | 3705 | -        | X                |
| 86  | MG   | 5     | 3707 | -        | X                |
| 86  | MG   | 5     | 3709 | -        | X                |
| 86  | MG   | 5     | 3710 | -        | X                |
| 86  | MG   | 5     | 3712 | -        | X                |
| 86  | MG   | 5     | 3714 | -        | X                |
| 86  | MG   | 5     | 3715 | -        | X                |
| 86  | MG   | 5     | 3716 | -        | X                |
| 86  | MG   | 5     | 3717 | -        | X                |
| 86  | MG   | 5     | 3718 | -        | X                |
| 86  | MG   | 5     | 3719 | -        | X                |
| 86  | MG   | 5     | 3720 | -        | X                |
| 86  | MG   | 5     | 3722 | -        | X                |
| 86  | MG   | 5     | 3727 | -        | X                |
| 86  | MG   | 5     | 3728 | -        | X                |
| 86  | MG   | 5     | 3729 | -        | X                |
| 86  | MG   | 5     | 3735 | -        | X                |
| 86  | MG   | 5     | 3736 | -        | X                |
| 86  | MG   | 5     | 3738 | -        | X                |
| 86  | MG   | 5     | 3739 | -        | X                |
| 86  | MG   | 5     | 3740 | -        | X                |
| 86  | MG   | 5     | 3742 | -        | X                |
| 86  | MG   | 5     | 3743 | -        | X                |
| 86  | MG   | 5     | 3744 | -        | X                |
| 86  | MG   | 5     | 3745 | -        | X                |
| 86  | MG   | 5     | 3746 | -        | X                |
| 86  | MG   | 5     | 3747 | -        | X                |
| 86  | MG   | 5     | 3748 | -        | X                |
| 86  | MG   | 5     | 3749 | -        | X                |
| 86  | MG   | 5     | 3752 | -        | X                |
| 86  | MG   | 5     | 3753 | -        | X                |
| 86  | MG   | 5     | 3756 | -        | X                |
| 86  | MG   | 5     | 3759 | -        | X                |
| 86  | MG   | 5     | 3762 | -        | X                |
| 86  | MG   | 5     | 3763 | -        | X                |
| 86  | MG   | 5     | 3765 | -        | X                |
| 86  | MG   | 5     | 3767 | -        | X                |
| 86  | MG   | 5     | 3768 | -        | X                |
| 86  | MG   | 5     | 3771 | -        | X                |
| 86  | MG   | 5     | 3773 | -        | X                |
| 86  | MG   | 5     | 3775 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 5     | 3776 | -        | X                |
| 86  | MG   | 5     | 3777 | -        | X                |
| 86  | MG   | 5     | 3780 | -        | X                |
| 86  | MG   | 5     | 3781 | -        | X                |
| 86  | MG   | 5     | 3784 | -        | X                |
| 86  | MG   | 5     | 3785 | -        | X                |
| 86  | MG   | 5     | 3786 | -        | X                |
| 86  | MG   | 5     | 3788 | -        | X                |
| 86  | MG   | 5     | 3789 | -        | X                |
| 86  | MG   | 5     | 3790 | -        | X                |
| 86  | MG   | 5     | 3791 | -        | X                |
| 86  | MG   | 5     | 3792 | -        | X                |
| 86  | MG   | 5     | 3793 | -        | X                |
| 86  | MG   | 5     | 3794 | -        | X                |
| 86  | MG   | 5     | 3795 | -        | X                |
| 86  | MG   | 5     | 3796 | -        | X                |
| 86  | MG   | 5     | 3797 | -        | X                |
| 86  | MG   | 5     | 3799 | -        | X                |
| 86  | MG   | 5     | 3802 | -        | X                |
| 86  | MG   | 5     | 3804 | -        | X                |
| 86  | MG   | 5     | 3805 | -        | X                |
| 86  | MG   | 5     | 3808 | -        | X                |
| 86  | MG   | 5     | 3809 | -        | X                |
| 86  | MG   | 5     | 3810 | -        | X                |
| 86  | MG   | 5     | 3813 | -        | X                |
| 86  | MG   | 5     | 3814 | -        | X                |
| 86  | MG   | 5     | 3815 | -        | X                |
| 86  | MG   | 5     | 3816 | -        | X                |
| 86  | MG   | 5     | 3820 | -        | X                |
| 86  | MG   | 5     | 3822 | -        | X                |
| 86  | MG   | 5     | 3825 | -        | X                |
| 86  | MG   | 5     | 3827 | -        | X                |
| 86  | MG   | 5     | 3828 | -        | X                |
| 86  | MG   | 5     | 3829 | -        | X                |
| 86  | MG   | 5     | 3830 | -        | X                |
| 86  | MG   | 5     | 3834 | -        | X                |
| 86  | MG   | 5     | 3835 | -        | X                |
| 86  | MG   | 5     | 3836 | -        | X                |
| 86  | MG   | 5     | 3838 | -        | X                |
| 86  | MG   | 5     | 3839 | -        | X                |
| 86  | MG   | 5     | 3840 | -        | X                |
| 86  | MG   | 5     | 3842 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 5     | 3843 | -        | X                |
| 86  | MG   | 5     | 3844 | -        | X                |
| 86  | MG   | 5     | 3845 | -        | X                |
| 86  | MG   | 5     | 3846 | -        | X                |
| 86  | MG   | 5     | 3847 | -        | X                |
| 86  | MG   | 5     | 3848 | -        | X                |
| 86  | MG   | 5     | 3850 | -        | X                |
| 86  | MG   | 5     | 3852 | -        | X                |
| 86  | MG   | 5     | 3853 | -        | X                |
| 86  | MG   | 5     | 3854 | -        | X                |
| 86  | MG   | 5     | 3856 | -        | X                |
| 86  | MG   | 5     | 3857 | -        | X                |
| 86  | MG   | 5     | 3858 | -        | X                |
| 86  | MG   | 5     | 3859 | -        | X                |
| 86  | MG   | 5     | 3861 | -        | X                |
| 86  | MG   | 5     | 3863 | -        | X                |
| 86  | MG   | 5     | 3864 | -        | X                |
| 86  | MG   | 5     | 3865 | -        | X                |
| 86  | MG   | 5     | 3866 | -        | X                |
| 86  | MG   | 5     | 3867 | -        | X                |
| 86  | MG   | 5     | 3868 | -        | X                |
| 86  | MG   | 5     | 3869 | -        | X                |
| 86  | MG   | 5     | 3870 | -        | X                |
| 86  | MG   | 5     | 3871 | -        | X                |
| 86  | MG   | 5     | 3872 | -        | X                |
| 86  | MG   | 5     | 3874 | -        | X                |
| 86  | MG   | 5     | 3877 | -        | X                |
| 86  | MG   | 5     | 3878 | -        | X                |
| 86  | MG   | 5     | 3879 | -        | X                |
| 86  | MG   | 5     | 3880 | -        | X                |
| 86  | MG   | 5     | 3881 | -        | X                |
| 86  | MG   | 5     | 3882 | -        | X                |
| 86  | MG   | 5     | 3883 | -        | X                |
| 86  | MG   | 5     | 3884 | -        | X                |
| 86  | MG   | 5     | 3885 | -        | X                |
| 86  | MG   | 5     | 3886 | -        | X                |
| 86  | MG   | 5     | 3887 | -        | X                |
| 86  | MG   | 5     | 3888 | -        | X                |
| 86  | MG   | 5     | 3889 | -        | X                |
| 86  | MG   | 5     | 3890 | -        | X                |
| 86  | MG   | 5     | 3891 | -        | X                |
| 86  | MG   | 5     | 3893 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 5     | 3894 | -        | X                |
| 86  | MG   | 5     | 3895 | -        | X                |
| 86  | MG   | 5     | 3896 | -        | X                |
| 86  | MG   | 5     | 3898 | -        | X                |
| 86  | MG   | 5     | 3899 | -        | X                |
| 86  | MG   | 5     | 4255 | -        | X                |
| 86  | MG   | 5     | 4256 | -        | X                |
| 86  | MG   | 5     | 4257 | -        | X                |
| 86  | MG   | 5     | 4258 | -        | X                |
| 86  | MG   | 5     | 4259 | -        | X                |
| 86  | MG   | 5     | 4261 | -        | X                |
| 86  | MG   | 6     | 1901 | -        | X                |
| 86  | MG   | 6     | 1902 | -        | X                |
| 86  | MG   | 6     | 1903 | -        | X                |
| 86  | MG   | 6     | 1904 | -        | X                |
| 86  | MG   | 6     | 1905 | -        | X                |
| 86  | MG   | 6     | 1906 | -        | X                |
| 86  | MG   | 6     | 1907 | -        | X                |
| 86  | MG   | 6     | 1908 | -        | X                |
| 86  | MG   | 6     | 1909 | -        | X                |
| 86  | MG   | 6     | 1910 | -        | X                |
| 86  | MG   | 6     | 1911 | -        | X                |
| 86  | MG   | 6     | 1912 | -        | X                |
| 86  | MG   | 6     | 1913 | -        | X                |
| 86  | MG   | 6     | 1914 | -        | X                |
| 86  | MG   | 6     | 1917 | -        | X                |
| 86  | MG   | 6     | 1918 | -        | X                |
| 86  | MG   | 6     | 1919 | -        | X                |
| 86  | MG   | 6     | 1920 | -        | X                |
| 86  | MG   | 6     | 1921 | -        | X                |
| 86  | MG   | 6     | 1922 | -        | X                |
| 86  | MG   | 6     | 1923 | -        | X                |
| 86  | MG   | 6     | 1925 | -        | X                |
| 86  | MG   | 6     | 1926 | -        | X                |
| 86  | MG   | 6     | 1927 | -        | X                |
| 86  | MG   | 6     | 1928 | -        | X                |
| 86  | MG   | 6     | 1929 | -        | X                |
| 86  | MG   | 6     | 1930 | -        | X                |
| 86  | MG   | 6     | 1931 | -        | X                |
| 86  | MG   | 6     | 1932 | -        | X                |
| 86  | MG   | 6     | 1933 | -        | X                |
| 86  | MG   | 6     | 1934 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 6     | 1935 | -        | X                |
| 86  | MG   | 6     | 1936 | -        | X                |
| 86  | MG   | 6     | 1937 | -        | X                |
| 86  | MG   | 6     | 1938 | -        | X                |
| 86  | MG   | 6     | 1939 | -        | X                |
| 86  | MG   | 6     | 1940 | -        | X                |
| 86  | MG   | 6     | 1941 | -        | X                |
| 86  | MG   | 6     | 1942 | -        | X                |
| 86  | MG   | 6     | 1943 | -        | X                |
| 86  | MG   | 6     | 1944 | -        | X                |
| 86  | MG   | 6     | 1945 | -        | X                |
| 86  | MG   | 6     | 1946 | -        | X                |
| 86  | MG   | 6     | 1947 | -        | X                |
| 86  | MG   | 6     | 1948 | -        | X                |
| 86  | MG   | 6     | 1949 | -        | X                |
| 86  | MG   | 6     | 1950 | -        | X                |
| 86  | MG   | 6     | 1951 | -        | X                |
| 86  | MG   | 6     | 1952 | -        | X                |
| 86  | MG   | 6     | 1953 | -        | X                |
| 86  | MG   | 6     | 1954 | -        | X                |
| 86  | MG   | 6     | 1955 | -        | X                |
| 86  | MG   | 6     | 1956 | -        | X                |
| 86  | MG   | 6     | 1957 | -        | X                |
| 86  | MG   | 6     | 1958 | -        | X                |
| 86  | MG   | 6     | 1959 | -        | X                |
| 86  | MG   | 6     | 1960 | -        | X                |
| 86  | MG   | 6     | 1961 | -        | X                |
| 86  | MG   | 6     | 1962 | -        | X                |
| 86  | MG   | 6     | 1963 | -        | X                |
| 86  | MG   | 6     | 1964 | -        | X                |
| 86  | MG   | 6     | 1965 | -        | X                |
| 86  | MG   | 6     | 1966 | -        | X                |
| 86  | MG   | 6     | 1967 | -        | X                |
| 86  | MG   | 6     | 1969 | -        | X                |
| 86  | MG   | 6     | 1970 | -        | X                |
| 86  | MG   | 6     | 1972 | -        | X                |
| 86  | MG   | 6     | 1973 | -        | X                |
| 86  | MG   | 6     | 1974 | -        | X                |
| 86  | MG   | 6     | 1976 | -        | X                |
| 86  | MG   | 6     | 1977 | -        | X                |
| 86  | MG   | 6     | 1979 | -        | X                |
| 86  | MG   | 6     | 1980 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 6     | 1981 | -        | X                |
| 86  | MG   | 6     | 1982 | -        | X                |
| 86  | MG   | 6     | 1984 | -        | X                |
| 86  | MG   | 6     | 1985 | -        | X                |
| 86  | MG   | 6     | 1986 | -        | X                |
| 86  | MG   | 6     | 1987 | -        | X                |
| 86  | MG   | 6     | 1988 | -        | X                |
| 86  | MG   | 6     | 1990 | -        | X                |
| 86  | MG   | 6     | 1992 | -        | X                |
| 86  | MG   | 6     | 1995 | -        | X                |
| 86  | MG   | 6     | 1996 | -        | X                |
| 86  | MG   | 6     | 1999 | -        | X                |
| 86  | MG   | 6     | 2003 | -        | X                |
| 86  | MG   | 6     | 2005 | -        | X                |
| 86  | MG   | 6     | 2006 | -        | X                |
| 86  | MG   | 6     | 2007 | -        | X                |
| 86  | MG   | 6     | 2008 | -        | X                |
| 86  | MG   | 6     | 2010 | -        | X                |
| 86  | MG   | 6     | 2011 | -        | X                |
| 86  | MG   | 6     | 2012 | -        | X                |
| 86  | MG   | 6     | 2013 | -        | X                |
| 86  | MG   | 6     | 2014 | -        | X                |
| 86  | MG   | 6     | 2015 | -        | X                |
| 86  | MG   | 6     | 2019 | -        | X                |
| 86  | MG   | 6     | 2020 | -        | X                |
| 86  | MG   | 6     | 2021 | -        | X                |
| 86  | MG   | 6     | 2023 | -        | X                |
| 86  | MG   | 6     | 2025 | -        | X                |
| 86  | MG   | 6     | 2026 | -        | X                |
| 86  | MG   | 6     | 2028 | -        | X                |
| 86  | MG   | 6     | 2032 | -        | X                |
| 86  | MG   | 6     | 2033 | -        | X                |
| 86  | MG   | 6     | 2034 | -        | X                |
| 86  | MG   | 6     | 2035 | -        | X                |
| 86  | MG   | 6     | 2037 | -        | X                |
| 86  | MG   | 6     | 2039 | -        | X                |
| 86  | MG   | 6     | 2040 | -        | X                |
| 86  | MG   | 6     | 2041 | -        | X                |
| 86  | MG   | 6     | 2043 | -        | X                |
| 86  | MG   | 6     | 2045 | -        | X                |
| 86  | MG   | 6     | 2046 | -        | X                |
| 86  | MG   | 6     | 2048 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | 6     | 2049 | -        | X                |
| 86  | MG   | 7     | 201  | -        | X                |
| 86  | MG   | 7     | 202  | -        | X                |
| 86  | MG   | 7     | 203  | -        | X                |
| 86  | MG   | 7     | 204  | -        | X                |
| 86  | MG   | 7     | 205  | -        | X                |
| 86  | MG   | 7     | 206  | -        | X                |
| 86  | MG   | 7     | 207  | -        | X                |
| 86  | MG   | 7     | 208  | -        | X                |
| 86  | MG   | 7     | 209  | -        | X                |
| 86  | MG   | 7     | 210  | -        | X                |
| 86  | MG   | 7     | 211  | -        | X                |
| 86  | MG   | 7     | 212  | -        | X                |
| 86  | MG   | 7     | 213  | -        | X                |
| 86  | MG   | 7     | 214  | -        | X                |
| 86  | MG   | 7     | 215  | -        | X                |
| 86  | MG   | 7     | 216  | -        | X                |
| 86  | MG   | 8     | 201  | -        | X                |
| 86  | MG   | 8     | 202  | -        | X                |
| 86  | MG   | 8     | 203  | -        | X                |
| 86  | MG   | 8     | 204  | -        | X                |
| 86  | MG   | 8     | 205  | -        | X                |
| 86  | MG   | 8     | 206  | -        | X                |
| 86  | MG   | 8     | 207  | -        | X                |
| 86  | MG   | 8     | 210  | -        | X                |
| 86  | MG   | 8     | 211  | -        | X                |
| 86  | MG   | 8     | 212  | -        | X                |
| 86  | MG   | 8     | 213  | -        | X                |
| 86  | MG   | 8     | 214  | -        | X                |
| 86  | MG   | D0    | 201  | -        | X                |
| 86  | MG   | L3    | 401  | -        | X                |
| 86  | MG   | L3    | 402  | -        | X                |
| 86  | MG   | L4    | 401  | -        | X                |
| 86  | MG   | L4    | 402  | -        | X                |
| 86  | MG   | L7    | 302  | -        | X                |
| 86  | MG   | M0    | 301  | -        | X                |
| 86  | MG   | M3    | 202  | -        | X                |
| 86  | MG   | M3    | 203  | -        | X                |
| 86  | MG   | M5    | 301  | -        | X                |
| 86  | MG   | M7    | 202  | -        | X                |
| 86  | MG   | M7    | 204  | -        | X                |
| 86  | MG   | M7    | 206  | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 86  | MG   | N0    | 201  | -        | X                |
| 86  | MG   | N3    | 201  | -        | X                |
| 86  | MG   | N8    | 201  | -        | X                |
| 86  | MG   | O4    | 201  | -        | X                |
| 86  | MG   | O7    | 102  | -        | X                |
| 86  | MG   | S2    | 301  | -        | X                |
| 86  | MG   | S8    | 301  | -        | X                |
| 86  | MG   | SM    | 301  | -        | X                |
| 86  | MG   | c1    | 201  | -        | X                |
| 86  | MG   | d3    | 201  | -        | X                |
| 86  | MG   | l2    | 301  | -        | X                |
| 86  | MG   | l2    | 302  | -        | X                |
| 86  | MG   | l3    | 401  | -        | X                |
| 86  | MG   | l3    | 402  | -        | X                |
| 86  | MG   | l7    | 302  | -        | X                |
| 86  | MG   | m5    | 301  | -        | X                |
| 86  | MG   | m5    | 302  | -        | X                |
| 86  | MG   | m6    | 201  | -        | X                |
| 86  | MG   | m7    | 201  | -        | X                |
| 86  | MG   | m7    | 203  | -        | X                |
| 86  | MG   | m7    | 204  | -        | X                |
| 86  | MG   | m7    | 205  | -        | X                |
| 86  | MG   | n0    | 201  | -        | X                |
| 86  | MG   | n3    | 201  | -        | X                |
| 86  | MG   | n6    | 201  | -        | X                |
| 86  | MG   | n8    | 201  | -        | X                |
| 86  | MG   | n8    | 202  | -        | X                |
| 86  | MG   | n8    | 204  | -        | X                |
| 86  | MG   | n8    | 205  | -        | X                |
| 86  | MG   | o1    | 202  | -        | X                |
| 86  | MG   | o3    | 201  | -        | X                |
| 86  | MG   | o3    | 202  | -        | X                |
| 86  | MG   | o4    | 201  | -        | X                |
| 86  | MG   | s8    | 301  | -        | X                |
| 86  | MG   | s8    | 302  | -        | X                |
| 87  | OHX  | 1     | 3900 | -        | X                |
| 87  | OHX  | 1     | 3959 | -        | X                |
| 87  | OHX  | 1     | 3960 | -        | X                |
| 87  | OHX  | 1     | 3961 | -        | X                |
| 87  | OHX  | 1     | 3978 | -        | X                |
| 87  | OHX  | 1     | 3979 | -        | X                |
| 87  | OHX  | 1     | 3984 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 87  | OHX  | 1     | 3991 | -        | X                |
| 87  | OHX  | 1     | 3996 | -        | X                |
| 87  | OHX  | 1     | 3997 | -        | X                |
| 87  | OHX  | 1     | 4004 | -        | X                |
| 87  | OHX  | 1     | 4006 | -        | X                |
| 87  | OHX  | 1     | 4007 | -        | X                |
| 87  | OHX  | 1     | 4009 | -        | X                |
| 87  | OHX  | 1     | 4011 | -        | X                |
| 87  | OHX  | 1     | 4013 | -        | X                |
| 87  | OHX  | 1     | 4014 | -        | X                |
| 87  | OHX  | 1     | 4019 | -        | X                |
| 87  | OHX  | 1     | 4020 | -        | X                |
| 87  | OHX  | 1     | 4021 | -        | X                |
| 87  | OHX  | 1     | 4023 | -        | X                |
| 87  | OHX  | 1     | 4026 | -        | X                |
| 87  | OHX  | 1     | 4033 | -        | X                |
| 87  | OHX  | 1     | 4038 | -        | X                |
| 87  | OHX  | 1     | 4040 | -        | X                |
| 87  | OHX  | 1     | 4042 | -        | X                |
| 87  | OHX  | 1     | 4043 | -        | X                |
| 87  | OHX  | 1     | 4044 | -        | X                |
| 87  | OHX  | 1     | 4046 | -        | X                |
| 87  | OHX  | 1     | 4047 | -        | X                |
| 87  | OHX  | 1     | 4049 | -        | X                |
| 87  | OHX  | 1     | 4050 | -        | X                |
| 87  | OHX  | 1     | 4051 | -        | X                |
| 87  | OHX  | 1     | 4052 | -        | X                |
| 87  | OHX  | 1     | 4054 | -        | X                |
| 87  | OHX  | 1     | 4059 | -        | X                |
| 87  | OHX  | 1     | 4061 | -        | X                |
| 87  | OHX  | 1     | 4062 | -        | X                |
| 87  | OHX  | 1     | 4066 | -        | X                |
| 87  | OHX  | 1     | 4067 | -        | X                |
| 87  | OHX  | 1     | 4068 | -        | X                |
| 87  | OHX  | 1     | 4069 | -        | X                |
| 87  | OHX  | 1     | 4071 | -        | X                |
| 87  | OHX  | 1     | 4072 | -        | X                |
| 87  | OHX  | 1     | 4073 | -        | X                |
| 87  | OHX  | 1     | 4074 | -        | X                |
| 87  | OHX  | 1     | 4075 | -        | X                |
| 87  | OHX  | 1     | 4077 | -        | X                |
| 87  | OHX  | 1     | 4079 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 87  | OHX  | 1     | 4080 | -        | X                |
| 87  | OHX  | 1     | 4081 | -        | X                |
| 87  | OHX  | 1     | 4082 | -        | X                |
| 87  | OHX  | 1     | 4084 | -        | X                |
| 87  | OHX  | 1     | 4085 | -        | X                |
| 87  | OHX  | 1     | 4086 | -        | X                |
| 87  | OHX  | 1     | 4087 | -        | X                |
| 87  | OHX  | 1     | 4091 | -        | X                |
| 87  | OHX  | 1     | 4092 | -        | X                |
| 87  | OHX  | 1     | 4096 | -        | X                |
| 87  | OHX  | 1     | 4099 | -        | X                |
| 87  | OHX  | 1     | 4100 | -        | X                |
| 87  | OHX  | 1     | 4101 | -        | X                |
| 87  | OHX  | 1     | 4102 | -        | X                |
| 87  | OHX  | 1     | 4103 | -        | X                |
| 87  | OHX  | 1     | 4104 | -        | X                |
| 87  | OHX  | 1     | 4109 | -        | X                |
| 87  | OHX  | 1     | 4112 | -        | X                |
| 87  | OHX  | 1     | 4113 | -        | X                |
| 87  | OHX  | 1     | 4114 | -        | X                |
| 87  | OHX  | 1     | 4115 | -        | X                |
| 87  | OHX  | 1     | 4116 | -        | X                |
| 87  | OHX  | 1     | 4117 | -        | X                |
| 87  | OHX  | 1     | 4118 | -        | X                |
| 87  | OHX  | 1     | 4119 | -        | X                |
| 87  | OHX  | 1     | 4120 | -        | X                |
| 87  | OHX  | 1     | 4121 | -        | X                |
| 87  | OHX  | 1     | 4123 | -        | X                |
| 87  | OHX  | 1     | 4124 | -        | X                |
| 87  | OHX  | 1     | 4125 | -        | X                |
| 87  | OHX  | 1     | 4126 | -        | X                |
| 87  | OHX  | 1     | 4127 | -        | X                |
| 87  | OHX  | 1     | 4130 | -        | X                |
| 87  | OHX  | 1     | 4131 | -        | X                |
| 87  | OHX  | 1     | 4132 | -        | X                |
| 87  | OHX  | 1     | 4133 | -        | X                |
| 87  | OHX  | 1     | 4134 | -        | X                |
| 87  | OHX  | 1     | 4135 | -        | X                |
| 87  | OHX  | 1     | 4137 | -        | X                |
| 87  | OHX  | 1     | 4138 | -        | X                |
| 87  | OHX  | 1     | 4139 | -        | X                |
| 87  | OHX  | 1     | 4140 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 87  | OHX  | 1     | 4142 | -        | X                |
| 87  | OHX  | 1     | 4143 | -        | X                |
| 87  | OHX  | 1     | 4144 | -        | X                |
| 87  | OHX  | 1     | 4145 | -        | X                |
| 87  | OHX  | 1     | 4146 | -        | X                |
| 87  | OHX  | 1     | 4147 | -        | X                |
| 87  | OHX  | 1     | 4148 | -        | X                |
| 87  | OHX  | 1     | 4150 | -        | X                |
| 87  | OHX  | 1     | 4151 | -        | X                |
| 87  | OHX  | 1     | 4152 | -        | X                |
| 87  | OHX  | 1     | 4153 | -        | X                |
| 87  | OHX  | 1     | 4154 | -        | X                |
| 87  | OHX  | 1     | 4155 | -        | X                |
| 87  | OHX  | 1     | 4157 | -        | X                |
| 87  | OHX  | 1     | 4158 | -        | X                |
| 87  | OHX  | 1     | 4159 | -        | X                |
| 87  | OHX  | 1     | 4161 | -        | X                |
| 87  | OHX  | 1     | 4162 | -        | X                |
| 87  | OHX  | 1     | 4163 | -        | X                |
| 87  | OHX  | 1     | 4164 | -        | X                |
| 87  | OHX  | 1     | 4165 | -        | X                |
| 87  | OHX  | 1     | 4167 | -        | X                |
| 87  | OHX  | 1     | 4168 | -        | X                |
| 87  | OHX  | 1     | 4169 | -        | X                |
| 87  | OHX  | 1     | 4171 | -        | X                |
| 87  | OHX  | 1     | 4172 | -        | X                |
| 87  | OHX  | 1     | 4173 | -        | X                |
| 87  | OHX  | 1     | 4174 | -        | X                |
| 87  | OHX  | 1     | 4175 | -        | X                |
| 87  | OHX  | 1     | 4176 | -        | X                |
| 87  | OHX  | 1     | 4177 | -        | X                |
| 87  | OHX  | 1     | 4178 | -        | X                |
| 87  | OHX  | 1     | 4179 | -        | X                |
| 87  | OHX  | 1     | 4180 | -        | X                |
| 87  | OHX  | 1     | 4181 | -        | X                |
| 87  | OHX  | 1     | 4182 | -        | X                |
| 87  | OHX  | 1     | 4184 | -        | X                |
| 87  | OHX  | 1     | 4185 | -        | X                |
| 87  | OHX  | 1     | 4186 | -        | X                |
| 87  | OHX  | 1     | 4187 | -        | X                |
| 87  | OHX  | 1     | 4188 | -        | X                |
| 87  | OHX  | 1     | 4189 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 87  | OHX  | 1     | 4190 | -        | X                |
| 87  | OHX  | 1     | 4191 | -        | X                |
| 87  | OHX  | 1     | 4192 | -        | X                |
| 87  | OHX  | 1     | 4193 | -        | X                |
| 87  | OHX  | 1     | 4194 | -        | X                |
| 87  | OHX  | 1     | 4195 | -        | X                |
| 87  | OHX  | 1     | 4196 | -        | X                |
| 87  | OHX  | 1     | 4197 | -        | X                |
| 87  | OHX  | 1     | 4199 | -        | X                |
| 87  | OHX  | 1     | 4200 | -        | X                |
| 87  | OHX  | 1     | 4201 | -        | X                |
| 87  | OHX  | 1     | 4202 | -        | X                |
| 87  | OHX  | 1     | 4204 | -        | X                |
| 87  | OHX  | 1     | 4206 | -        | X                |
| 87  | OHX  | 1     | 4207 | -        | X                |
| 87  | OHX  | 1     | 4208 | -        | X                |
| 87  | OHX  | 1     | 4209 | -        | X                |
| 87  | OHX  | 1     | 4210 | -        | X                |
| 87  | OHX  | 1     | 4211 | -        | X                |
| 87  | OHX  | 1     | 4212 | -        | X                |
| 87  | OHX  | 1     | 4213 | -        | X                |
| 87  | OHX  | 1     | 4214 | -        | X                |
| 87  | OHX  | 1     | 4216 | -        | X                |
| 87  | OHX  | 1     | 4217 | -        | X                |
| 87  | OHX  | 2     | 2056 | -        | X                |
| 87  | OHX  | 2     | 2060 | -        | X                |
| 87  | OHX  | 2     | 2072 | -        | X                |
| 87  | OHX  | 2     | 2073 | -        | X                |
| 87  | OHX  | 2     | 2077 | -        | X                |
| 87  | OHX  | 2     | 2082 | -        | X                |
| 87  | OHX  | 2     | 2084 | -        | X                |
| 87  | OHX  | 2     | 2089 | -        | X                |
| 87  | OHX  | 2     | 2090 | -        | X                |
| 87  | OHX  | 2     | 2099 | -        | X                |
| 87  | OHX  | 2     | 2100 | -        | X                |
| 87  | OHX  | 2     | 2101 | -        | X                |
| 87  | OHX  | 2     | 2103 | -        | X                |
| 87  | OHX  | 2     | 2106 | -        | X                |
| 87  | OHX  | 2     | 2107 | -        | X                |
| 87  | OHX  | 2     | 2111 | -        | X                |
| 87  | OHX  | 2     | 2114 | -        | X                |
| 87  | OHX  | 2     | 2117 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 87  | OHX  | 2     | 2118 | -        | X                |
| 87  | OHX  | 2     | 2121 | -        | X                |
| 87  | OHX  | 2     | 2123 | -        | X                |
| 87  | OHX  | 2     | 2124 | -        | X                |
| 87  | OHX  | 2     | 2126 | -        | X                |
| 87  | OHX  | 2     | 2129 | -        | X                |
| 87  | OHX  | 2     | 2131 | -        | X                |
| 87  | OHX  | 2     | 2132 | -        | X                |
| 87  | OHX  | 2     | 2133 | -        | X                |
| 87  | OHX  | 2     | 2134 | -        | X                |
| 87  | OHX  | 2     | 2135 | -        | X                |
| 87  | OHX  | 2     | 2138 | -        | X                |
| 87  | OHX  | 2     | 2141 | -        | X                |
| 87  | OHX  | 2     | 2143 | -        | X                |
| 87  | OHX  | 2     | 2145 | -        | X                |
| 87  | OHX  | 2     | 2146 | -        | X                |
| 87  | OHX  | 2     | 2147 | -        | X                |
| 87  | OHX  | 2     | 2150 | -        | X                |
| 87  | OHX  | 2     | 2151 | -        | X                |
| 87  | OHX  | 2     | 2152 | -        | X                |
| 87  | OHX  | 2     | 2155 | -        | X                |
| 87  | OHX  | 2     | 2157 | -        | X                |
| 87  | OHX  | 2     | 2158 | -        | X                |
| 87  | OHX  | 2     | 2160 | -        | X                |
| 87  | OHX  | 2     | 2161 | -        | X                |
| 87  | OHX  | 2     | 2162 | -        | X                |
| 87  | OHX  | 2     | 2164 | -        | X                |
| 87  | OHX  | 2     | 2166 | -        | X                |
| 87  | OHX  | 2     | 2167 | -        | X                |
| 87  | OHX  | 2     | 2169 | -        | X                |
| 87  | OHX  | 2     | 2170 | -        | X                |
| 87  | OHX  | 2     | 2171 | -        | X                |
| 87  | OHX  | 2     | 2172 | -        | X                |
| 87  | OHX  | 2     | 2173 | -        | X                |
| 87  | OHX  | 2     | 2174 | -        | X                |
| 87  | OHX  | 2     | 2176 | -        | X                |
| 87  | OHX  | 2     | 2177 | -        | X                |
| 87  | OHX  | 3     | 222  | -        | X                |
| 87  | OHX  | 3     | 223  | -        | X                |
| 87  | OHX  | 3     | 224  | -        | X                |
| 87  | OHX  | 3     | 225  | -        | X                |
| 87  | OHX  | 3     | 226  | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 87  | OHX  | 4     | 225  | -        | X                |
| 87  | OHX  | 4     | 226  | -        | X                |
| 87  | OHX  | 4     | 229  | -        | X                |
| 87  | OHX  | 4     | 230  | -        | X                |
| 87  | OHX  | 4     | 231  | -        | X                |
| 87  | OHX  | 4     | 232  | -        | X                |
| 87  | OHX  | 4     | 233  | -        | X                |
| 87  | OHX  | 5     | 3931 | -        | X                |
| 87  | OHX  | 5     | 3985 | -        | X                |
| 87  | OHX  | 5     | 3994 | -        | X                |
| 87  | OHX  | 5     | 3997 | -        | X                |
| 87  | OHX  | 5     | 4005 | -        | X                |
| 87  | OHX  | 5     | 4027 | -        | X                |
| 87  | OHX  | 5     | 4028 | -        | X                |
| 87  | OHX  | 5     | 4033 | -        | X                |
| 87  | OHX  | 5     | 4034 | -        | X                |
| 87  | OHX  | 5     | 4040 | -        | X                |
| 87  | OHX  | 5     | 4043 | -        | X                |
| 87  | OHX  | 5     | 4045 | -        | X                |
| 87  | OHX  | 5     | 4046 | -        | X                |
| 87  | OHX  | 5     | 4047 | -        | X                |
| 87  | OHX  | 5     | 4048 | -        | X                |
| 87  | OHX  | 5     | 4052 | -        | X                |
| 87  | OHX  | 5     | 4053 | -        | X                |
| 87  | OHX  | 5     | 4055 | -        | X                |
| 87  | OHX  | 5     | 4060 | -        | X                |
| 87  | OHX  | 5     | 4062 | -        | X                |
| 87  | OHX  | 5     | 4063 | -        | X                |
| 87  | OHX  | 5     | 4066 | -        | X                |
| 87  | OHX  | 5     | 4069 | -        | X                |
| 87  | OHX  | 5     | 4070 | -        | X                |
| 87  | OHX  | 5     | 4071 | -        | X                |
| 87  | OHX  | 5     | 4072 | -        | X                |
| 87  | OHX  | 5     | 4073 | -        | X                |
| 87  | OHX  | 5     | 4074 | -        | X                |
| 87  | OHX  | 5     | 4076 | -        | X                |
| 87  | OHX  | 5     | 4077 | -        | X                |
| 87  | OHX  | 5     | 4080 | -        | X                |
| 87  | OHX  | 5     | 4083 | -        | X                |
| 87  | OHX  | 5     | 4086 | -        | X                |
| 87  | OHX  | 5     | 4087 | -        | X                |
| 87  | OHX  | 5     | 4088 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 87  | OHX  | 5     | 4089 | -        | X                |
| 87  | OHX  | 5     | 4090 | -        | X                |
| 87  | OHX  | 5     | 4092 | -        | X                |
| 87  | OHX  | 5     | 4093 | -        | X                |
| 87  | OHX  | 5     | 4094 | -        | X                |
| 87  | OHX  | 5     | 4096 | -        | X                |
| 87  | OHX  | 5     | 4098 | -        | X                |
| 87  | OHX  | 5     | 4099 | -        | X                |
| 87  | OHX  | 5     | 4101 | -        | X                |
| 87  | OHX  | 5     | 4102 | -        | X                |
| 87  | OHX  | 5     | 4104 | -        | X                |
| 87  | OHX  | 5     | 4107 | -        | X                |
| 87  | OHX  | 5     | 4108 | -        | X                |
| 87  | OHX  | 5     | 4110 | -        | X                |
| 87  | OHX  | 5     | 4112 | -        | X                |
| 87  | OHX  | 5     | 4113 | -        | X                |
| 87  | OHX  | 5     | 4114 | -        | X                |
| 87  | OHX  | 5     | 4115 | -        | X                |
| 87  | OHX  | 5     | 4117 | -        | X                |
| 87  | OHX  | 5     | 4118 | -        | X                |
| 87  | OHX  | 5     | 4120 | -        | X                |
| 87  | OHX  | 5     | 4121 | -        | X                |
| 87  | OHX  | 5     | 4124 | -        | X                |
| 87  | OHX  | 5     | 4125 | -        | X                |
| 87  | OHX  | 5     | 4127 | -        | X                |
| 87  | OHX  | 5     | 4128 | -        | X                |
| 87  | OHX  | 5     | 4129 | -        | X                |
| 87  | OHX  | 5     | 4130 | -        | X                |
| 87  | OHX  | 5     | 4132 | -        | X                |
| 87  | OHX  | 5     | 4134 | -        | X                |
| 87  | OHX  | 5     | 4135 | -        | X                |
| 87  | OHX  | 5     | 4136 | -        | X                |
| 87  | OHX  | 5     | 4137 | -        | X                |
| 87  | OHX  | 5     | 4138 | -        | X                |
| 87  | OHX  | 5     | 4139 | -        | X                |
| 87  | OHX  | 5     | 4140 | -        | X                |
| 87  | OHX  | 5     | 4141 | -        | X                |
| 87  | OHX  | 5     | 4142 | -        | X                |
| 87  | OHX  | 5     | 4143 | -        | X                |
| 87  | OHX  | 5     | 4145 | -        | X                |
| 87  | OHX  | 5     | 4146 | -        | X                |
| 87  | OHX  | 5     | 4147 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 87  | OHX  | 5     | 4148 | -        | X                |
| 87  | OHX  | 5     | 4149 | -        | X                |
| 87  | OHX  | 5     | 4150 | -        | X                |
| 87  | OHX  | 5     | 4151 | -        | X                |
| 87  | OHX  | 5     | 4152 | -        | X                |
| 87  | OHX  | 5     | 4154 | -        | X                |
| 87  | OHX  | 5     | 4155 | -        | X                |
| 87  | OHX  | 5     | 4156 | -        | X                |
| 87  | OHX  | 5     | 4157 | -        | X                |
| 87  | OHX  | 5     | 4158 | -        | X                |
| 87  | OHX  | 5     | 4159 | -        | X                |
| 87  | OHX  | 5     | 4160 | -        | X                |
| 87  | OHX  | 5     | 4161 | -        | X                |
| 87  | OHX  | 5     | 4162 | -        | X                |
| 87  | OHX  | 5     | 4163 | -        | X                |
| 87  | OHX  | 5     | 4164 | -        | X                |
| 87  | OHX  | 5     | 4165 | -        | X                |
| 87  | OHX  | 5     | 4166 | -        | X                |
| 87  | OHX  | 5     | 4167 | -        | X                |
| 87  | OHX  | 5     | 4168 | -        | X                |
| 87  | OHX  | 5     | 4171 | -        | X                |
| 87  | OHX  | 5     | 4173 | -        | X                |
| 87  | OHX  | 5     | 4174 | -        | X                |
| 87  | OHX  | 5     | 4175 | -        | X                |
| 87  | OHX  | 5     | 4176 | -        | X                |
| 87  | OHX  | 5     | 4177 | -        | X                |
| 87  | OHX  | 5     | 4178 | -        | X                |
| 87  | OHX  | 5     | 4180 | -        | X                |
| 87  | OHX  | 5     | 4181 | -        | X                |
| 87  | OHX  | 5     | 4183 | -        | X                |
| 87  | OHX  | 5     | 4185 | -        | X                |
| 87  | OHX  | 5     | 4186 | -        | X                |
| 87  | OHX  | 5     | 4187 | -        | X                |
| 87  | OHX  | 5     | 4188 | -        | X                |
| 87  | OHX  | 5     | 4189 | -        | X                |
| 87  | OHX  | 5     | 4190 | -        | X                |
| 87  | OHX  | 5     | 4191 | -        | X                |
| 87  | OHX  | 5     | 4192 | -        | X                |
| 87  | OHX  | 5     | 4193 | -        | X                |
| 87  | OHX  | 5     | 4194 | -        | X                |
| 87  | OHX  | 5     | 4195 | -        | X                |
| 87  | OHX  | 5     | 4197 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 87  | OHX  | 5     | 4198 | -        | X                |
| 87  | OHX  | 5     | 4199 | -        | X                |
| 87  | OHX  | 5     | 4201 | -        | X                |
| 87  | OHX  | 5     | 4203 | -        | X                |
| 87  | OHX  | 5     | 4204 | -        | X                |
| 87  | OHX  | 5     | 4205 | -        | X                |
| 87  | OHX  | 5     | 4206 | -        | X                |
| 87  | OHX  | 5     | 4207 | -        | X                |
| 87  | OHX  | 5     | 4208 | -        | X                |
| 87  | OHX  | 5     | 4209 | -        | X                |
| 87  | OHX  | 5     | 4210 | -        | X                |
| 87  | OHX  | 5     | 4211 | -        | X                |
| 87  | OHX  | 5     | 4212 | -        | X                |
| 87  | OHX  | 5     | 4213 | -        | X                |
| 87  | OHX  | 5     | 4214 | -        | X                |
| 87  | OHX  | 5     | 4215 | -        | X                |
| 87  | OHX  | 5     | 4217 | -        | X                |
| 87  | OHX  | 5     | 4219 | -        | X                |
| 87  | OHX  | 5     | 4220 | -        | X                |
| 87  | OHX  | 5     | 4221 | -        | X                |
| 87  | OHX  | 5     | 4222 | -        | X                |
| 87  | OHX  | 5     | 4223 | -        | X                |
| 87  | OHX  | 5     | 4224 | -        | X                |
| 87  | OHX  | 5     | 4225 | -        | X                |
| 87  | OHX  | 5     | 4226 | -        | X                |
| 87  | OHX  | 5     | 4228 | -        | X                |
| 87  | OHX  | 5     | 4229 | -        | X                |
| 87  | OHX  | 5     | 4230 | -        | X                |
| 87  | OHX  | 5     | 4231 | -        | X                |
| 87  | OHX  | 5     | 4232 | -        | X                |
| 87  | OHX  | 5     | 4233 | -        | X                |
| 87  | OHX  | 5     | 4234 | -        | X                |
| 87  | OHX  | 5     | 4235 | -        | X                |
| 87  | OHX  | 5     | 4236 | -        | X                |
| 87  | OHX  | 5     | 4237 | -        | X                |
| 87  | OHX  | 5     | 4238 | -        | X                |
| 87  | OHX  | 5     | 4239 | -        | X                |
| 87  | OHX  | 5     | 4241 | -        | X                |
| 87  | OHX  | 5     | 4242 | -        | X                |
| 87  | OHX  | 5     | 4245 | -        | X                |
| 87  | OHX  | 5     | 4246 | -        | X                |
| 87  | OHX  | 5     | 4247 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 87  | OHX  | 5     | 4248 | -        | X                |
| 87  | OHX  | 5     | 4249 | -        | X                |
| 87  | OHX  | 5     | 4250 | -        | X                |
| 87  | OHX  | 5     | 4251 | -        | X                |
| 87  | OHX  | 5     | 4252 | -        | X                |
| 87  | OHX  | 6     | 2106 | -        | X                |
| 87  | OHX  | 6     | 2111 | -        | X                |
| 87  | OHX  | 6     | 2113 | -        | X                |
| 87  | OHX  | 6     | 2118 | -        | X                |
| 87  | OHX  | 6     | 2120 | -        | X                |
| 87  | OHX  | 6     | 2124 | -        | X                |
| 87  | OHX  | 6     | 2127 | -        | X                |
| 87  | OHX  | 6     | 2128 | -        | X                |
| 87  | OHX  | 6     | 2129 | -        | X                |
| 87  | OHX  | 6     | 2130 | -        | X                |
| 87  | OHX  | 6     | 2131 | -        | X                |
| 87  | OHX  | 6     | 2135 | -        | X                |
| 87  | OHX  | 6     | 2136 | -        | X                |
| 87  | OHX  | 6     | 2139 | -        | X                |
| 87  | OHX  | 6     | 2141 | -        | X                |
| 87  | OHX  | 6     | 2143 | -        | X                |
| 87  | OHX  | 6     | 2144 | -        | X                |
| 87  | OHX  | 6     | 2147 | -        | X                |
| 87  | OHX  | 6     | 2150 | -        | X                |
| 87  | OHX  | 6     | 2151 | -        | X                |
| 87  | OHX  | 6     | 2152 | -        | X                |
| 87  | OHX  | 6     | 2153 | -        | X                |
| 87  | OHX  | 6     | 2154 | -        | X                |
| 87  | OHX  | 6     | 2156 | -        | X                |
| 87  | OHX  | 6     | 2159 | -        | X                |
| 87  | OHX  | 6     | 2160 | -        | X                |
| 87  | OHX  | 6     | 2163 | -        | X                |
| 87  | OHX  | 6     | 2164 | -        | X                |
| 87  | OHX  | 6     | 2166 | -        | X                |
| 87  | OHX  | 6     | 2168 | -        | X                |
| 87  | OHX  | 6     | 2169 | -        | X                |
| 87  | OHX  | 6     | 2171 | -        | X                |
| 87  | OHX  | 6     | 2172 | -        | X                |
| 87  | OHX  | 6     | 2173 | -        | X                |
| 87  | OHX  | 6     | 2174 | -        | X                |
| 87  | OHX  | 6     | 2176 | -        | X                |
| 87  | OHX  | 6     | 2177 | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 87  | OHX  | 6     | 2178 | -        | X                |
| 87  | OHX  | 6     | 2179 | -        | X                |
| 87  | OHX  | 6     | 2180 | -        | X                |
| 87  | OHX  | 6     | 2181 | -        | X                |
| 87  | OHX  | 6     | 2182 | -        | X                |
| 87  | OHX  | 6     | 2183 | -        | X                |
| 87  | OHX  | 6     | 2184 | -        | X                |
| 87  | OHX  | 6     | 2186 | -        | X                |
| 87  | OHX  | 6     | 2187 | -        | X                |
| 87  | OHX  | 6     | 2188 | -        | X                |
| 87  | OHX  | 6     | 2189 | -        | X                |
| 87  | OHX  | 6     | 2190 | -        | X                |
| 87  | OHX  | 6     | 2191 | -        | X                |
| 87  | OHX  | 6     | 2192 | -        | X                |
| 87  | OHX  | 6     | 2193 | -        | X                |
| 87  | OHX  | 6     | 2194 | -        | X                |
| 87  | OHX  | 6     | 2196 | -        | X                |
| 87  | OHX  | 6     | 2197 | -        | X                |
| 87  | OHX  | 6     | 2198 | -        | X                |
| 87  | OHX  | 6     | 2199 | -        | X                |
| 87  | OHX  | 6     | 2200 | -        | X                |
| 87  | OHX  | 6     | 2201 | -        | X                |
| 87  | OHX  | 6     | 2202 | -        | X                |
| 87  | OHX  | 6     | 2203 | -        | X                |
| 87  | OHX  | 6     | 2206 | -        | X                |
| 87  | OHX  | 6     | 2207 | -        | X                |
| 87  | OHX  | 7     | 225  | -        | X                |
| 87  | OHX  | 7     | 226  | -        | X                |
| 87  | OHX  | 7     | 227  | -        | X                |
| 87  | OHX  | 8     | 221  | -        | X                |
| 87  | OHX  | 8     | 223  | -        | X                |
| 87  | OHX  | 8     | 226  | -        | X                |
| 87  | OHX  | 8     | 227  | -        | X                |
| 87  | OHX  | 8     | 228  | -        | X                |
| 87  | OHX  | 8     | 229  | -        | X                |
| 87  | OHX  | 8     | 230  | -        | X                |
| 87  | OHX  | D9    | 102  | -        | X                |
| 87  | OHX  | L3    | 403  | -        | X                |
| 87  | OHX  | M7    | 207  | -        | X                |
| 87  | OHX  | M7    | 208  | -        | X                |
| 87  | OHX  | M9    | 202  | -        | X                |
| 87  | OHX  | O3    | 201  | -        | X                |

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| Mol | Type | Chain | Res  | Geometry | Electron density |
|-----|------|-------|------|----------|------------------|
| 87  | OHX  | O9    | 101  | -        | X                |
| 87  | OHX  | l4    | 403  | -        | X                |
| 87  | OHX  | l5    | 305  | -        | X                |
| 87  | OHX  | m4    | 201  | -        | X                |
| 87  | OHX  | m7    | 206  | -        | X                |
| 87  | OHX  | o7    | 503  | -        | X                |
| 87  | OHX  | s1    | 303  | -        | X                |
| 87  | OHX  | s9    | 201  | -        | X                |
| 88  | ZN   | d7    | 101  | -        | X                |
| 89  | 3KD  | 5     | 4254 | -        | X                |

## 2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 411211 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a RNA chain called *Saccharomyces cerevisiae* chromosome XII cosmid 9634.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | 2     | 1750     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 37283 | 16668 | 6591 | 12274 | 1750 |         |         |       |
| 1   | 6     | 1795     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 38238 | 17095 | 6758 | 12590 | 1795 |         |         |       |

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | S0    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1577  | 1014 | 278 | 283 | 2 |         |         |       |
| 2   | s0    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1583  | 1017 | 281 | 283 | 2 |         |         |       |

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | S1    | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1709  | 1084 | 310 | 311 | 4 |         |         |       |
| 3   | s1    | 216      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1722  | 1091 | 312 | 315 | 4 |         |         |       |

- Molecule 4 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | S2    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1047 | 289 | 297 | 2 |         |         |       |
| 4   | s2    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1047 | 289 | 297 | 2 |         |         |       |

- Molecule 5 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | S3    | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1734  | 1101 | 313 | 314 | 6 |         |         |       |
| 5   | s3    | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1734  | 1101 | 313 | 314 | 6 |         |         |       |

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6   | S4    | 260      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2068  | 1316 | 389 | 360 | 3 |         |         |       |
| 6   | s4    | 260      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2068  | 1316 | 389 | 360 | 3 |         |         |       |

- Molecule 7 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 7   | S5    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1609  | 1007 | 300 | 299 | 3 |         |         |       |
| 7   | s5    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1609  | 1007 | 300 | 299 | 3 |         |         |       |

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 8   | S6    | 226      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1799  | 1129 | 346 | 321 | 3 |         |         |       |
| 8   | s6    | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1755  | 1102 | 337 | 313 | 3 |         |         |       |

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 9   | S7    | 184      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1481  | 951 | 265 | 265 |  |         |         |       |
| 9   | s7    | 186      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1491  | 957 | 267 | 267 |  |         |         |       |

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | S8    | 188      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1489  | 925 | 298 | 264 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | s8    | 188      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1489  | 925 | 298 | 264 | 2 |         |         |       |

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | S9    | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1494  | 943 | 289 | 261 | 1 |         |         |       |
| 11  | s9    | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1494  | 943 | 289 | 261 | 1 |         |         |       |

- Molecule 12 is a protein called 40S ribosomal protein S10-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | C0    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 773   | 500 | 126 | 145 | 2 |         |         |       |
| 12  | c0    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 491 | 125 | 144 | 2 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C0    | 89      | ALA      | GLY    | conflict | UNP Q08745 |
| c0    | 89      | ALA      | GLY    | conflict | UNP Q08745 |

- Molecule 13 is a protein called 40S ribosomal protein S11-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | C1    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1214  | 775 | 230 | 206 | 3 |         |         |       |
| 13  | c1    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1168  | 747 | 221 | 197 | 3 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C1    | 147     | ALA      | GLY    | conflict | UNP P0CX47 |
| c1    | 147     | ALA      | GLY    | conflict | UNP P0CX47 |

- Molecule 14 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | C2    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 892   | 562 | 156 | 172 | 2 |         |         |       |
| 14  | c2    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 892   | 562 | 156 | 172 | 2 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C2    | 104     | ALA      | GLY    | conflict | UNP P48589 |
| C2    | 110     | ALA      | GLY    | conflict | UNP P48589 |
| c2    | 104     | ALA      | GLY    | conflict | UNP P48589 |
| c2    | 110     | ALA      | GLY    | conflict | UNP P48589 |

- Molecule 15 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | C3    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1192  | 759 | 224 | 207 | 2 |         |         |       |
| 15  | c3    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1192  | 759 | 224 | 207 | 2 |         |         |       |

- Molecule 16 is a protein called 40S ribosomal protein S14-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | C4    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 891   | 545 | 182 | 163 | 1 |         |         |       |
| 16  | c4    | 128      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 949   | 582 | 188 | 176 | 3 |         |         |       |

- Molecule 17 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | C5    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 977   | 622 | 182 | 166 | 7 |         |         |       |
| 17  | c5    | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1039  | 658 | 196 | 178 | 7 |         |         |       |

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 18  | C6    | 141      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1105  | 708 | 203 | 194 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 18  | c6    | 142      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1111  | 711 | 204 | 196 |         |         |       |

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | C7    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 926   | 577 | 177 | 170 | 2 |         |         |       |
| 19  | c7    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 906   | 563 | 174 | 167 | 2 |         |         |       |

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | C8    | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1192  | 743 | 237 | 210 | 2 |         |         |       |
| 20  | c8    | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1192  | 743 | 237 | 210 | 2 |         |         |       |

- Molecule 21 is a protein called 40S ribosomal protein S19-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | C9    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1112  | 694 | 208 | 208 | 2 |         |         |       |
| 21  | c9    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1112  | 694 | 208 | 208 | 2 |         |         |       |

- Molecule 22 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22  | D0    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 855   | 539 | 156 | 159 | 1 |         |         |       |
| 22  | d0    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 882   | 554 | 161 | 166 | 1 |         |         |       |

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23  | D1    | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 684   | 420 | 125 | 137 | 2 |         |         |       |
| 23  | d1    | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 684   | 420 | 125 | 137 | 2 |         |         |       |



- Molecule 24 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24  | D2    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1021  | 650 | 188 | 180 | 3 |         |         |       |
| 24  | d2    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1021  | 650 | 188 | 180 | 3 |         |         |       |

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25  | D3    | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1121  | 708 | 220 | 191 | 2 |         |         |       |
| 25  | d3    | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1121  | 708 | 220 | 191 | 2 |         |         |       |

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 26  | D4    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1073  | 676 | 208 | 189 |         |         |       |
| 26  | d4    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1073  | 676 | 208 | 189 |         |         |       |

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 27  | D5    | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 563   | 360 | 104 | 99 |         |         |       |
| 27  | d5    | 69       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 558   | 357 | 103 | 98 |         |         |       |

- Molecule 28 is a protein called 40S ribosomal protein S26-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | D6    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 769   | 475 | 160 | 129 | 5 |         |         |       |
| 28  | d6    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 769   | 475 | 160 | 129 | 5 |         |         |       |

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | D7    | 81       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 610   | 382 | 110 | 113 | 5 |         |         |       |
| 29  | d7    | 81       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 610   | 382 | 110 | 113 | 5 |         |         |       |

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30  | D8    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 497   | 306 | 99 | 91 | 1 |         |         |       |
| 30  | d8    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 497   | 306 | 99 | 91 | 1 |         |         |       |

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31  | D9    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 442   | 274 | 92 | 72 | 4 |         |         |       |
| 31  | d9    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 442   | 274 | 92 | 72 | 4 |         |         |       |

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 32  | E0    | 60       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 475   | 299 | 98 | 77 | 1 |         |         |       |

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 33  | E1    | 71       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 566   | 362 | 106 | 94 | 4 |         |         |       |
| 33  | e1    | 76       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 608   | 388 | 117 | 99 | 4 |         |         |       |

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 34  | SR    | 318      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2441  | 1544 | 419 | 470 | 8 |         |         |       |
| 34  | sR    | 318      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2442  | 1544 | 418 | 472 | 8 |         |         |       |

- Molecule 35 is a protein called Suppressor protein STM1.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 35  | SM    | 159      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1104  | 652 | 221 | 231 |         |         |       |

- Molecule 36 is a RNA chain called TPA\_inf: Saccharomyces cerevisiae S288c chromosome XII, complete sequence.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 36  | 1     | 3149     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 67355 | 30086 | 12142 | 21978 | 3149 |         |         |       |
| 36  | 5     | 3150     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 67376 | 30095 | 12145 | 21987 | 3149 |         |         |       |

- Molecule 37 is a RNA chain called TPA\_inf: Saccharomyces cerevisiae S288c chromosome XII, complete sequence.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 37  | 3     | 121      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2579  | 1152 | 461 | 845 | 121 |         |         |       |
| 37  | 7     | 121      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2579  | 1152 | 461 | 845 | 121 |         |         |       |

- Molecule 38 is a RNA chain called Saccharomyces cerevisiae genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97.

| Mol | Chain | Residues | Atoms |      |     |      |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|---------|-------|
| 38  | 4     | 158      | Total | C    | N   | O    | P   | 0       | 0       | 0     |
|     |       |          | 3353  | 1500 | 586 | 1109 | 158 |         |         |       |
| 38  | 8     | 158      | Total | C    | N   | O    | P   | 0       | 0       | 0     |
|     |       |          | 3353  | 1500 | 586 | 1109 | 158 |         |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 39  | L2    | 252      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1914  | 1191 | 388 | 334 | 1 |         |         |       |
| 39  | l2    | 252      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1912  | 1190 | 388 | 333 | 1 |         |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 40  | L3    | 386      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3075  | 1950 | 584 | 533 | 8 |         |         |       |
| 40  | l3    | 386      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3075  | 1950 | 584 | 533 | 8 |         |         |       |

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 41  | L4    | 361      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2748  | 1729 | 522 | 494 | 3 |         |         |       |
| 41  | l4    | 361      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2748  | 1729 | 522 | 494 | 3 |         |         |       |

- Molecule 42 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 42  | L5    | 296      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2375  | 1501 | 414 | 458 | 2 |         |         |       |
| 42  | l5    | 294      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2359  | 1489 | 412 | 456 | 2 |         |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | L6    | 156      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1239  | 800 | 222 | 216 | 1 |         |         |       |
| 43  | l6    | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1248  | 806 | 224 | 217 | 1 |         |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 44  | L7    | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1784  | 1151 | 324 | 308 | 1 |         |         |       |
| 44  | l7    | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1791  | 1155 | 325 | 310 | 1 |         |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 45  | L8    | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1804  | 1151 | 323 | 327 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 45  | l8    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1763  | 1130 | 316 | 314 | 3 |         |         |       |

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | L9    | 191      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1518  | 963 | 274 | 277 | 4 |         |         |       |
| 46  | l9    | 191      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1518  | 963 | 274 | 277 | 4 |         |         |       |

- Molecule 47 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 47  | M0    | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1705  | 1083 | 322 | 294 | 6 |         |         |       |
| 47  | m0    | 213      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1722  | 1094 | 325 | 297 | 6 |         |         |       |

- Molecule 48 is a protein called 60S ribosomal protein L11-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | M1    | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1353  | 847 | 253 | 249 | 4 |         |         |       |
| 48  | m1    | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1353  | 847 | 253 | 249 | 4 |         |         |       |

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 49  | M3    | 193      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1543  | 962 | 315 | 266 |  |         |         |       |
| 49  | m3    | 194      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1548  | 965 | 316 | 267 |  |         |         |       |

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50  | M4    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1053  | 675 | 199 | 177 | 2 |         |         |       |
| 50  | m4    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1059  | 678 | 200 | 179 | 2 |         |         |       |

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 51  | M5    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1720  | 1077 | 361 | 281 | 1 |         |         |       |
| 51  | m5    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1720  | 1077 | 361 | 281 | 1 |         |         |       |

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 52  | M6    | 197      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1555  | 1003 | 289 | 262 | 1 |         |         |       |
| 52  | m6    | 197      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1555  | 1003 | 289 | 262 | 1 |         |         |       |

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 53  | M7    | 183      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1420  | 882 | 281 | 257 |         |         |       |
| 53  | m7    | 155      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1227  | 764 | 238 | 225 |         |         |       |

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 54  | M8    | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1441  | 908 | 290 | 241 | 2 |         |         |       |
| 54  | m8    | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1441  | 908 | 290 | 241 | 2 |         |         |       |

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 55  | M9    | 188      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1521  | 935 | 326 | 260 |         |         |       |
| 55  | m9    | 188      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1521  | 935 | 326 | 260 |         |         |       |

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 56  | N0    | 172      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1445  | 930 | 267 | 244 | 4 |         |         |       |
| 56  | n0    | 172      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1445  | 930 | 267 | 244 | 4 |         |         |       |

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 57  | N1    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1276  | 805 | 246 | 221 | 4 |         |         |       |
| 57  | n1    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1276  | 805 | 246 | 221 | 4 |         |         |       |

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 58  | N2    | 100      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 796   | 516 | 131 | 149 |  |         |         |       |
| 58  | n2    | 98       | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 778   | 505 | 127 | 146 |  |         |         |       |

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 59  | N3    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1003  | 628 | 189 | 179 | 7 |         |         |       |
| 59  | n3    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1003  | 628 | 189 | 179 | 7 |         |         |       |

- Molecule 60 is a protein called 60S ribosomal protein L24-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 60  | N4    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 699   | 443 | 137 | 118 | 1 |         |         |       |
| 60  | n4    | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1038  | 651 | 206 | 180 | 1 |         |         |       |

- Molecule 61 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 61  | N5    | 121      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 620 | 169 | 173 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 61  | n5    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 959   | 617 | 168 | 172 | 2 |         |         |       |

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 62  | N6    | 126      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 993   | 625 | 192 | 176 |  |         |         |       |
| 62  | n6    | 126      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 993   | 625 | 192 | 176 |  |         |         |       |

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 63  | N7    | 135      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1092  | 710 | 202 | 180 |  |         |         |       |
| 63  | n7    | 135      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1092  | 710 | 202 | 180 |  |         |         |       |

- Molecule 64 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 64  | N8    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1173  | 749 | 231 | 190 | 3 |         |         |       |
| 64  | n8    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1173  | 749 | 231 | 190 | 3 |         |         |       |

- Molecule 65 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|--|---------|---------|-------|
| 65  | N9    | 58       | Total | C   | N   | O  |  | 0       | 0       | 0     |
|     |       |          | 462   | 289 | 100 | 73 |  |         |         |       |
| 65  | n9    | 58       | Total | C   | N   | O  |  | 0       | 0       | 0     |
|     |       |          | 462   | 289 | 100 | 73 |  |         |         |       |

- Molecule 66 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 66  | O0    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 743   | 479 | 124 | 139 | 1 |         |         |       |
| 66  | o0    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 767   | 492 | 128 | 146 | 1 |         |         |       |



- Molecule 67 is a protein called 60S ribosomal protein L31-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 67  | O1    | 109      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 876   | 556 | 167 | 152 | 1 |         |         |       |
| 67  | o1    | 109      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 883   | 559 | 167 | 156 | 1 |         |         |       |

- Molecule 68 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 68  | O2    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1020  | 647 | 205 | 167 | 1 |         |         |       |
| 68  | o2    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1020  | 647 | 205 | 167 | 1 |         |         |       |

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 69  | O3    | 106      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 850   | 540 | 165 | 144 | 1 |         |         |       |
| 69  | o3    | 106      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 850   | 540 | 165 | 144 | 1 |         |         |       |

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 70  | O4    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 880   | 545 | 179 | 152 | 4 |         |         |       |
| 70  | o4    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 880   | 545 | 179 | 152 | 4 |         |         |       |

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 71  | O5    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 969   | 615 | 186 | 167 | 1 |         |         |       |
| 71  | o5    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 965   | 612 | 185 | 167 | 1 |         |         |       |

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 72  | O6    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 771   | 481 | 156 | 132 | 2 |         |         |       |
| 72  | o6    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 770   | 481 | 156 | 131 | 2 |         |         |       |

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 73  | O7    | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 681   | 414 | 148 | 114 | 5 |         |         |       |
| 73  | o7    | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 681   | 414 | 148 | 114 | 5 |         |         |       |

- Molecule 74 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 74  | O8    | 77       | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 612   | 391 | 115 | 106 |  |         |         |       |
| 74  | o8    | 77       | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 608   | 388 | 114 | 106 |  |         |         |       |

- Molecule 75 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 75  | O9    | 50       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 436   | 272 | 97 | 65 | 2 |         |         |       |
| 75  | o9    | 50       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 436   | 272 | 97 | 65 | 2 |         |         |       |

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 76  | Q0    | 52       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 417   | 259 | 86 | 67 | 5 |         |         |       |
| 76  | q0    | 52       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 417   | 259 | 86 | 67 | 5 |         |         |       |

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 77  | Q1    | 25       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 233   | 142 | 63 | 27 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 77  | q1    | 25       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 233   | 142 | 63 | 27 | 1 |         |         |       |

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 78  | Q2    | 105      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 847   | 534 | 170 | 138 | 5 |         |         |       |
| 78  | q2    | 105      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 847   | 534 | 170 | 138 | 5 |         |         |       |

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 79  | Q3    | 91       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 694   | 429 | 138 | 121 | 6 |         |         |       |
| 79  | q3    | 91       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 694   | 429 | 138 | 121 | 6 |         |         |       |

- Molecule 80 is a protein called 40S ribosomal protein S30-A.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 80  | e0    | 62       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 491   | 309 | 101 | 80 | 1 |         |         |       |

- Molecule 81 is a protein called Suppressor protein STM1.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 81  | sM    | 104      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 681   | 404 | 140 | 137 |         |         |       |

- Molecule 82 is a protein called unknown protein chain m2.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 82  | m2    | 150      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 750   | 450 | 150 | 150 |         |         |       |

- Molecule 83 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 83  | p0    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1077  | 687 | 192 | 195 | 3 |         |         |       |

- Molecule 84 is a protein called unknown protein chain p1.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 84  | p1    | 47       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 235   | 141 | 47 | 47 |         |         |       |

- Molecule 85 is a protein called unknown protein chain p2.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 85  | p2    | 46       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 230   | 138 | 46 | 46 |         |         |       |

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 86  | L7    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 86  | m6    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 86  | n8    | 5        | Total | Mg  | 0       | 0       |
|     |       |          | 5     | 5   |         |         |
| 86  | o1    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 86  | N5    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 86  | 6     | 149      | Total | Mg  | 0       | 0       |
|     |       |          | 149   | 149 |         |         |
| 86  | sM    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 86  | O4    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 86  | m5    | 3        | Total | Mg  | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 86  | l3    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 86  | M1    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 86  | l4    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 86  | 2     | 123      | Total<br>123 | Mg<br>123 | 0       | 0       |
| 86  | n0    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | L4    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 86  | l7    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 86  | M5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | S2    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | L8    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | D3    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | M9    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | q0    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | SM    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | o4    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | M0    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 86  | c1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | n6    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | 5     | 506      | Total<br>506 | Mg<br>506 | 0       | 0       |
| 86  | L5    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 86  | O7    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | Q2    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | 1     | 477      | Total<br>477 | Mg<br>477 | 0       | 0       |
| 86  | D0    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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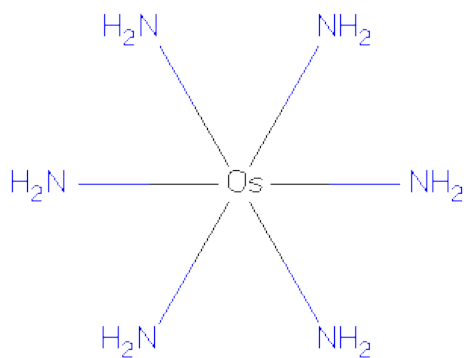
| Mol | Chain | Residues | Atoms       |          | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 86  | S8    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 86  | m1    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 86  | M8    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 86  | q3    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 86  | o3    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 86  | d3    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 86  | M3    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 86  | N3    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 86  | 4     | 21       | Total<br>21 | Mg<br>21 | 0       | 0       |
| 86  | D4    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 86  | L2    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 86  | l5    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 86  | m7    | 5        | Total<br>5  | Mg<br>5  | 0       | 0       |
| 86  | M7    | 6        | Total<br>6  | Mg<br>6  | 0       | 0       |
| 86  | N8    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 86  | s1    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 86  | l9    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 86  | s8    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 86  | O8    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 86  | c7    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 86  | 7     | 16       | Total<br>16 | Mg<br>16 | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |          | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 86  | n3    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 86  | q1    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 86  | L3    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 86  | d4    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 86  | s4    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 86  | l2    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 86  | 8     | 14       | Total<br>14 | Mg<br>14 | 0       | 0       |
| 86  | M6    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 86  | N0    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 86  | 3     | 14       | Total<br>14 | Mg<br>14 | 0       | 0       |

- Molecule 87 is osmium (III) hexammine (three-letter code: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



| Mol | Chain | Residues | Atoms      |        |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|---------|
| 87  | 2     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | S8    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | C3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | C5    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | C8    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | D3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | D9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | SR    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms      |        |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|---------|
| 87  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | L3    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | L3    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | L3    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | L4    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | M0    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | M5    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | M6    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | M7    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 87  | M7    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | M8    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | M9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | N1    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | N9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | O2    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | O3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | O7    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | O7    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | O9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | Q2    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | s1    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | s1    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | s4    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | s8    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | s9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | c1    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | c3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | c5    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | c8    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | d4    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | d9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | sR    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 13    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 13    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 14    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 14    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 15    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | 15    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 87  | l5    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | l9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | m0    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | m0    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | m1    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | m4    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | m5    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | m6    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | m7    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | m8    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | m9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | n3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | n6    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | n9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | o2    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | o3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | o7    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | o7    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 87  | q2    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 88  | q0    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 88  | D6    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 88  | Q2    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 88  | e1    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 88  | Q3    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 88  | D9    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 88  | E1    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 88  | Q0    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 88  | d7    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 88  | q3    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 88  | d9    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 88  | D7    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 88  | d6    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 88  | o7    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 88  | O7    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 88  | q2    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

- Molecule 89 is (1S,2S,12bS,12cS)-2,4,5,7,12b,12c-hexahydro-1H-[1,3]dioxolo[4,5-j]pyrrolo[3,2,1-de]phenanthridine-1,2-diol (three-letter code: 3KD) (formula: C<sub>16</sub>H<sub>17</sub>NO<sub>4</sub>).

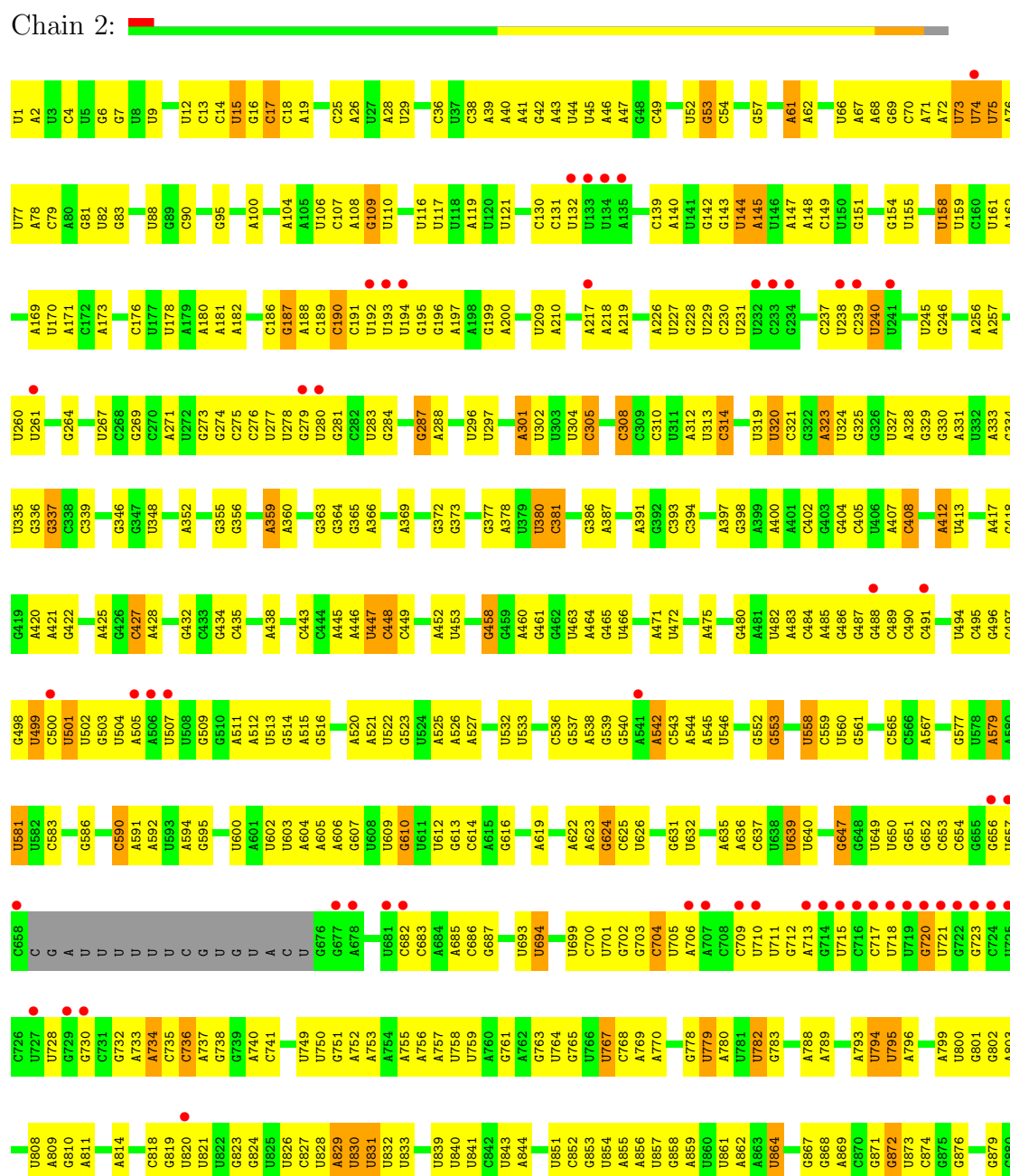
Image  
Not Available

| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 89  | 1     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 21    | 16 | 1 | 4 |         |         |
| 89  | 5     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 21    | 16 | 1 | 4 |         |         |

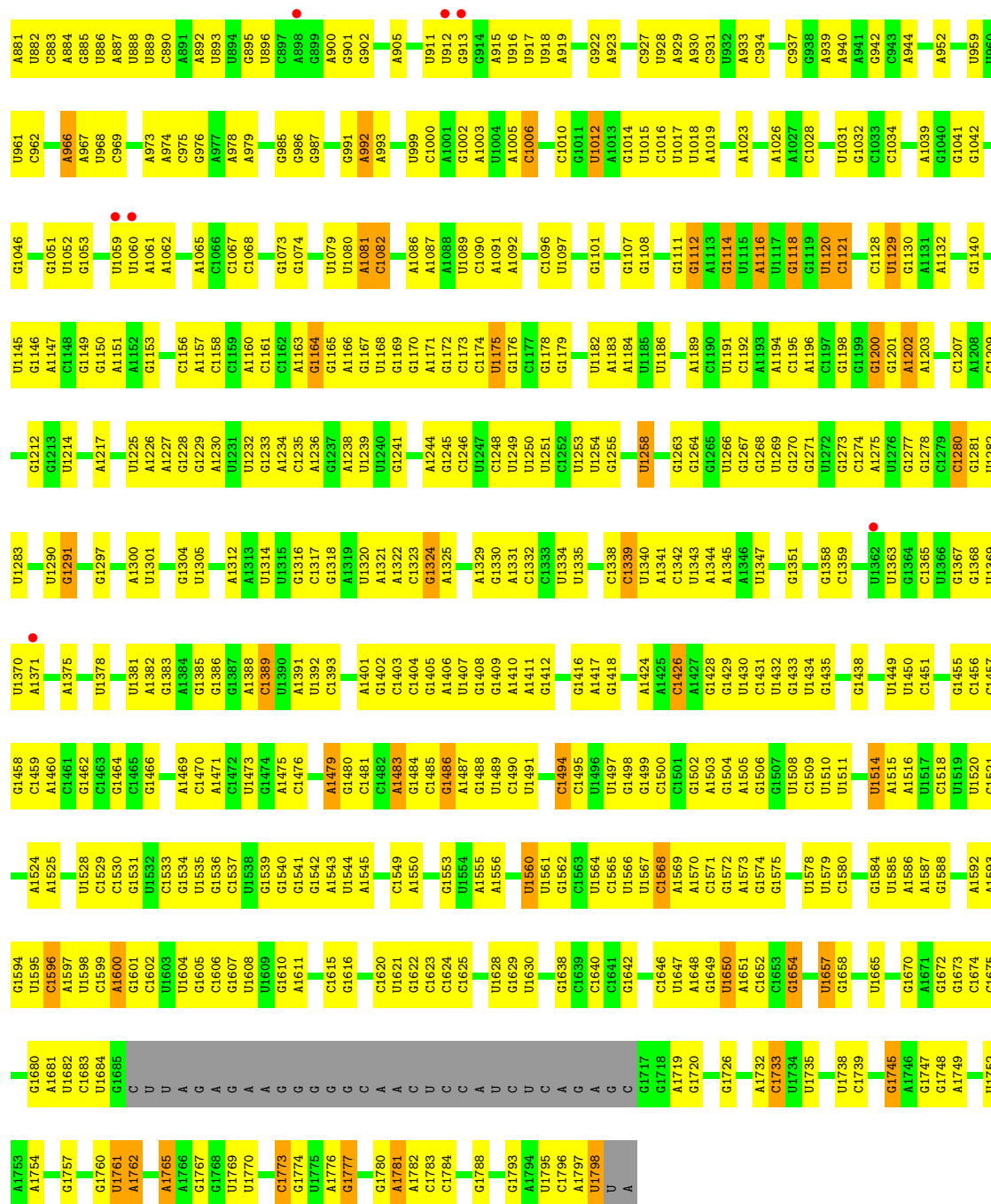
### 3 Residue-property plots

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

- Molecule 1: *Saccharomyces cerevisiae* chromosome XII cosmid 9634

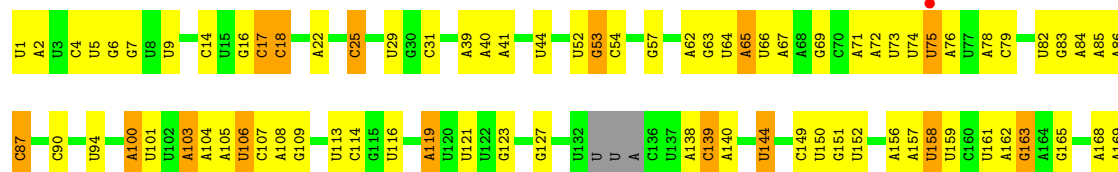


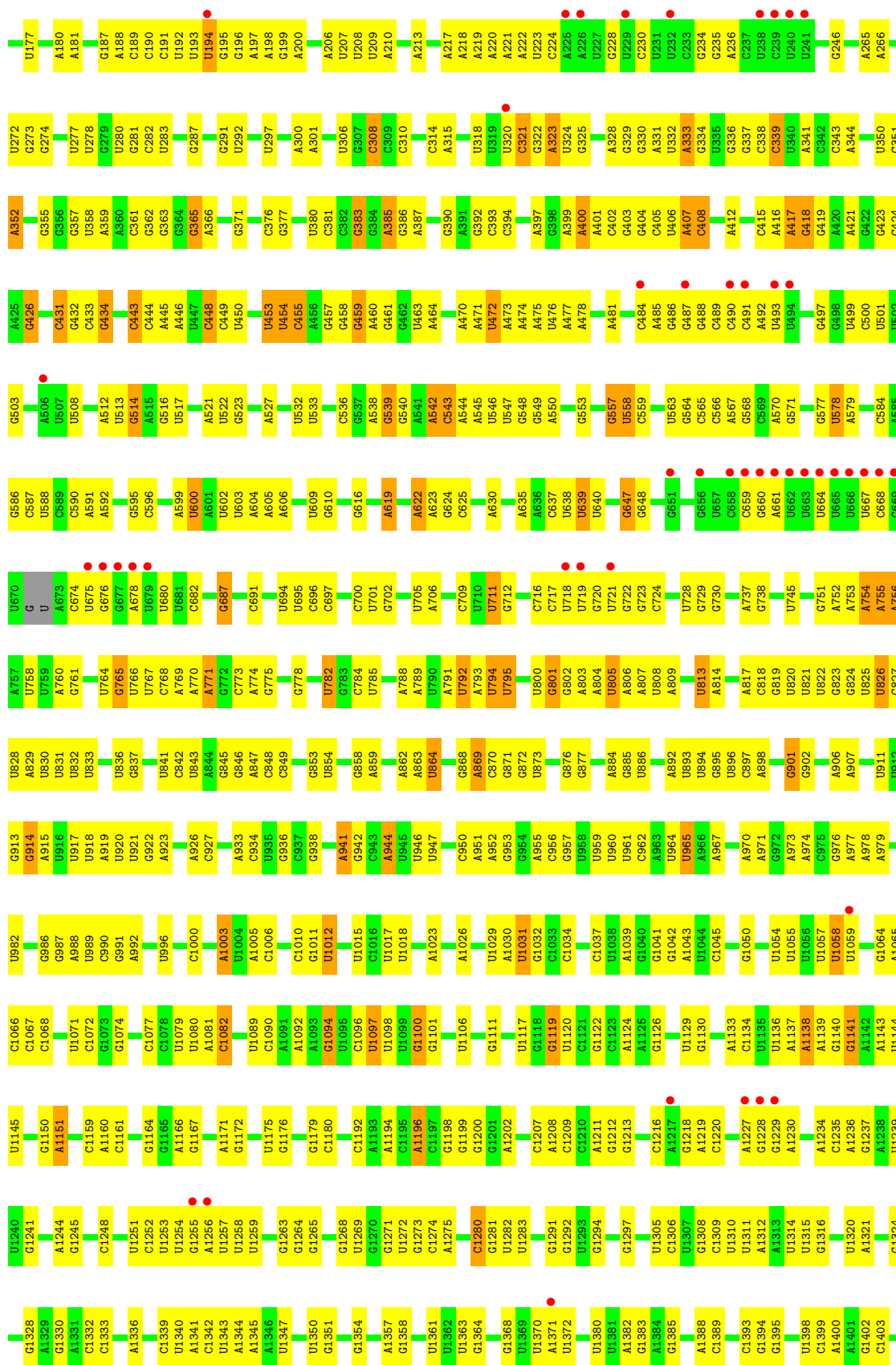


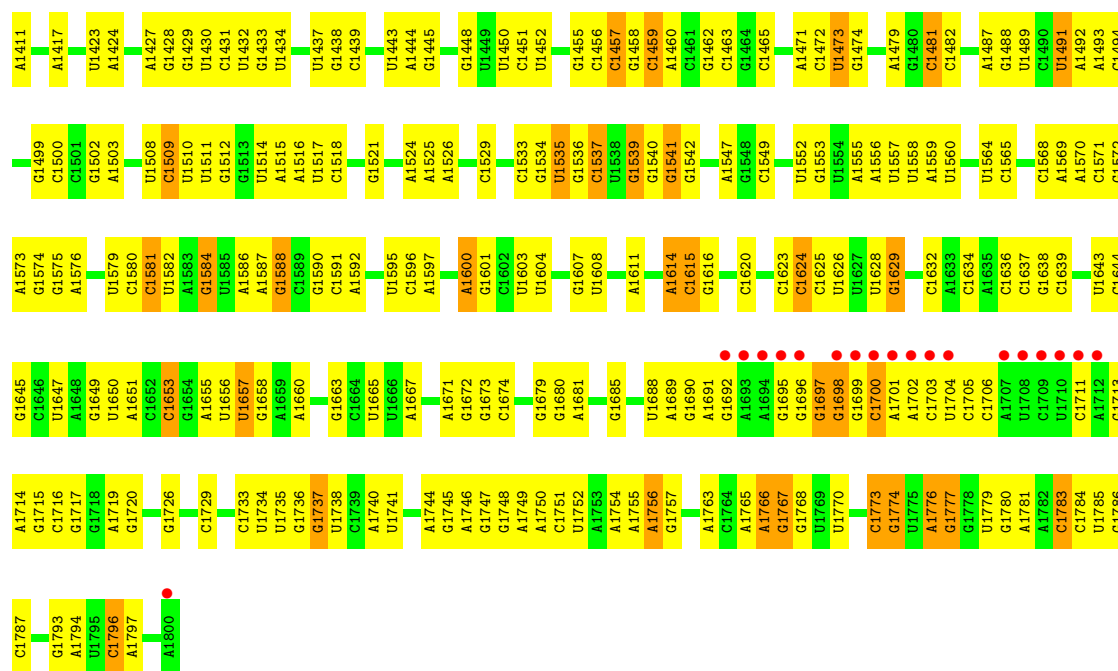


• Molecule 1: *Saccharomyces cerevisiae* chromosome XII cosmid 9634

Chain 6:

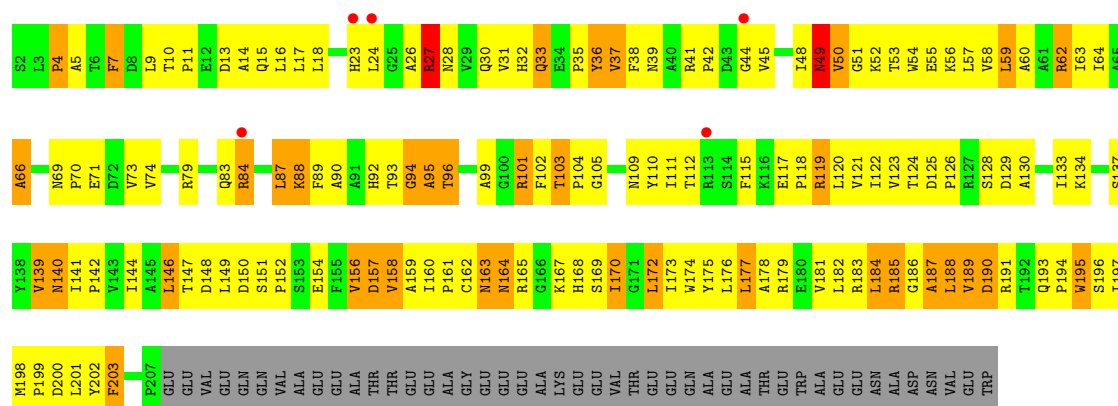






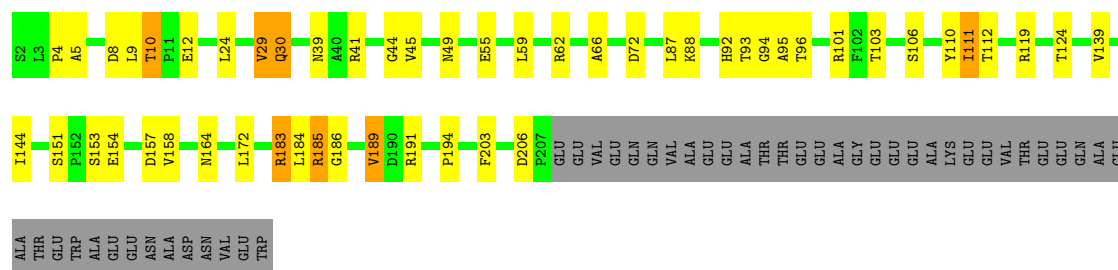
• Molecule 2: 40S ribosomal protein S0-A

Chain S0: 



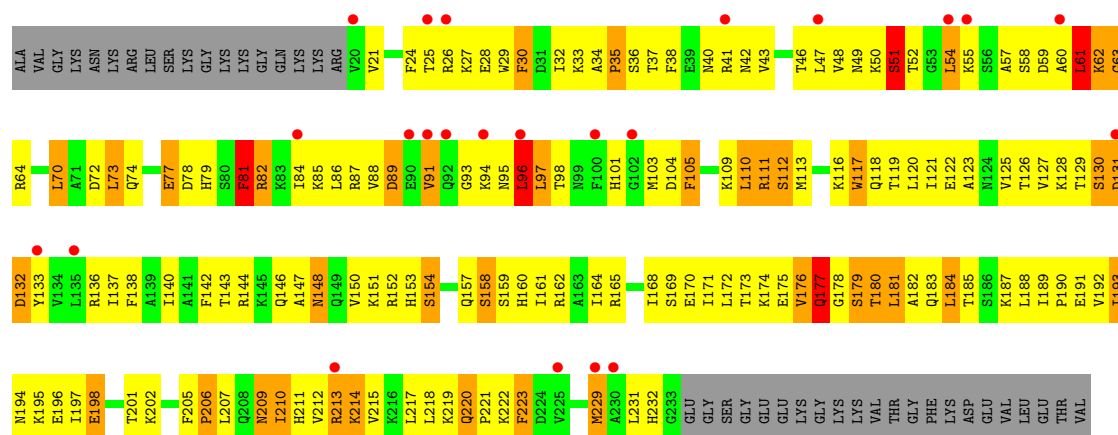
• Molecule 2: 40S ribosomal protein S0-A

Chain s0: 



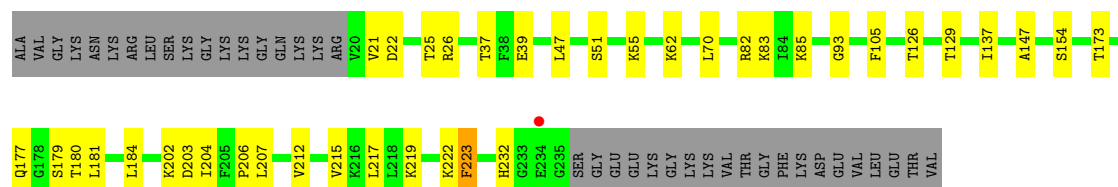
• Molecule 3: 40S ribosomal protein S1-A

Chain S1: 



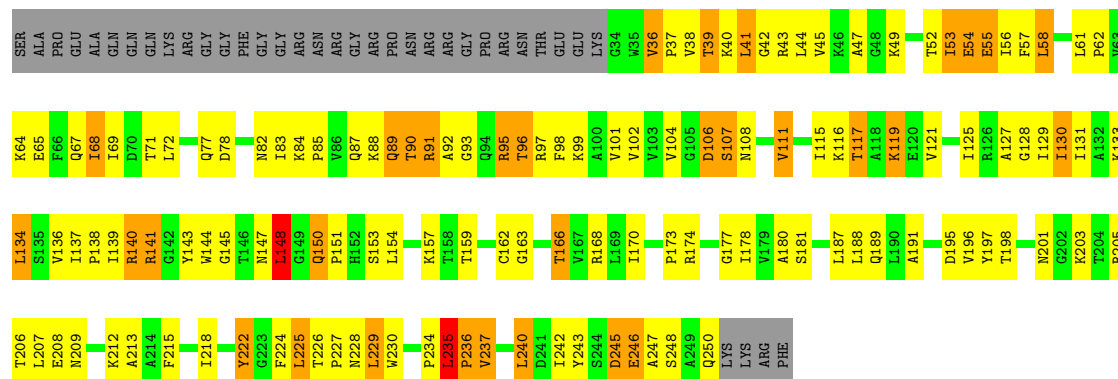
• Molecule 3: 40S ribosomal protein S1-A

Chain s1:



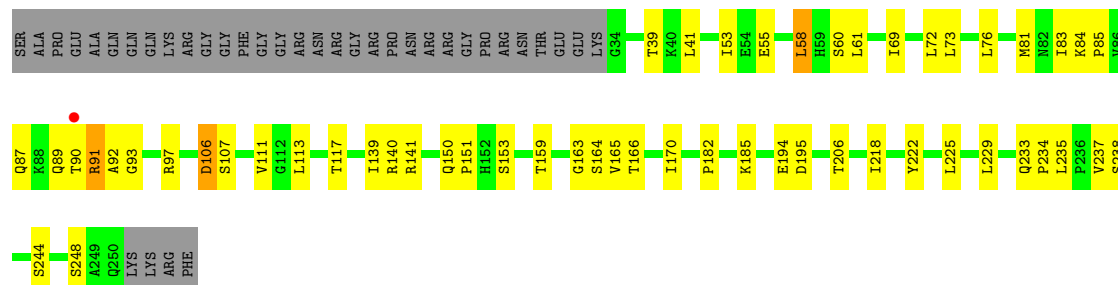
• Molecule 4: 40S ribosomal protein S2

Chain S2:



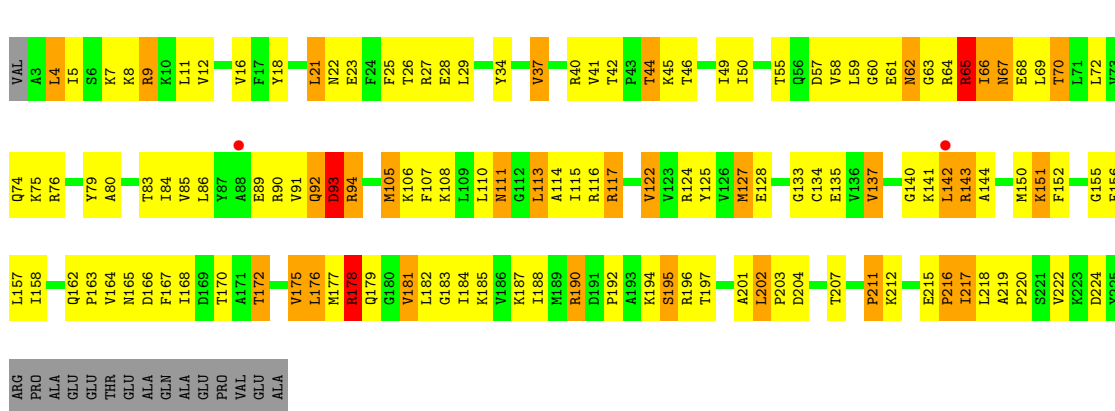
• Molecule 4: 40S ribosomal protein S2

Chain s2:



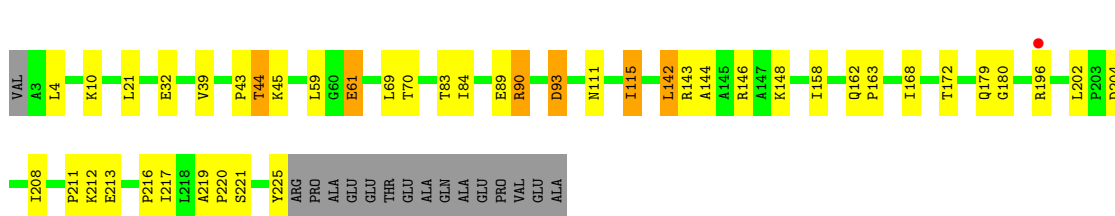
- Molecule 5: 40S ribosomal protein S3

Chain S3:



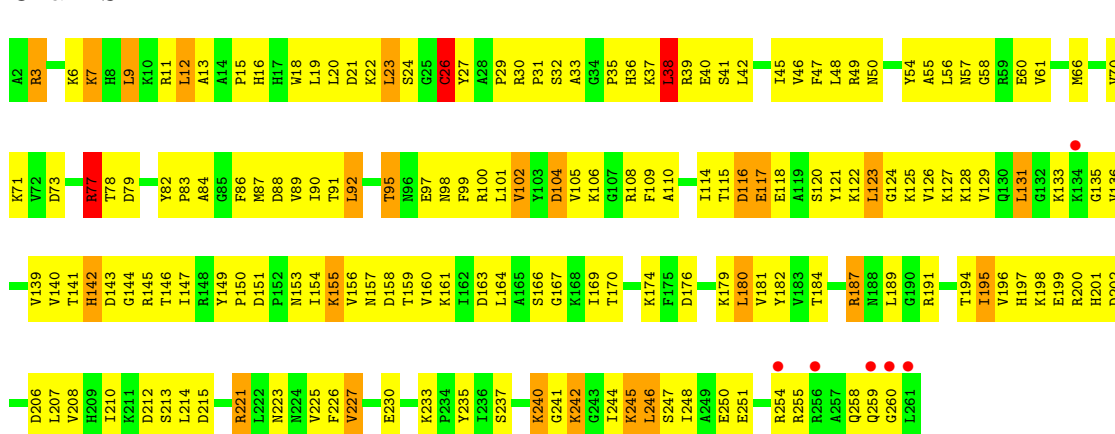
- Molecule 5: 40S ribosomal protein S3

Chain s3:



- Molecule 6: 40S ribosomal protein S4-A

Chain S4:



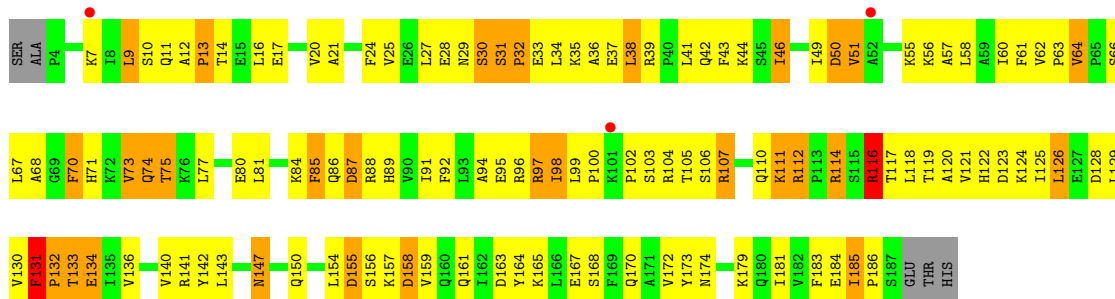
- Molecule 6: 40S ribosomal protein S4-A

Chain s4:



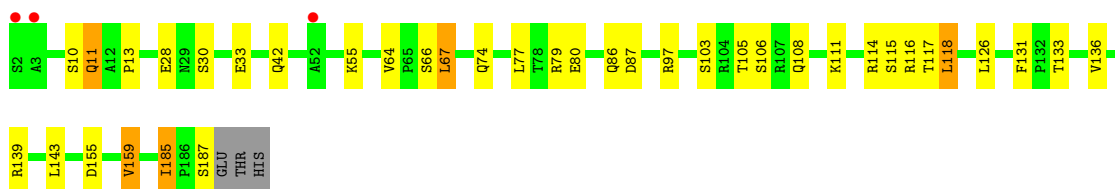
- Molecule 7: 40S ribosomal protein S5





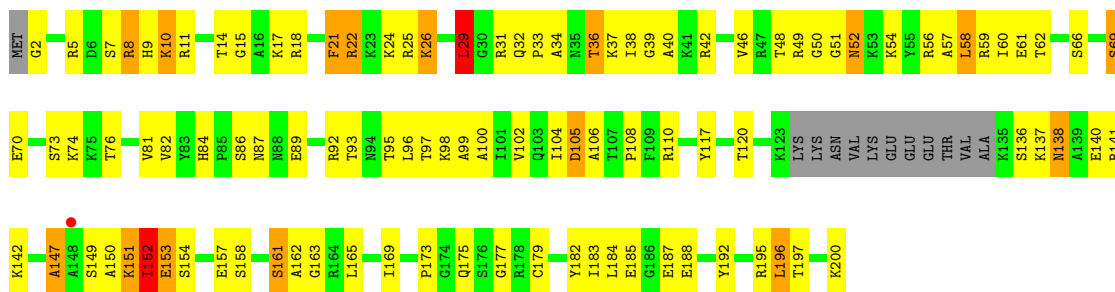
• Molecule 9: 40S ribosomal protein S7-A

Chain s7:



• Molecule 10: 40S ribosomal protein S8-A

Chain S8:



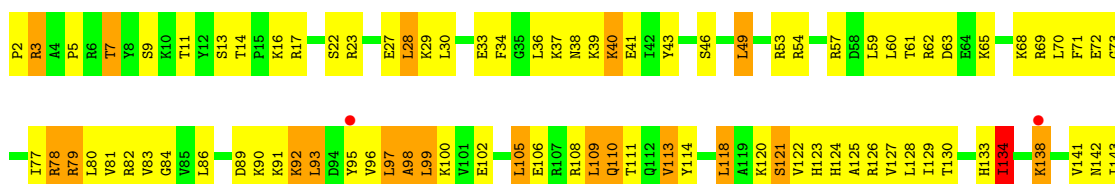
• Molecule 10: 40S ribosomal protein S8-A

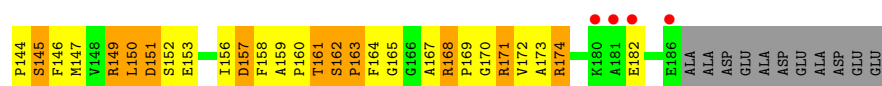
Chain s8:



• Molecule 11: 40S ribosomal protein S9-A

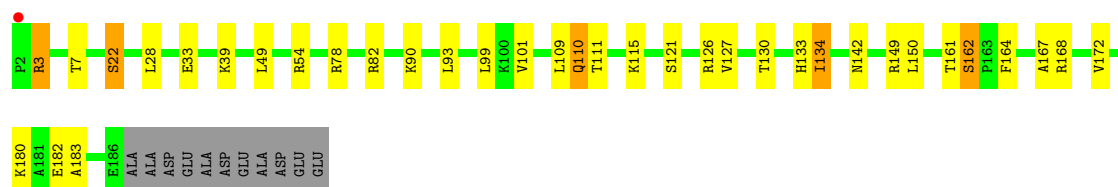
Chain S9:





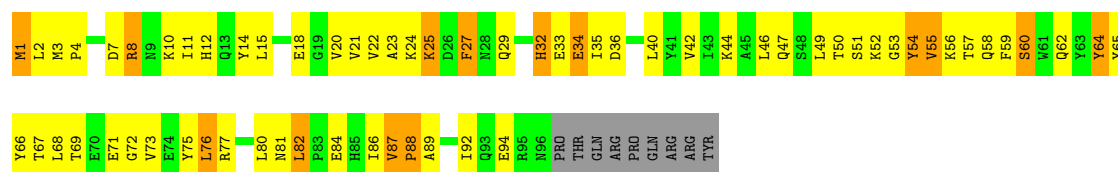
- Molecule 11: 40S ribosomal protein S9-A

Chain s9:



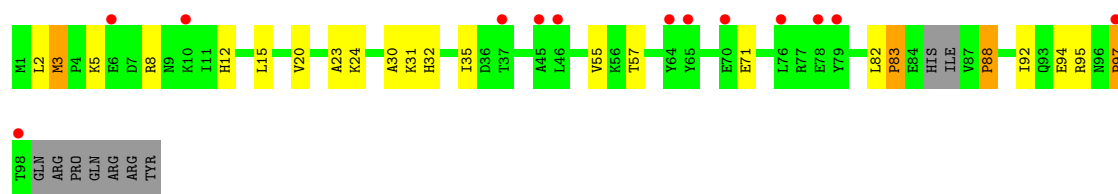
- Molecule 12: 40S ribosomal protein S10-A

Chain C0:



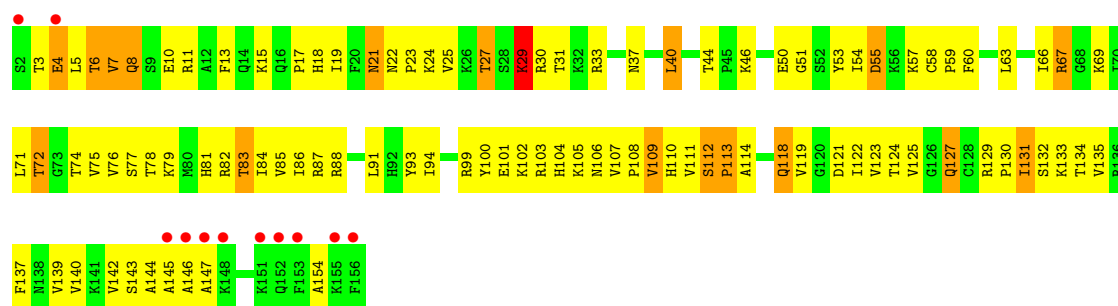
- Molecule 12: 40S ribosomal protein S10-A

Chain c0:



- Molecule 13: 40S ribosomal protein S11-A

Chain C1:



- Molecule 13: 40S ribosomal protein S11-A

Chain c1:





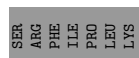
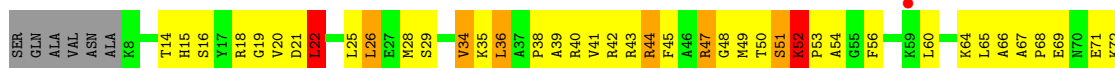




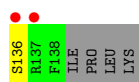
- Chain c4: 



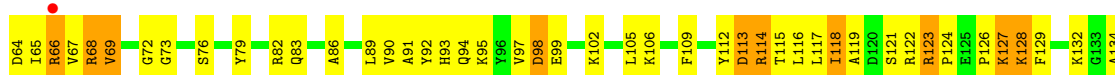
- Chain C5:



- Chain c5: 



- Chain C6:

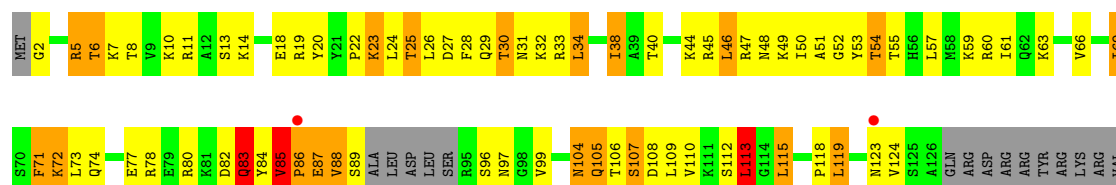


- Chain c6: 



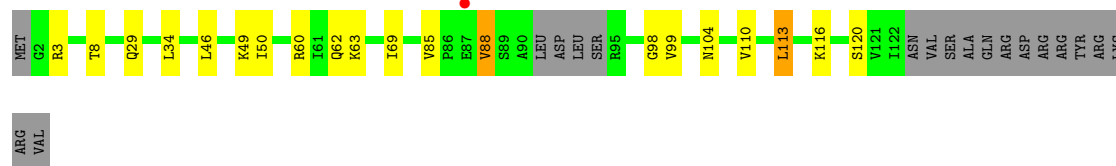
- Molecule 19: 40S ribosomal protein S17-A

Chain C7:



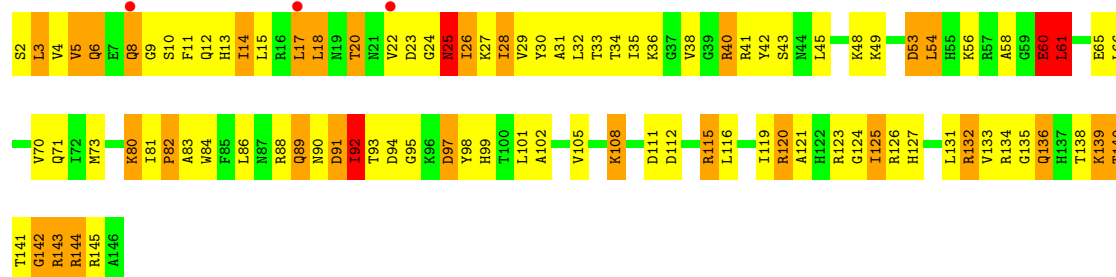
- Molecule 19: 40S ribosomal protein S17-A

Chain c7:



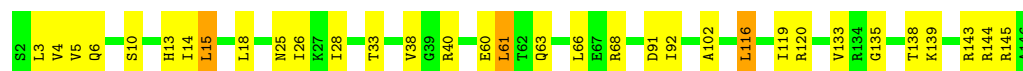
- Molecule 20: 40S ribosomal protein S18-A

Chain C8:



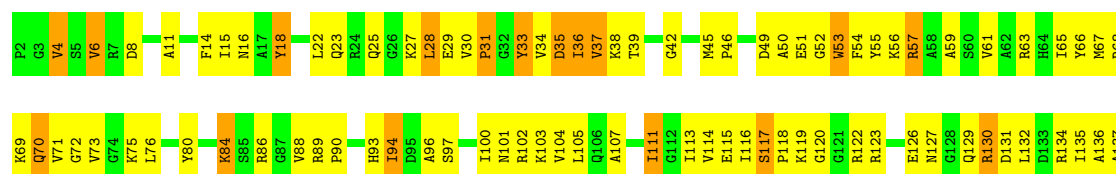
- Molecule 20: 40S ribosomal protein S18-A

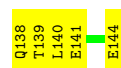
Chain c8:



- Molecule 21: 40S ribosomal protein S19-A

Chain C9:





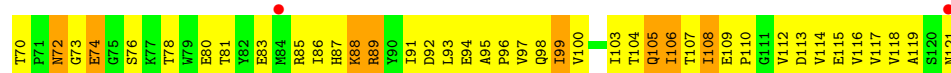
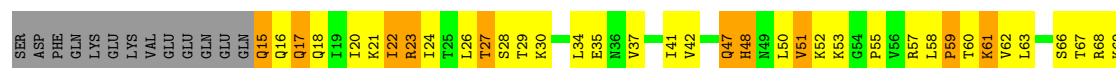
- Molecule 21: 40S ribosomal protein S19-A

Chain c9:



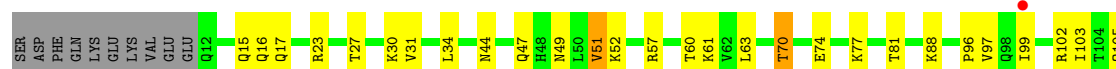
- Molecule 22: 40S ribosomal protein S20

Chain D0:



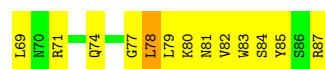
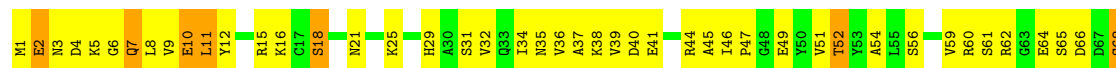
- Molecule 22: 40S ribosomal protein S20

Chain d0:



- Molecule 23: 40S ribosomal protein S21-A

Chain D1:



- Molecule 23: 40S ribosomal protein S21-A

Chain d1:



- Molecule 24: 40S ribosomal protein S22-A

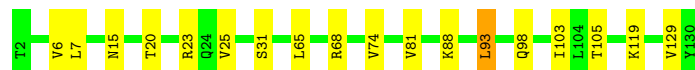
Chain D2:





- Molecule 24: 40S ribosomal protein S22-A

Chain d2:



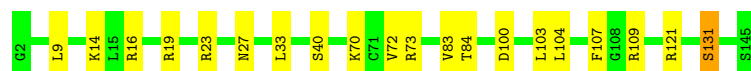
- Molecule 25: 40S ribosomal protein S23-A

Chain D3:



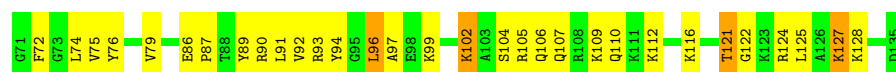
- Molecule 25: 40S ribosomal protein S23-A

Chain d3:



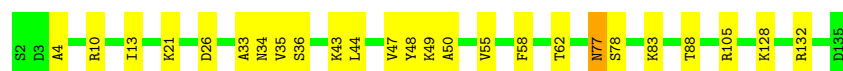
- Molecule 26: 40S ribosomal protein S24-A

Chain D4:



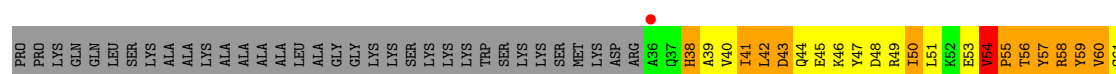
- Molecule 26: 40S ribosomal protein S24-A

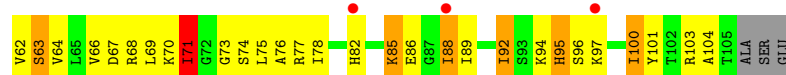
Chain d4:



- Molecule 27: 40S ribosomal protein S25-A

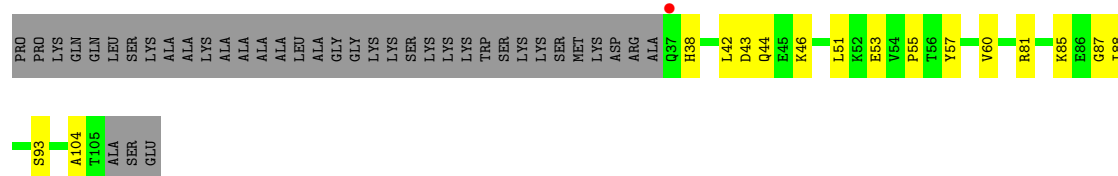
Chain D5:





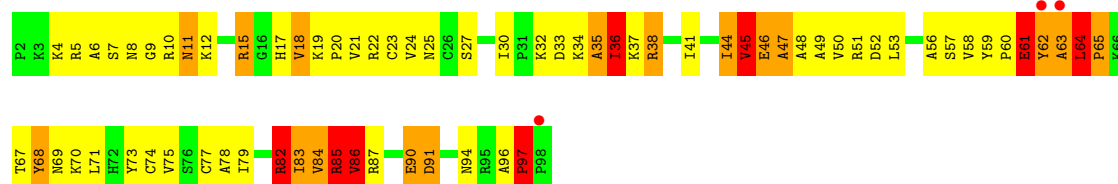
- Molecule 27: 40S ribosomal protein S25-A

Chain d5:



- Molecule 28: 40S ribosomal protein S26-B

Chain D6:



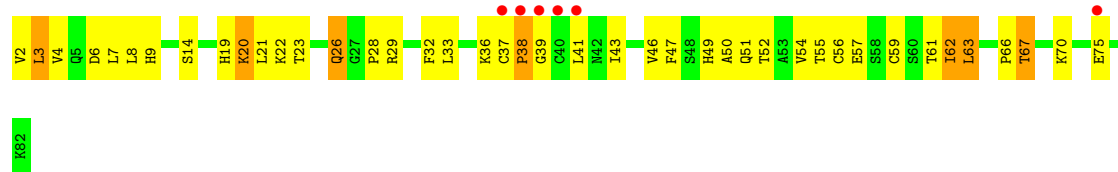
- Molecule 28: 40S ribosomal protein S26-B

Chain d6:



- Molecule 29: 40S ribosomal protein S27-A

Chain D7:



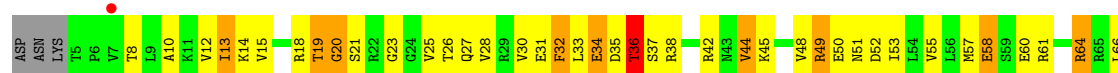
- Molecule 29: 40S ribosomal protein S27-A

Chain d7:



- Molecule 30: 40S ribosomal protein S28-A

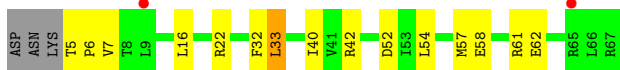
Chain D8:



R67

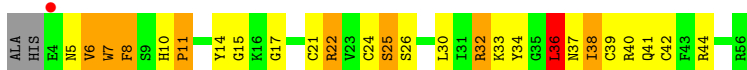
- Molecule 30: 40S ribosomal protein S28-A

Chain d8:



- Molecule 31: 40S ribosomal protein S29-A

Chain D9:



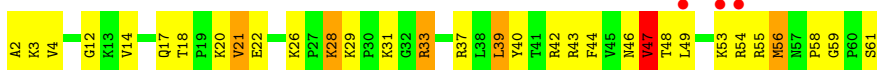
- Molecule 31: 40S ribosomal protein S29-A

Chain d9:



- Molecule 32: 40S ribosomal protein S30-A

Chain E0:



- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain E1:



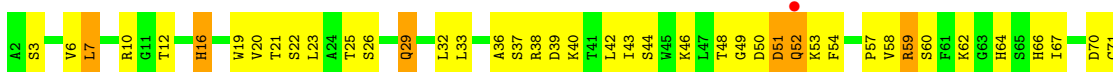
- Molecule 33: Ubiquitin-40S ribosomal protein S31

Chain e1:



- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

Chain SR:







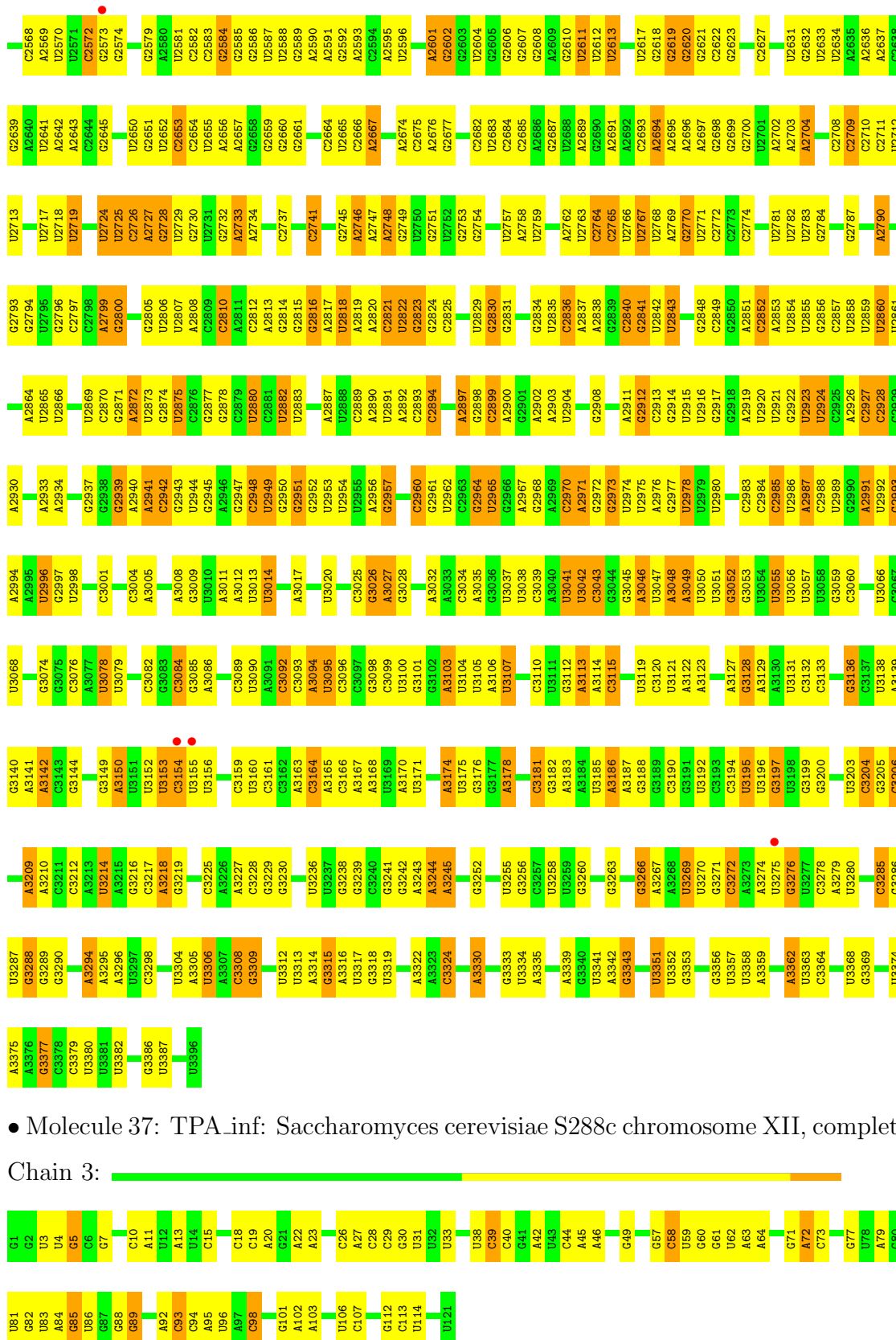


|       |       |       |         |       |       |       |   |   |       |       |       |       |       |       |
|-------|-------|-------|---------|-------|-------|-------|---|---|-------|-------|-------|-------|-------|-------|
| U     | C     | A2404 | C2339   | C2267 | C2197 | A2119 | G | U | G1835 | U1740 | C1639 | G1560 | U1484 | G1413 |
| C     | C2405 | U2340 | U2340   | U2268 | U2200 | A2120 | C | G | U1837 | A1741 | C1639 | G1561 | G1485 | G1414 |
| G     | A2341 | U2341 | U2269   | U2269 | U2201 | G2121 | C | A | G1838 | U1742 | G1655 | G1562 | G1486 | U1415 |
| G     | C2407 | U2342 | U2270   | U2270 | U2202 | G2122 | U | A | U1839 | G1743 | G1656 | U1563 | G1487 | C1416 |
| C     | U2408 | U2343 | U2271   | U2271 | U2203 | G2123 | C | U | U1840 | G1744 | C1657 | U1564 | G1488 | G1417 |
| G     | U2409 | U2344 | U2272   | U2272 | U2204 | A2124 | G | C | A1841 | G1745 | C1658 | U1565 | A1418 | A1418 |
| C     | U2410 | A2345 | U2273   | U2273 | U2205 | A2125 | U | G | U1842 | G1746 | C1659 | U1566 | A1419 | A1419 |
| C     | U2411 | U2346 | U2274   | U2274 | U2206 | U2126 | G | C | C1843 | A1747 | C1660 | U1567 | C1420 | C1420 |
| C     | U2412 | U2347 | U2275   | U2275 | U2207 | U2127 | U | C | C1844 | A1748 | U1661 | U1568 | G1492 | G1421 |
| A     | A2413 | C2348 | U2276   | U2276 | U2208 | C2128 | A | C | U1845 | A1749 | G1662 | U1569 | G1493 |       |
| G     | A2414 | A2349 | U2277   | U2277 | U2209 | U2129 | G | U | G1846 | A1752 | G1663 | U1570 | U1494 | A1428 |
| U     | U2415 | U2350 | U2278   | U2278 | U2210 | G2130 | G | C | C1847 | U1753 | G1664 | U1571 | U1495 | A1428 |
| G     | U2416 | U2351 | U2279   | U2279 | U2211 | U2131 | U | C | G1848 | U1754 | G1665 | U1572 | C1496 | G1429 |
| A     | U2417 | U2352 | U2280   | U2280 | U2212 | U2132 | U | G | C1849 | U1755 | G1666 | U1573 |       |       |
| A     | U2418 | U2353 | U2281   | U2281 | U2213 | G2133 | C | G | A1858 | G1770 | G1667 | U1574 | G1500 | A1433 |
| A     | U2419 | U2354 | U2282   | U2282 | U2214 | G2134 | U | C |       | G1771 | C1668 | C1574 | U1501 | G1434 |
| U     | C2420 | U2355 | U2283   | U2283 | U2215 | G2135 | C | G | A1859 | G1772 | C1669 | U1575 | U1502 | A1435 |
| U     | U2421 | U2356 | U2284   | U2284 | U2216 | A2136 | U | G | A1860 | G1773 | C1670 | U1576 | A1503 | U1436 |
| C     | U2422 | U2357 | U2285   | U2285 | U2217 | U2137 | U | C | U1861 | G1774 | G1671 | G1577 | A1504 | G1437 |
| C     | U2423 | U2358 | U2286   | U2286 | U2218 | U2138 | G | U | G1862 | G1775 | G1672 | C1578 | A1505 |       |
| C     | U2424 | U2359 | U2287   | U2287 | U2219 | U2139 | U | C | U1863 | G1776 | G1673 | C1579 | A1506 | G1440 |
| A     | A2425 | U2360 | U2288   | U2288 | U2220 | U2140 | A | U | A1864 | G1777 | G1674 | A1580 | A1507 | G1441 |
| A     | U2426 | U2361 | U2289   | U2289 | U2221 | U2141 | C | C | U1865 | G1778 | G1675 | A1581 | A1508 | G1442 |
| C     | U2427 | U2362 | U2290   | U2290 | U2222 | A2142 | C | U | U1866 | G1779 | G1676 | C1582 | A1509 | U1443 |
| C     | U2428 | U2363 | U2291   | U2291 | U2223 | A2143 | C | U | U1867 | G1780 | G1677 | G1583 | G1510 | G1444 |
| C     | U2429 | U2364 | U2292   | U2292 | U2224 | A2144 | C | C | U1868 | G1781 | G1678 | G1584 | G1511 |       |
| C     | U2430 | U2365 | U2293   | U2293 | U2225 | A2145 | C | C | U1869 | G1782 | G1679 | G1585 | G1512 | U1445 |
| C     | U2431 | U2366 | U2294   | U2294 | U2226 | U2146 | G | U | U1870 | G1783 | G1680 | G1586 | A1446 | A1446 |
| C     | U2432 | U2367 | U2295   | U2295 | U2227 | U2147 | U | C | A1871 | G1784 | G1681 | G1587 | A1447 | U1448 |
| U     | U2433 | U2368 | U2296   | U2296 | U2228 | U2148 | C | C | U1872 | G1785 | G1682 | G1588 | A1449 | A1449 |
| U     | U2434 | U2369 | U2297   | U2297 | U2229 | U2149 | C | C | U1873 | G1786 | G1683 | G1589 | A1450 | G1450 |
| U     | U2435 | U2370 | U2298   | U2298 | U2230 | U2150 | C | C | U1874 | G1787 | G1684 | G1590 | G1520 | C1451 |
| U     | U2436 | U2371 | U2299   | U2299 | U2231 | U2151 | C | C | U1875 | G1788 | G1685 | G1591 | G1521 | G1452 |
| A     | U2437 | U2372 | U2300   | U2300 | U2232 | U2152 | C | U | U1876 | G1789 | G1686 | G1592 | G1522 | A1453 |
| U2501 | U2501 | U2373 | U2301   | U2301 | U2233 | G2155 | C | U | U1877 | G1790 | G1687 | G1593 | G1523 | U1454 |
| A2502 | A2502 | U2374 | U2302   | U2302 | U2234 | C2156 | U | C | U1878 | G1791 | G1688 | G1594 | G1524 | U1455 |
| G2503 | G2503 | U2375 | U2303   | U2303 | U2235 | G2157 | C | C | U1879 | G1792 | G1689 | G1595 | G1525 |       |
| U2504 | U2504 | U2376 | U2304   | U2304 | U2236 | G2158 | C | C | U1880 | G1793 | G1690 | G1596 | G1526 |       |
| U2505 | U2505 | U2377 | U2305   | U2305 | U2237 | U2159 | C | C | U1881 | G1794 | G1691 | G1597 | G1527 |       |
| U2506 | U2506 | U2378 | U2306   | U2306 | U2238 | G2160 | C | U | U1882 | G1795 | G1692 | G1598 | G1528 | C1459 |
| U2510 | U2510 | U2379 | U2307   | U2307 | U2239 | G2161 | C | U | U1883 | G1796 | G1693 | G1599 | A1529 | A1460 |
| A2511 | A2511 | U2380 | U2308   | U2308 | U2240 | U2162 | C | U | U1884 | G1797 | G1694 | G1600 | A1530 | A1461 |
| C2512 | C2512 | U2381 | U2309   | U2309 | U2241 | G2163 | C | A | U1885 | G1798 | G1695 | G1601 | C1531 | A1462 |
| U2513 | U2513 | U2382 | U2310   | U2310 | U2242 | A2164 | U | C | U1886 | G1799 | G1696 | G1602 | U1463 | U1463 |
| U2514 | U2514 | U2383 | U2311   | U2311 | U2243 | G2165 | C | U | U1887 | G1800 | G1697 | G1603 | U1464 | G1464 |
| U     | U2515 | U2384 | U2312   | U2312 | U2244 | A2166 | A | U | U1888 | G1801 | G1698 | G1604 | A1532 | A1465 |
| U     | U2516 | U2385 | U2313   | U2313 | U2245 | A2167 | C | C | U1889 | G1802 | G1699 | G1605 | U1533 | G1466 |
| U     | U2517 | U2386 | U2314   | U2314 | U2246 | A2168 | C | C | U1890 | G1803 | G1700 | U1606 | A1534 | A1467 |
| A     | U2518 | U2387 | U2315   | U2315 | U2247 | G2169 | C | U | U1891 | G1804 | U1701 | U1607 | U1535 | G1468 |
| G     | U2519 | U2388 | U2316   | U2316 | U2248 | U2173 | C | U | U1892 | G1805 | U1702 | C1608 | A1536 | A1469 |
| A     | U2520 | U2389 | U2317   | U2317 | U2249 | U2174 | C | C | U1893 | G1806 | U1703 | C1609 | U1540 | C1470 |
| G2525 | G2525 | U2390 | U2318   | U2318 | U2250 | G2175 | C | C | U1894 | G1807 | G1712 | A1613 | U1471 | U1471 |
| G2526 | G2526 | U2391 | U2319   | U2319 | U2251 | U2176 | C | C | U1895 | G1808 | G1713 | C1614 | U1472 | U1472 |
| G2527 | G2527 | U2392 | U2320   | U2320 | U2252 | G2177 | C | U | U1896 | G1809 | G1714 | C1615 | U1473 | G1473 |
| G2528 | G2528 | U2393 | U2321   | U2321 | U2253 | U2178 | C | U | U1897 | G1810 | G1715 | U1616 | A1474 | A1474 |
| U2532 | U2532 | U2394 | U2322   | U2322 | U2254 | G2179 | C | C | U1898 | G1811 | G1716 | U1617 | G1475 | G1475 |
| G2533 | G2533 | U2395 | U2323   | U2323 | U2255 | C2181 | C | G | U1899 | G1812 | G1717 | U1618 | G1476 | G1476 |
| G2534 | G2534 | U2396 | U2324   | U2324 | U2256 | A2182 | C | U | A1900 | G1813 | G1718 | U1619 | U1551 | C1477 |
| A2535 | A2535 | U2397 | U2325   | U2325 | U2257 | U2183 | C | U | U1901 | G1814 | G1719 | U1620 | G1552 | A1478 |
| U2539 | U2539 | U2398 | U2326   | U2326 | U2258 | A2184 | C | U | U1902 | G1815 | G1720 | U1621 | U1553 | U1479 |
| A2540 | A2540 | U2399 | U2327   | U2327 | U2259 | U2185 | C | U | U1903 | G1816 | G1721 | U1622 | U1554 | U1480 |
| U2541 | U2541 | U2400 | U2328   | U2328 | U2260 | U2186 | C | U | U1904 | G1817 | G1722 | U1623 | U1555 | A1481 |
| U2542 | U2542 | U2401 | U2329   | U2329 | U2261 | U2187 | C | U | U1905 | G1818 | G1723 | U1624 | C1556 |       |
|       |       | U2402 | U2330   | U2330 | U2262 | U2188 | C | U | U1906 | G1819 | G1724 | C1631 |       |       |
|       |       | U2403 | U2331   | U2331 | U2263 | U2189 | C | U | U1907 | U1820 | C1632 | C1633 |       |       |
|       |       |       | U2332   | U2332 | U2264 | U2190 | C | U | U1908 | U1821 | C1633 | C1634 |       |       |
|       |       |       | U2333   | U2333 | U2265 | U2191 | C | U | U1909 | U1822 | C1634 | C1635 |       |       |
|       |       |       | U2334   | U2334 | U2266 | U2192 | C | U | A1910 | C1822 | C1635 | C1636 |       |       |
|       |       |       | U2335   | U2335 | U2267 | U2193 | C | U | U1911 | C1823 | C1636 | C1637 |       |       |
|       |       |       | U2336   | U2336 | U2268 | U2194 | C | U | U1912 | C1824 | C1637 | C1638 |       |       |
|       |       |       | U2337   | U2337 | U2269 | U2195 | C | U | U1913 | C1825 | C1638 | C1639 |       |       |
|       |       |       | U2338   | U2338 | U2270 | U2196 | C | U | U1914 | C1826 | C1639 | C1640 |       |       |
|       |       |       | U2339   | U2339 | U2271 | U2197 | C | U | U1915 | C1827 | C1640 | C1641 |       |       |
|       |       |       | U2340   | U2340 | U2272 | U2198 | C | U | U1916 | C1828 | C1641 | C1642 |       |       |
|       |       |       | U2341   | U2341 | U2273 | U2199 | C | U | U1917 | C1829 | C1642 | C1643 |       |       |
|       |       |       | U2342   | U2342 | U2274 | U2200 | C | U | U1918 | C1830 | C1643 | C1644 |       |       |
|       |       |       | U2343   | U2343 | U2275 | U2201 | C | U | U1919 | C1831 | C1644 | C1645 |       |       |
|       |       |       | U2344   | U2344 | U2276 | U2202 | C | U | U1920 | C1832 | C1645 | C1646 |       |       |
|       |       |       | U2345   | U2345 | U2277 | U2203 | C | U | U1921 | C1833 | C1646 | C1647 |       |       |
|       |       |       | U2346   | U2346 | U2278 | U2204 | C | U | U1922 | C1834 | C1647 | C1648 |       |       |
|       |       |       | U2347   | U2347 | U2279 | U2205 | C | U | U1923 | C1835 | C1648 | C1649 |       |       |
|       |       |       | U2348   | U2348 | U2280 | U2206 | C | U | U1924 | C1836 | C1649 | C1650 |       |       |
|       |       |       | U2349   | U2349 | U2281 | U2207 | C | U | U1925 | C1837 | C1650 | C1651 |       |       |
|       |       |       | U2350   | U2350 | U2282 | U2208 | C | U | U1926 | C1838 | C1651 | C1652 |       |       |
|       |       |       | U2351   | U2351 | U2283 | U2209 | C | U | U1927 | C1839 | C1652 | C1653 |       |       |
|       |       |       | U2352   | U2352 | U2284 | U2210 | C | U | U1928 | C1840 | C1653 | C1654 |       |       |
|       |       |       | U2353   | U2353 | U2285 | U2211 | C | U | U1929 | C1841 | C1654 | C1655 |       |       |
|       |       |       | U2354   | U2354 | U2286 | U2212 | C | U | U1930 | C1842 | C1655 | C1656 |       |       |
|       |       |       | U2355   | U2355 | U2287 | U2213 | C | U | U1931 | C1843 | C1656 | C1657 |       |       |
|       |       |       | U2356   | U2356 | U2288 | U2214 | C | U | U1932 | C1844 | C1657 | C1658 |       |       |
|       |       |       | U2357   | U2357 | U2289 | U2215 | C | U | U1933 | C1845 | C1658 | C1659 |       |       |
|       |       |       | U2358   | U2358 | U2290 | U2216 | C | U | U1934 | C1846 | C1659 | C1660 |       |       |
|       |       |       | U2359   | U2359 | U2291 | U2217 | C | U | U1935 | C1847 | C1660 | C1661 |       |       |
|       |       |       | U2360   | U2360 | U2292 | U2218 | C | U | U1936 | C1848 | C1661 | C1662 |       |       |
|       |       |       | U2361   | U2361 | U2293 | U2219 | C | U | U1937 | C1849 | C1662 | C1663 |       |       |
|       |       |       | U2362   | U2362 | U2294 | U2220 | C | U | U1938 | C1850 | C1663 | C1664 |       |       |
|       |       |       | U2363</ |       |       |       |   |   |       |       |       |       |       |       |



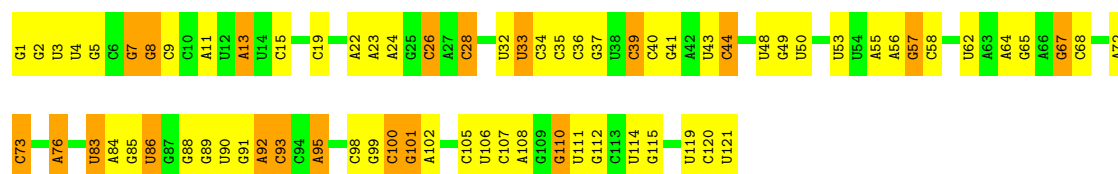
|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| U1329 | U1330 | U1331 | U1332 | U1333 | U1334 | U1335 | U1336 | U1337 | U1338 | U1339 | U1340 | U1345 | U1348 | U1349 | U1350 | U1351 | U1352 | U1353 | U1354 | U1355 | U1356 | U1357 | U1358 | U1359 | U1362 | U1363 | U1364 | U1365 | U1366 | U1367 | U1368 | U1369 | U1370 | U1371 | U1372 | U1373 | U1374 | U1375 | U1376 | U1377 | U1378 | U1379 | U1380 | U1381 | U1385 | U1386 | U1387 | U1388 | U1389 | U1390 | U1391 | U1392 | U1393 | U1394 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| G1241 | G1242 | G1243 | G1244 | G1245 | G1246 | G1249 | G1250 | G1251 | G1252 | G1253 | G1258 | G1259 | G1260 | G1261 | G1262 | G1263 | G1264 | G1265 | G1266 | G1270 | G1271 | G1276 | G1285 | G1286 | G1289 | G1290 | G1291 | G1292 | G1293 | G1294 | G1295 | G1296 | G1297 | G1298 | G1299 | G1300 | G1301 | G1302 | G1303 | G1304 | G1305 | G1306 | G1307 | G1308 | G1309 | G1310 | G1311 | G1312 | G1313 | G1314 | G1315 | G1316 | G1317 | G1318 | G1319 | G1320 | G1321 | G1322 | G1323 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| U1096 | U1097 | U1098 | U1099 | U1100 | U1101 | U1102 | U1103 | U1104 | U1105 | U1106 | U1107 | U1108 | U1109 | U1110 | U1111 | U1112 | U1113 | U1114 | U1115 | U1116 | U1117 | U1118 | U1119 | U1120 | U1121 | U1122 | U1123 | U1124 | U1125 | U1126 | U1127 | U1128 | U1129 | U1130 | U1131 | U1132 | U1133 | U1134 | U1135 | U1136 | U1137 | U1138 | U1139 | U1140 | U1141 | U1142 | U1143 | U1144 | U1145 | U1146 | U1147 | U1148 | U1149 | U1150 | U1151 | U1152 | U1153 | U1154 | U1155 | U1156 | U1157 | U1158 | U1159 | U1160 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| G1161 | G1162 | G1163 | G1164 | G1165 | G1166 | G1167 | G1168 | G1169 | G1170 | G1171 | G1172 | G1173 | G1174 | G1175 | G1176 | G1177 | G1178 | G1179 | G1180 | G1181 | G1182 | G1183 | G1184 | G1185 | G1186 | G1187 | G1188 | G1189 | G1190 | G1191 | G1192 | G1193 | G1194 | G1195 | G1196 | G1197 | G1198 | G1199 | G1200 | G1201 | G1202 | G1203 | G1204 | G1205 | G1206 | G1207 | G1208 | G1209 | G1210 | G1211 | G1212 | G1213 | G1214 | G1215 | G1216 | G1217 | G1218 | G1219 | G1220 | G1221 | G1222 | G1223 | G1224 | G1225 | G1226 | G1227 | G1228 | G1229 | G1230 | G1231 | G1232 | G1233 | G1234 | G1235 | G1236 | G1237 | G1238 | G1239 | G1240 | G1241 | G1242 | G1243 | G1244 | G1245 | G1246 | G1247 | G1248 | G1249 | G1250 | G1251 | G1252 | G1253 | G1254 | G1255 | G1256 | G1257 | G1258 | G1259 | G1260 | G1261 | G1262 | G1263 | G1264 | G1265 | G1266 | G1267 | G1268 | G1269 | G1270 | G1271 | G1272 | G1273 | G1274 | G1275 | G1276 | G1277 | G1278 | G1279 | G1280 | G1281 | G1282 | G1283 | G1284 | G1285 | G1286 | G1287 | G1288 | G1289 | G1290 | G1291 | G1292 | G1293 | G1294 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| U0963 | U0964 | U0965 | U0966 | U0967 | U0968 | U0969 | U0970 | U0971 | U0972 | U0973 | U0974 | U0975 | U0976 | U0977 | U0978 | U0979 | U0980 | U0981 | U0982 | U0983 | U0984 | U0985 | U0986 | U0987 | U0988 | U0989 | U0990 | U0991 | U0992 | U0993 | U0994 | U0995 | U0996 | U0997 | U0998 | U0999 | U1000 | U1001 | U1002 | U1003 | U1004 | U1005 | U1006 | U1007 | U1008 | U1009 | U1010 | U1011 | U1012 | U1013 | U1014 | U1015 | U1016 | U1017 | U1018 | U1019 | U1020 | U1021 | U1022 | U1023 | U1024 | U1025 | U1026 | U1027 | U1028 | U1029 | U1030 | U1031 | U1032 | U1033 | U1034 | U1035 | U1036 | U1037 | U1038 | U1039 | U1040 | U1041 | U1042 | U1043 | U1044 | U1045 | U1046 | U1047 | U1048 | U1049 | U1050 | U1051 | U1052 | U1053 | U1054 | U1055 | U1056 | U1057 | U1058 | U1059 | U1060 | U1061 | U1062 | U1063 | U1064 | U1065 | U1066 | U1067 | U1068 | U1069 | U1070 | U1071 | U1072 | U1073 | U1074 | U1075 | U1076 | U1077 | U1078 | U1079 | U1080 | U1081 | U1082 | U1083 | U1084 | U1085 | U1086 | U1087 | U1088 | U1089 | U1090 | U1091 | U1092 | U1093 | U1094 | U1095 | U1096 | U1097 | U1098 | U1099 | U1100 | U1101 | U1102 | U1103 | U1104 | U1105 | U1106 | U1107 | U1108 | U1109 | U1110 | U1111 | U1112 | U1113 | U1114 | U1115 | U1116 | U1117 | U1118 | U1119 | U1120 | U1121 | U1122 | U1123 | U1124 | U1125 | U1126 | U1127 | U1128 | U1129 | U1130 | U1131 | U1132 | U1133 | U1134 | U1135 | U1136 | U1137 | U1138 | U1139 | U1140 | U1141 | U1142 | U1143 | U1144 | U1145 | U1146 | U1147 | U1148 | U1149 | U1150 | U1151 | U1152 | U1153 | U1154 | U1155 | U1156 | U1157 | U1158 | U1159 | U1160 |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
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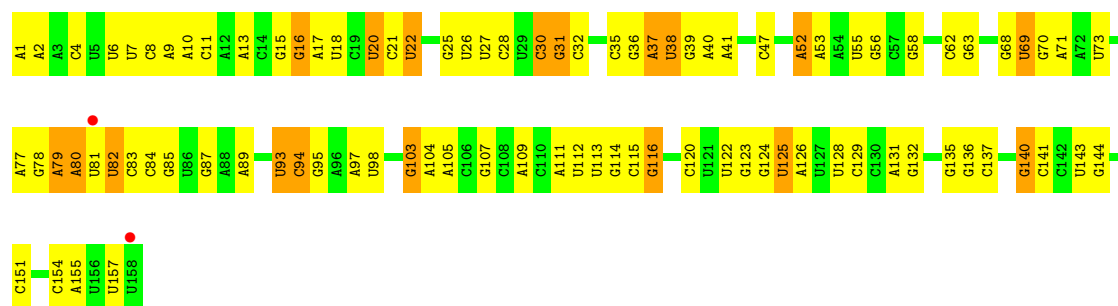
● Molecule 37: TPA\_inf: Saccharomyces cerevisiae S288c chromosome XII, complete sequence

Chain 7:



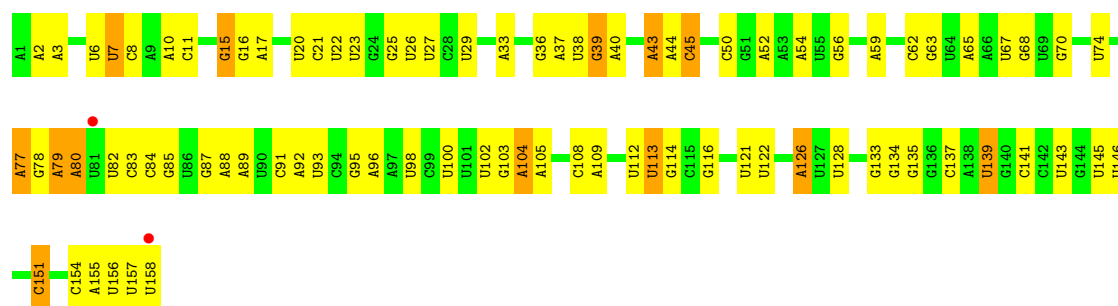
- Molecule 38: *Saccharomyces cerevisiae* genomic DNA containing ITS1, 5.8S rRNA gene, ITS2, 28S rRNA gene, strain Kw97

Chain 4:



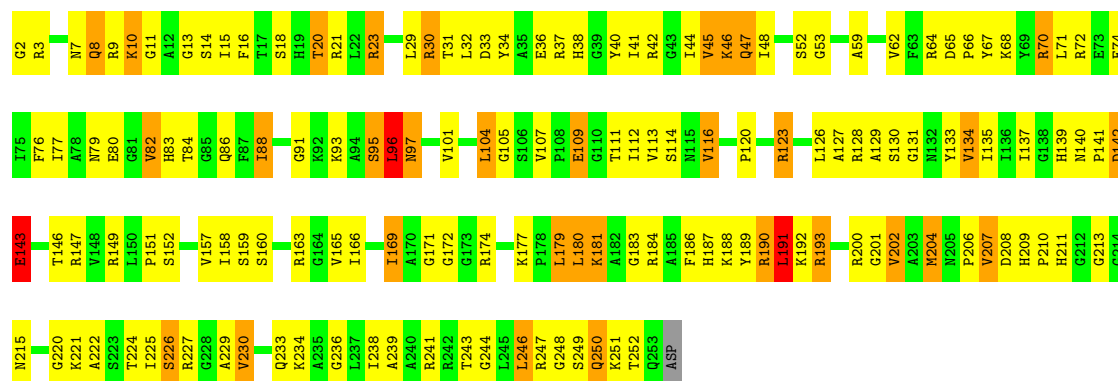
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Chain 8:



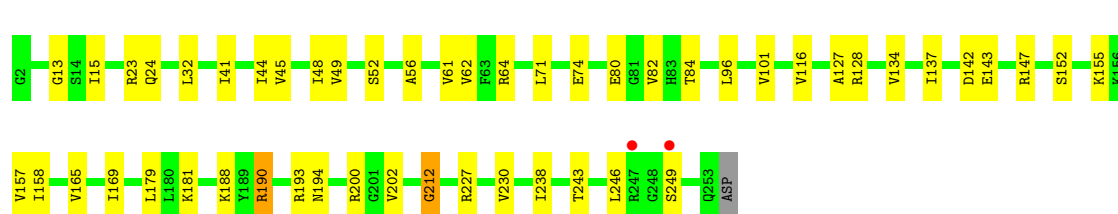
- Molecule 39: 60S ribosomal protein L2-A

Chain L2:



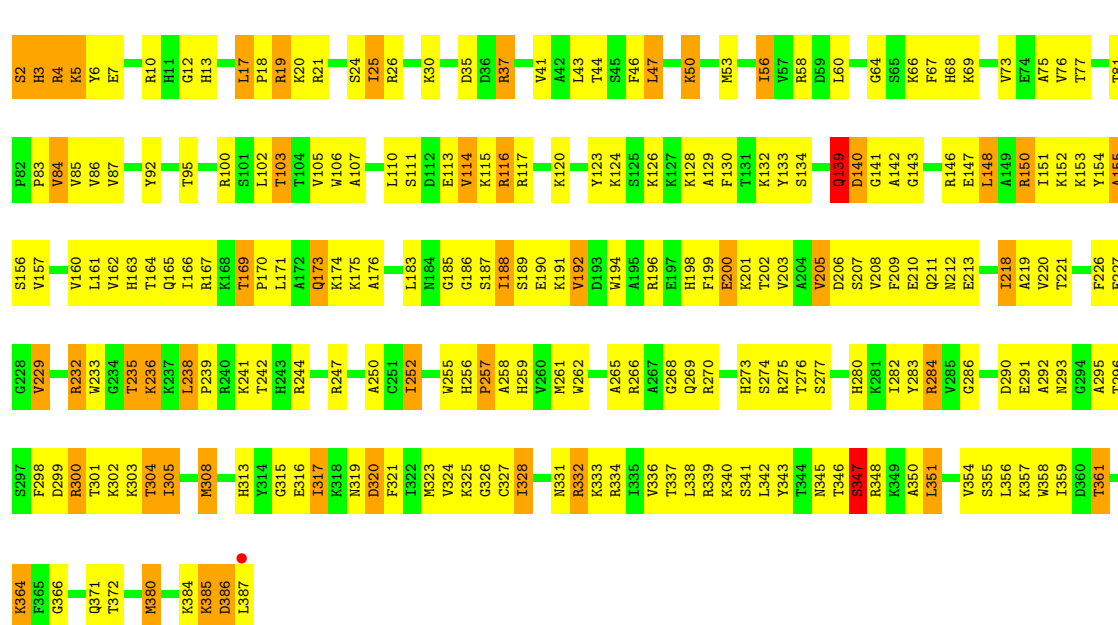
- Molecule 39: 60S ribosomal protein L2-A

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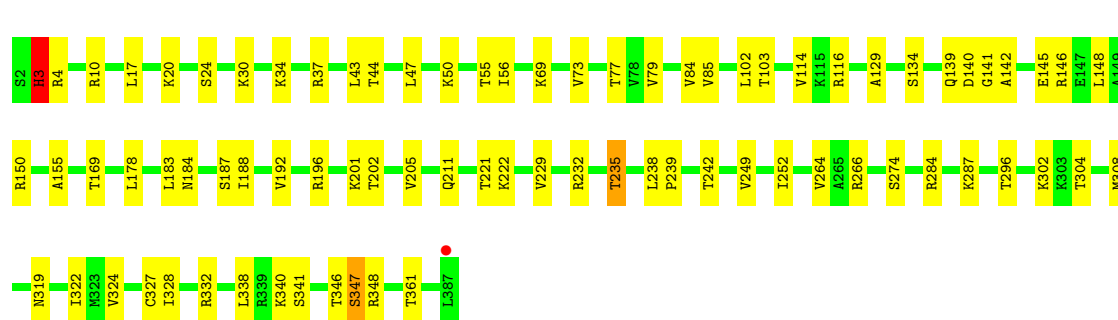
- Molecule 40: 60S ribosomal protein L3

Chain L3:



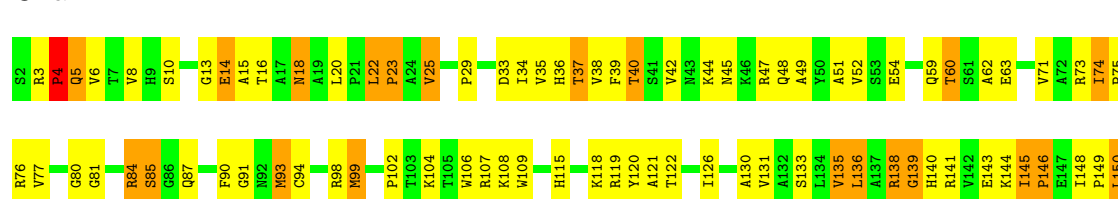
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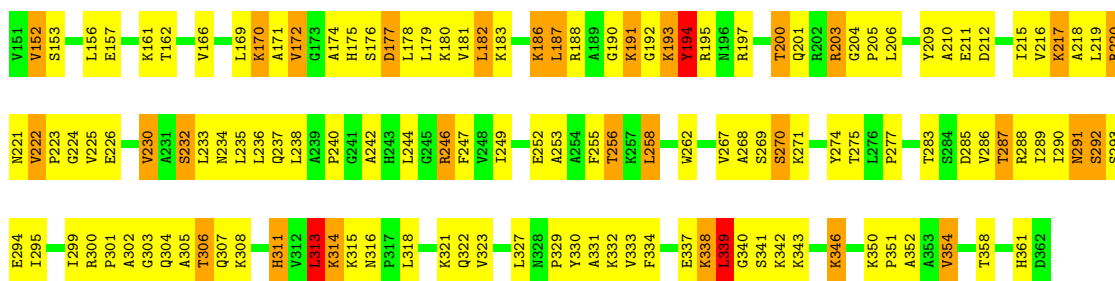


- Molecule 41: 60S ribosomal protein L4-A

Chain L4:

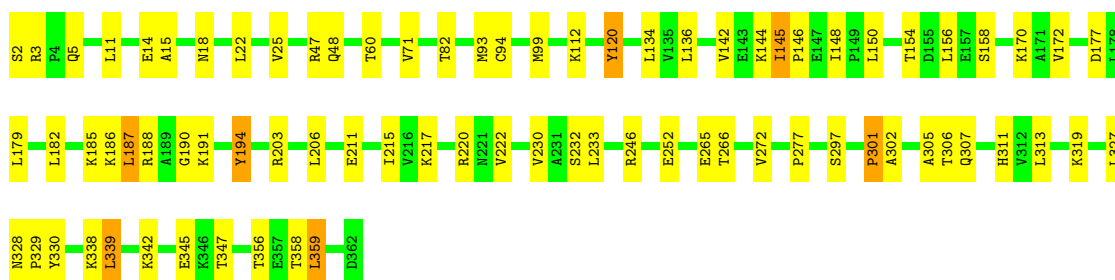






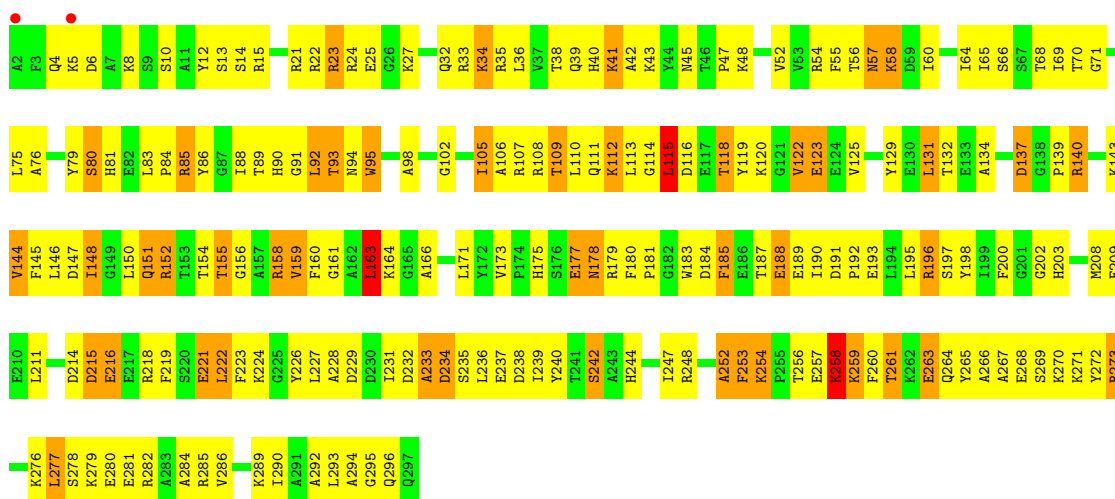
• Molecule 41: 60S ribosomal protein L4-A

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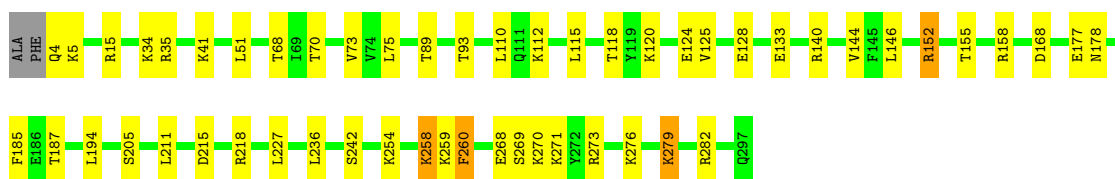
• Molecule 42: 60S ribosomal protein L5

Chain L5:



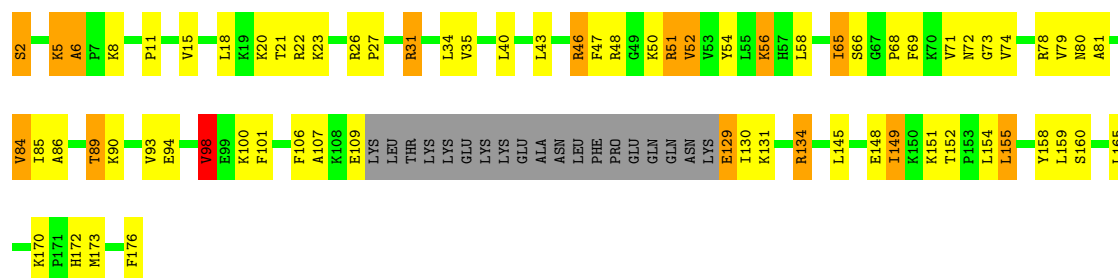
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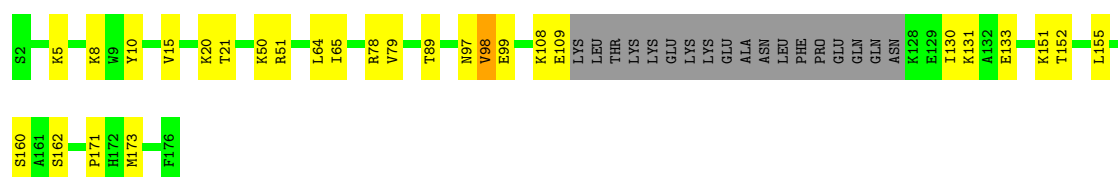
• Molecule 43: 60S ribosomal protein L6-A

Chain L6:



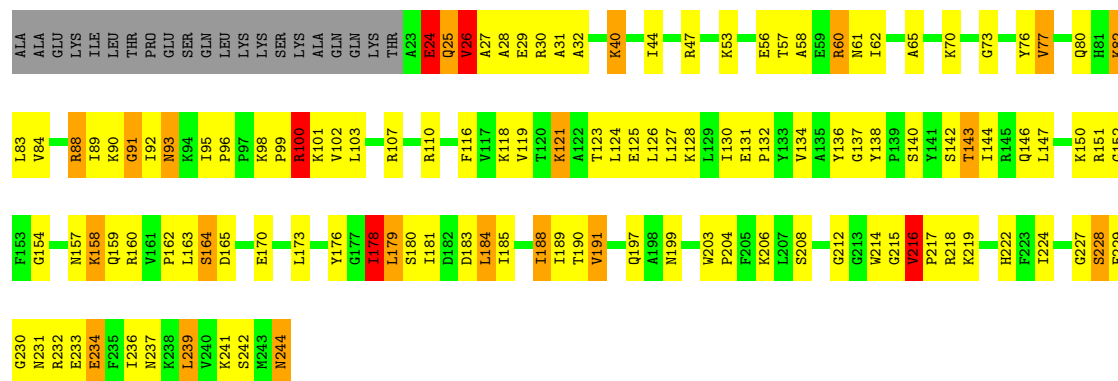
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Chain 16:



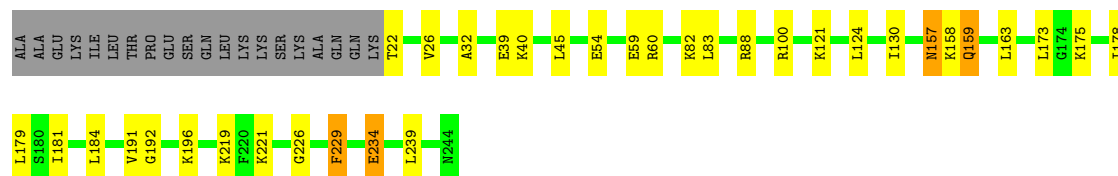
• Molecule 44: 60S ribosomal protein L7-A

Chain 17:



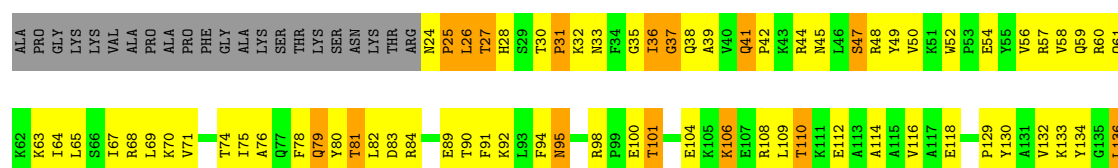
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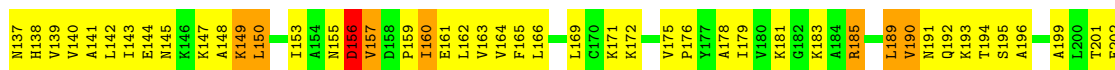
Chain 17:



• Molecule 45: 60S ribosomal protein L8-A

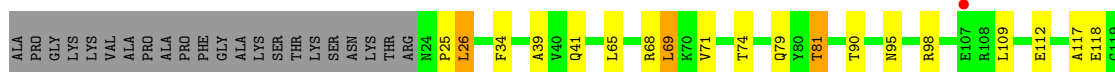
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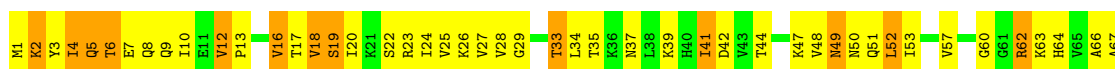
• Molecule 45: 60S ribosomal protein L8-A

Chain 18:



• Molecule 46: 60S ribosomal protein L9-A

Chain L9:



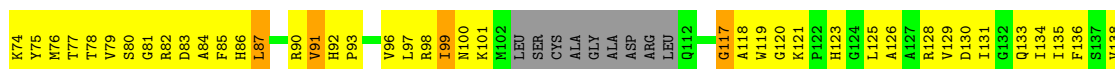
• Molecule 46: 60S ribosomal protein L9-A

Chain 19:



• Molecule 47: 60S ribosomal protein L10

Chain M0:





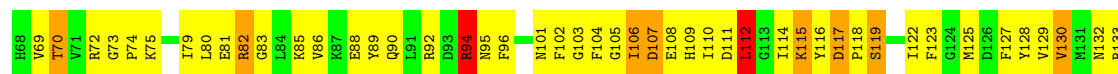
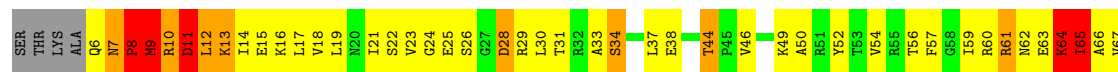
- Molecule 47: 60S ribosomal protein L10

Chain m0:



- Molecule 48: 60S ribosomal protein L11-B

Chain M1:



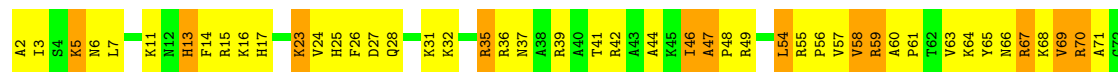
- Molecule 48: 60S ribosomal protein L11-B

Chain m1:



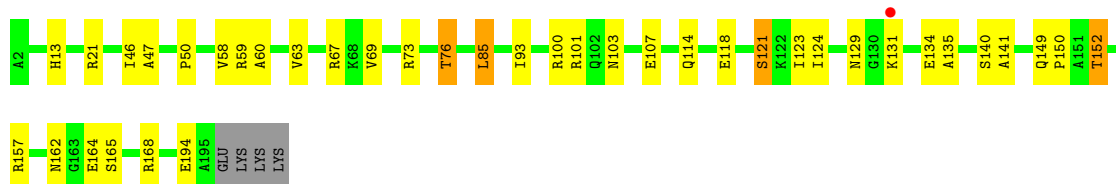
- Molecule 49: 60S ribosomal protein L13-A

Chain M3:



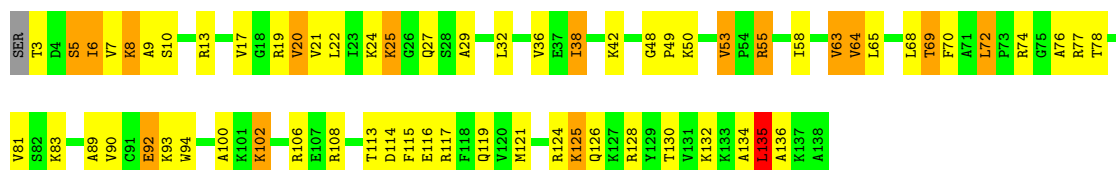
- Molecule 49: 60S ribosomal protein L13-A

Chain m3:



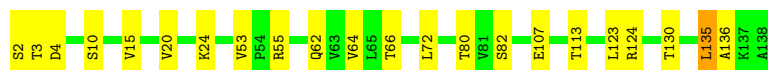
- Molecule 50: 60S ribosomal protein L14-A

Chain M4:



- Molecule 50: 60S ribosomal protein L14-A

Chain m4:



- Molecule 51: 60S ribosomal protein L15-A

Chain M5:



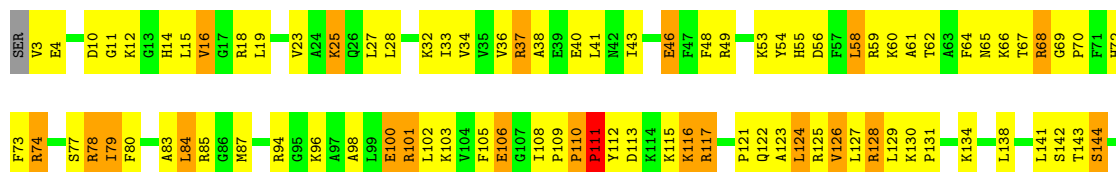
- Molecule 51: 60S ribosomal protein L15-A

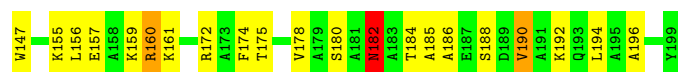
Chain m5:



- Molecule 52: 60S ribosomal protein L16-A

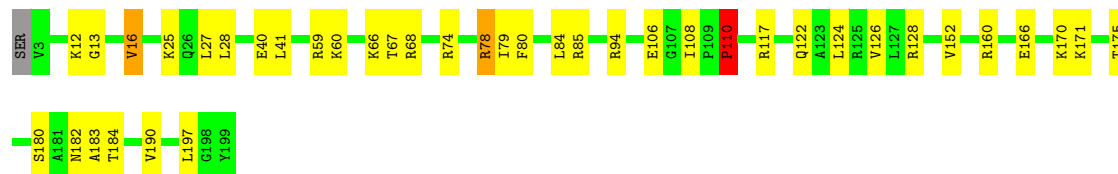
Chain M6:





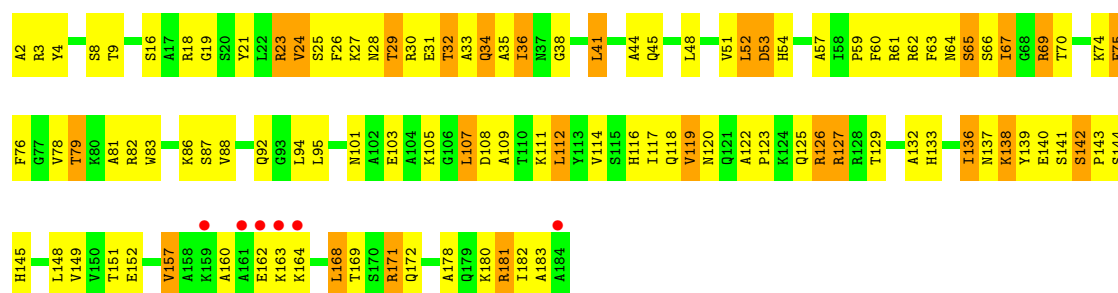
• Molecule 52: 60S ribosomal protein L16-A

Chain m6:



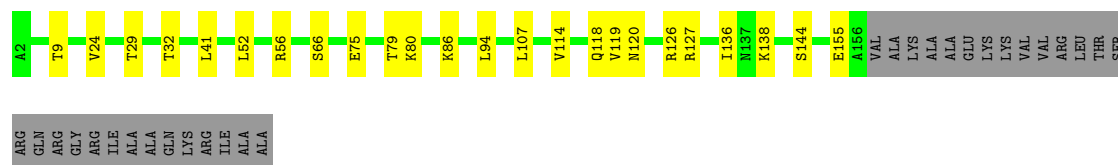
• Molecule 53: 60S ribosomal protein L17-A

Chain M7:



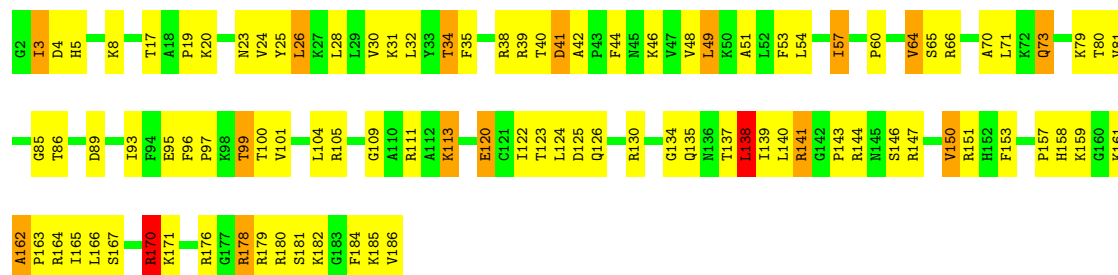
• Molecule 53: 60S ribosomal protein L17-A

Chain m7:



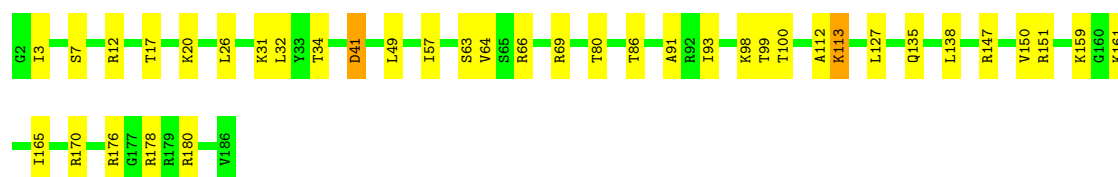
• Molecule 54: 60S ribosomal protein L18-A

Chain M8:



• Molecule 54: 60S ribosomal protein L18-A

Chain m8:



- Molecule 55: 60S ribosomal protein L19-A

Chain M9:



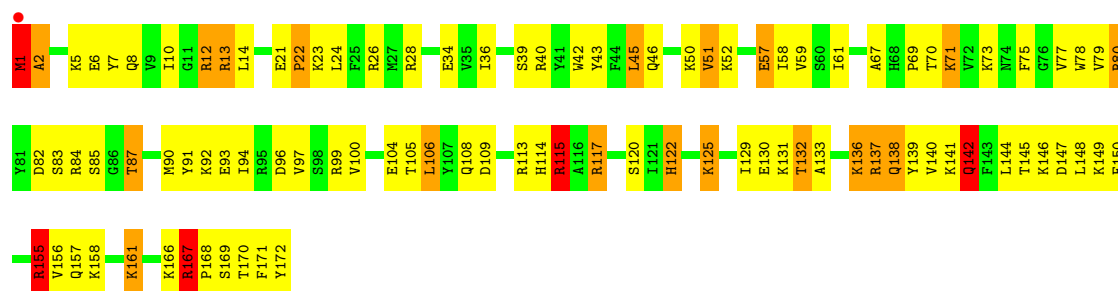
- Molecule 55: 60S ribosomal protein L19-A

Chain m9:



- Molecule 56: 60S ribosomal protein L20-A

Chain N0:



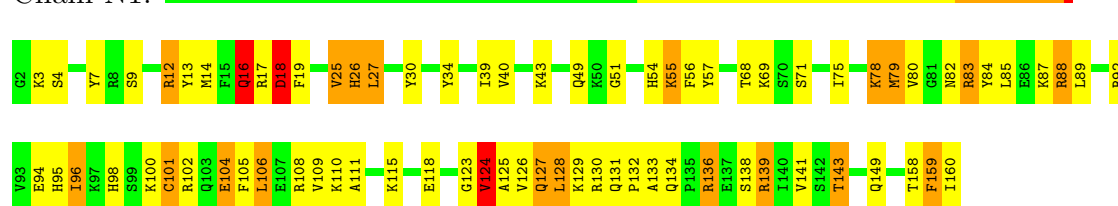
- Molecule 56: 60S ribosomal protein L20-A

Chain n0:



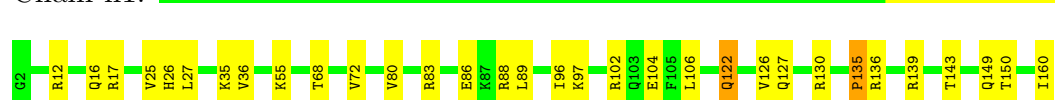
- Molecule 57: 60S ribosomal protein L21-A

Chain N1:



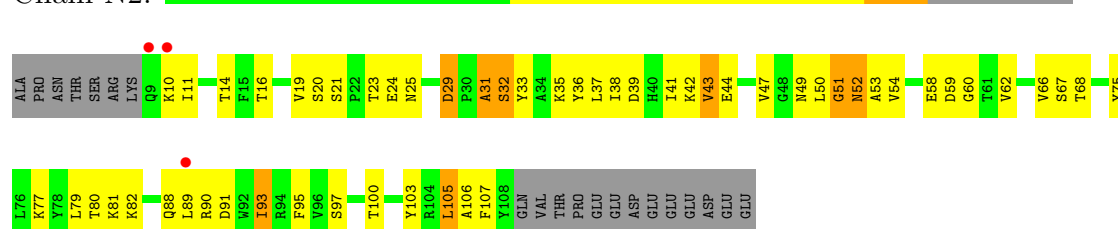
- Molecule 57: 60S ribosomal protein L21-A

Chain n1:



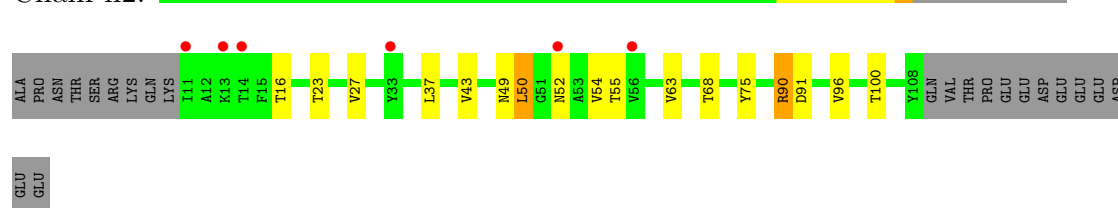
- Molecule 58: 60S ribosomal protein L22-A

Chain N2:



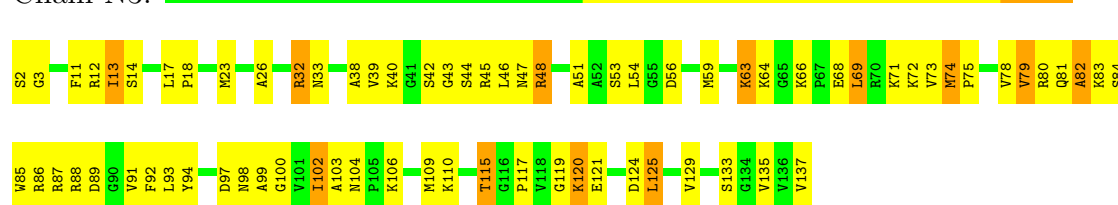
- Molecule 58: 60S ribosomal protein L22-A

Chain n2:



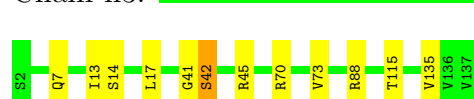
- Molecule 59: 60S ribosomal protein L23-A

Chain N3:



- Molecule 59: 60S ribosomal protein L23-A

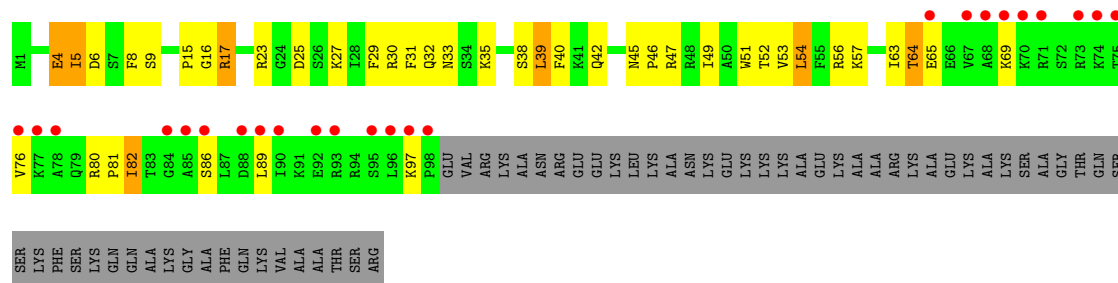
Chain n3:



- Molecule 60: 60S ribosomal protein L24-A

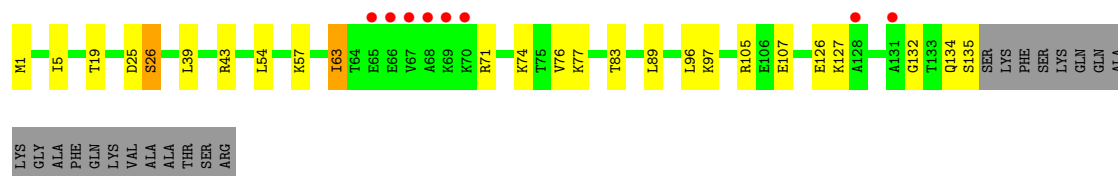
Chain N4:





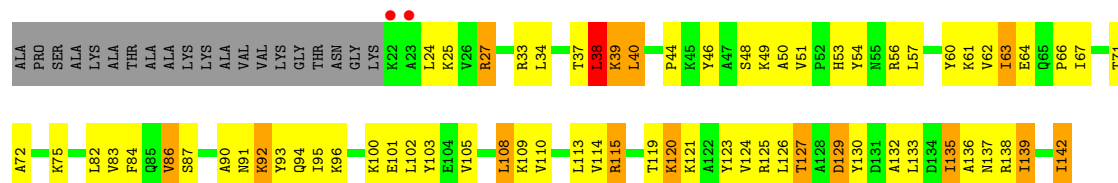
- Molecule 60: 60S ribosomal protein L24-A

Chain n4:



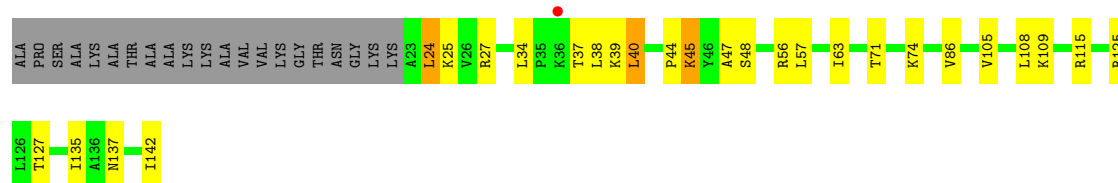
- Molecule 61: 60S ribosomal protein L25

Chain N5:



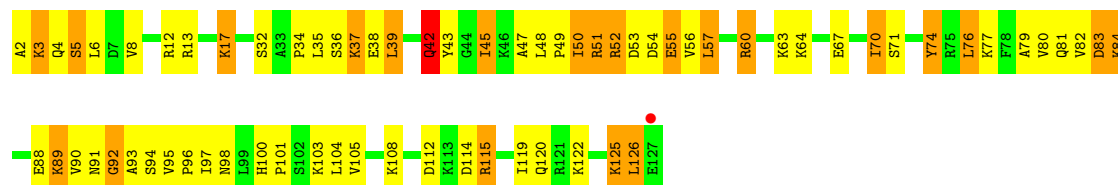
- Molecule 61: 60S ribosomal protein L25

Chain n5:



- Molecule 62: 60S ribosomal protein L26-A

Chain N6:



- Molecule 62: 60S ribosomal protein L26-A

Chain n6:



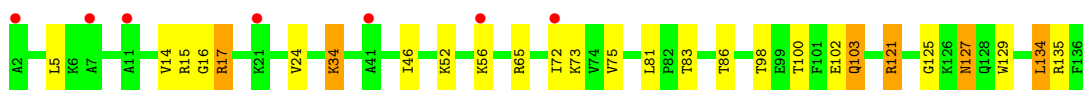
- Molecule 63: 60S ribosomal protein L27-A

Chain N7:



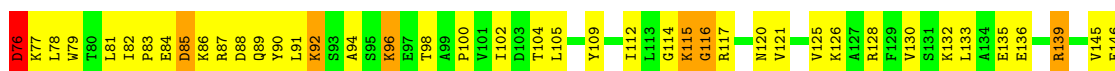
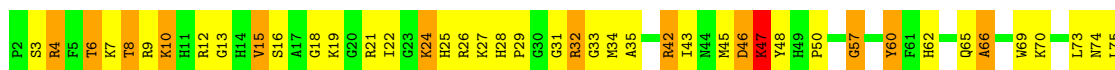
- Molecule 63: 60S ribosomal protein L27-A

Chain n7:



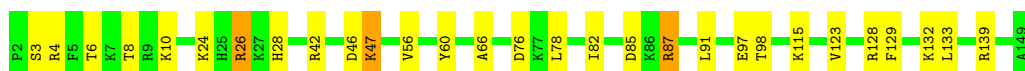
- Molecule 64: 60S ribosomal protein L28

Chain N8:



- Molecule 64: 60S ribosomal protein L28

Chain n8:



- Molecule 65: 60S ribosomal protein L29

Chain N9:



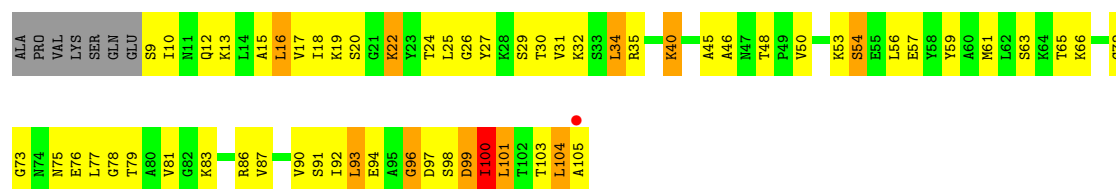
- Molecule 65: 60S ribosomal protein L29

Chain n9:



- Molecule 66: 60S ribosomal protein L30

Chain O0:



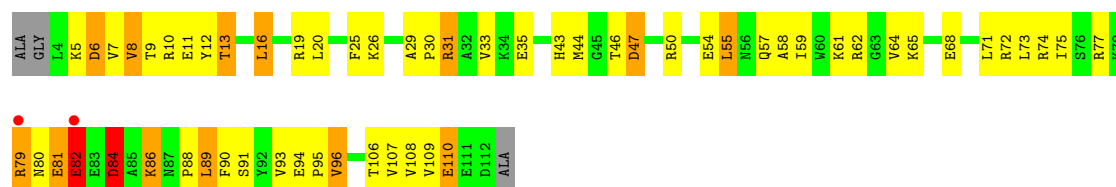
- Molecule 66: 60S ribosomal protein L30

Chain o0:



- Molecule 67: 60S ribosomal protein L31-A

Chain O1:



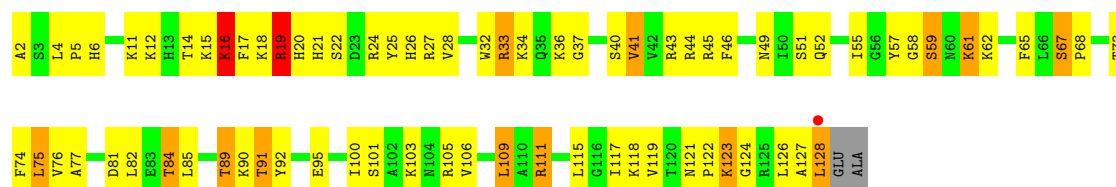
- Molecule 67: 60S ribosomal protein L31-A

Chain o1:



- Molecule 68: 60S ribosomal protein L32

Chain O2:



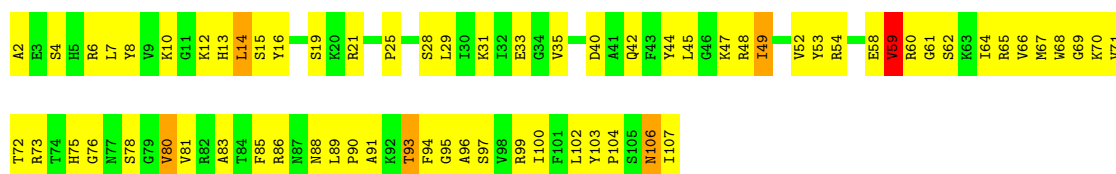
- Molecule 68: 60S ribosomal protein L32

Chain o2:



- Molecule 69: 60S ribosomal protein L33-A

Chain O3:



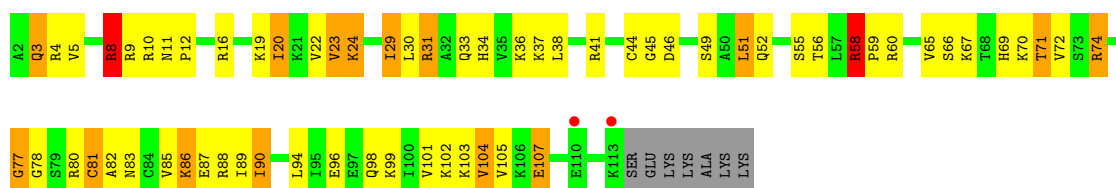
- Molecule 69: 60S ribosomal protein L33-A

Chain o3:



- Molecule 70: 60S ribosomal protein L34-A

Chain O4:



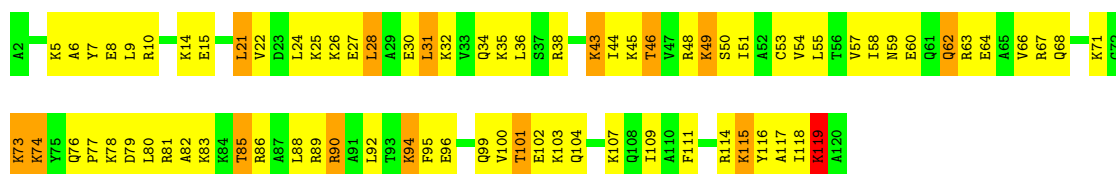
- Molecule 70: 60S ribosomal protein L34-A

Chain o4:



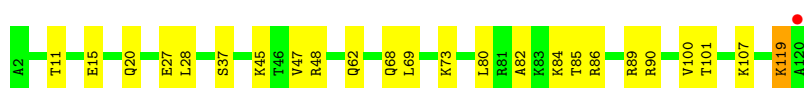
- Molecule 71: 60S ribosomal protein L35-A

Chain O5:



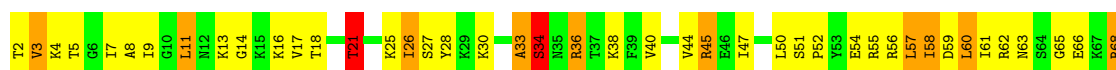
- Molecule 71: 60S ribosomal protein L35-A

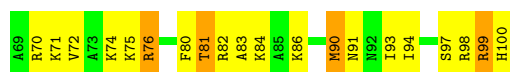
Chain o5:



- Molecule 72: 60S ribosomal protein L36-A

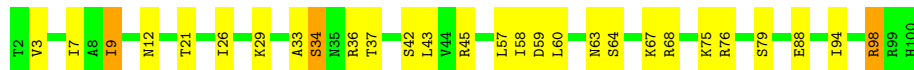
Chain O6:





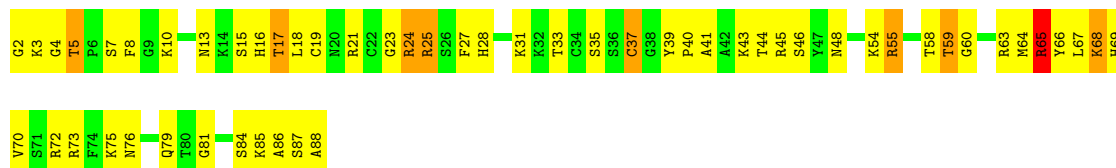
- Molecule 72: 60S ribosomal protein L36-A

Chain o6:



- Molecule 73: 60S ribosomal protein L37-A

Chain O7:



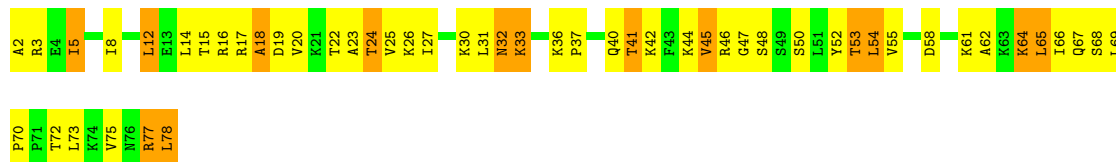
- Molecule 73: 60S ribosomal protein L37-A

Chain o7:



- Molecule 74: 60S ribosomal protein L38

Chain O8:



- Molecule 74: 60S ribosomal protein L38

Chain o8:



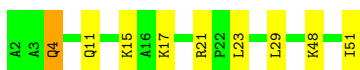
- Molecule 75: 60S ribosomal protein L39

Chain O9:



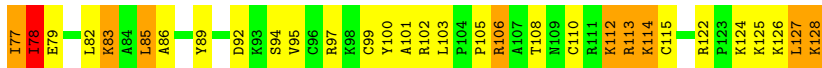
- Molecule 75: 60S ribosomal protein L39

Chain o9:



- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain Q0:



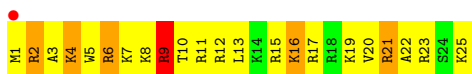
- Molecule 76: Ubiquitin-60S ribosomal protein L40

Chain q0:



- Molecule 77: 60S ribosomal protein L41-A

Chain Q1:



- Molecule 77: 60S ribosomal protein L41-A

Chain q1:



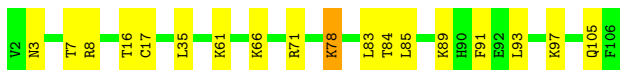
- Molecule 78: 60S ribosomal protein L42-A

Chain Q2:



- Molecule 78: 60S ribosomal protein L42-A

Chain q2:



- Molecule 79: 60S ribosomal protein L43-A

Chain Q3:





TYR PRO GLU ILE GLU ASP LEU VAL ASP ARG ILE GLU ASN PRO GLU LYS TYR ALA ALA ALA PRO ALA ALA THR SER ALA SER GLY ASP ALA ALA PRO ALA GLU GLU ALA ALA GLU GLU GLU GLU SER ASP ASP MET GLY PHE GLY LEU PHE ASP

- Molecule 84: unknown protein chain p1

Chain p1: 

There are no outlier residues recorded for this chain.

- Molecule 85: unknown protein chain p2

Chain p2: 

There are no outlier residues recorded for this chain.



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 435.26Å 287.54Å 304.02Å<br>90.00° 98.97° 90.00°             | Depositor        |
| Resolution (Å)  | 73.99 – 3.00<br>74.59 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (73.99-3.00)<br>99.9 (74.59-3.00)                     | Depositor<br>EDS |
| $R_{merge}$   | 0.29  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.30 (at 3.01Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: dev_1702)                            | Depositor        |
| R, $R_{free}$   | 0.211 , 0.259<br>0.263 , 0.304                              | Depositor<br>DCC |
| $R_{free}$ test set   | 28605 reflections (1.95%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 64.9  | Xtriage          |
| Anisotropy  | 0.199   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 35.2   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Outliers  | 0 of 1468952 reflections                                    | Xtriage          |
| $F_o, F_c$ correlation  | 0.91  | EDS              |
| Total number of atoms   | 411211  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 62.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3KD, ZN, OHX, MG

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

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$      |
| 1   | 2     | 0.71         | 1/41698 (0.0%)  | 1.27        | 275/64972 (0.4%) |
| 1   | 6     | 0.88         | 13/42765 (0.0%) | 1.38        | 436/66634 (0.7%) |
| 2   | S0    | 0.43         | 0/1617          | 0.66        | 0/2215           |
| 2   | s0    | 0.49         | 0/1623          | 0.71        | 0/2222           |
| 3   | S1    | 0.35         | 0/1735          | 0.63        | 1/2335 (0.0%)    |
| 3   | s1    | 0.48         | 0/1748          | 0.66        | 0/2352           |
| 4   | S2    | 0.49         | 0/1665          | 0.67        | 0/2263           |
| 4   | s2    | 0.57         | 0/1665          | 0.75        | 2/2263 (0.1%)    |
| 5   | S3    | 0.48         | 0/1759          | 0.66        | 1/2368 (0.0%)    |
| 5   | s3    | 0.42         | 0/1759          | 0.60        | 0/2368           |
| 6   | S4    | 0.46         | 0/2109          | 0.73        | 1/2839 (0.0%)    |
| 6   | s4    | 0.55         | 0/2109          | 0.78        | 1/2839 (0.0%)    |
| 7   | S5    | 0.36         | 0/1629          | 0.58        | 0/2202           |
| 7   | s5    | 0.44         | 0/1629          | 0.64        | 0/2202           |
| 8   | S6    | 0.44         | 0/1823          | 0.64        | 0/2439           |
| 8   | s6    | 0.54         | 0/1779          | 0.70        | 0/2379           |
| 9   | S7    | 0.42         | 0/1506          | 0.65        | 0/2028           |
| 9   | s7    | 0.45         | 0/1516          | 0.67        | 1/2043 (0.0%)    |
| 10  | S8    | 0.54         | 0/1514          | 0.72        | 1/2021 (0.0%)    |
| 10  | s8    | 0.60         | 0/1514          | 0.76        | 1/2021 (0.0%)    |
| 11  | S9    | 0.47         | 0/1519          | 0.64        | 0/2035           |
| 11  | s9    | 0.55         | 0/1519          | 0.76        | 2/2035 (0.1%)    |
| 12  | C0    | 0.42         | 0/790           | 0.70        | 1/1069 (0.1%)    |
| 12  | c0    | 0.36         | 0/777           | 0.63        | 3/1049 (0.3%)    |
| 13  | C1    | 0.55         | 0/1240          | 0.66        | 0/1675           |
| 13  | c1    | 0.61         | 0/1194          | 0.77        | 0/1610           |
| 14  | C2    | 0.38         | 0/900           | 0.62        | 0/1224           |
| 14  | c2    | 0.28         | 0/900           | 0.56        | 0/1224           |
| 15  | C3    | 0.47         | 0/1215          | 0.68        | 2/1638 (0.1%)    |
| 15  | c3    | 0.56         | 0/1215          | 0.73        | 0/1638           |
| 16  | C4    | 0.36         | 0/901           | 0.63        | 0/1217           |
| 16  | c4    | 0.52         | 0/960           | 0.72        | 0/1290           |

| Mol | Chain | Bond lengths |                  | Bond angles |                    |
|-----|-------|--------------|------------------|-------------|--------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5            |
| 17  | C5    | 0.44         | 0/998            | 0.68        | 0/1341             |
| 17  | c5    | 0.45         | 0/1060           | 0.66        | 0/1426             |
| 18  | C6    | 0.41         | 0/1125           | 0.69        | 2/1510 (0.1%)      |
| 18  | c6    | 0.49         | 0/1131           | 0.69        | 0/1518             |
| 19  | C7    | 0.41         | 0/935            | 0.62        | 0/1254             |
| 19  | c7    | 0.48         | 0/914            | 0.71        | 0/1224             |
| 20  | C8    | 0.42         | 0/1211           | 0.63        | 0/1628             |
| 20  | c8    | 0.49         | 0/1211           | 0.71        | 2/1628 (0.1%)      |
| 21  | C9    | 0.41         | 0/1130           | 0.63        | 0/1517             |
| 21  | c9    | 0.50         | 0/1130           | 0.70        | 2/1517 (0.1%)      |
| 22  | D0    | 0.45         | 0/865            | 0.64        | 0/1169             |
| 22  | d0    | 0.46         | 0/892            | 0.65        | 0/1205             |
| 23  | D1    | 0.44         | 0/693            | 0.62        | 0/935              |
| 23  | d1    | 0.54         | 0/693            | 0.71        | 0/935              |
| 24  | D2    | 0.48         | 0/1038           | 0.73        | 3/1395 (0.2%)      |
| 24  | d2    | 0.59         | 0/1038           | 0.74        | 1/1395 (0.1%)      |
| 25  | D3    | 0.60         | 0/1139           | 0.77        | 1/1518 (0.1%)      |
| 25  | d3    | 0.70         | 0/1139           | 0.89        | 3/1518 (0.2%)      |
| 26  | D4    | 0.44         | 0/1087           | 0.63        | 0/1449             |
| 26  | d4    | 0.53         | 0/1087           | 0.73        | 0/1449             |
| 27  | D5    | 0.39         | 0/571            | 0.68        | 0/768              |
| 27  | d5    | 0.41         | 0/566            | 0.63        | 0/761              |
| 28  | D6    | 0.43         | 0/782            | 0.67        | 0/1047             |
| 28  | d6    | 0.56         | 0/782            | 0.71        | 0/1047             |
| 29  | D7    | 0.42         | 0/620            | 0.66        | 0/838              |
| 29  | d7    | 0.46         | 0/620            | 0.66        | 0/838              |
| 30  | D8    | 0.35         | 0/499            | 0.57        | 0/670              |
| 30  | d8    | 0.44         | 0/499            | 0.64        | 0/670              |
| 31  | D9    | 0.50         | 0/452            | 0.70        | 1/600 (0.2%)       |
| 31  | d9    | 0.50         | 0/452            | 0.64        | 0/600              |
| 32  | E0    | 0.46         | 0/483            | 0.63        | 0/643              |
| 33  | E1    | 0.42         | 0/577            | 0.78        | 0/770              |
| 33  | e1    | 0.39         | 0/619            | 0.72        | 0/822              |
| 34  | SR    | 0.37         | 0/2494           | 0.57        | 0/3393             |
| 34  | sR    | 0.38         | 0/2495           | 0.56        | 0/3395             |
| 35  | SM    | 0.48         | 0/1113           | 0.70        | 2/1502 (0.1%)      |
| 36  | 1     | 1.16         | 153/75394 (0.2%) | 1.66        | 1837/117545 (1.6%) |
| 36  | 5     | 1.20         | 178/75414 (0.2%) | 1.67        | 1863/117575 (1.6%) |
| 37  | 3     | 0.95         | 2/2883 (0.1%)    | 1.47        | 39/4491 (0.9%)     |
| 37  | 7     | 1.16         | 5/2883 (0.2%)    | 1.62        | 57/4491 (1.3%)     |
| 38  | 4     | 1.13         | 5/3746 (0.1%)    | 1.66        | 86/5832 (1.5%)     |
| 38  | 8     | 0.98         | 2/3746 (0.1%)    | 1.48        | 42/5832 (0.7%)     |
| 39  | L2    | 0.74         | 0/1948           | 0.84        | 3/2617 (0.1%)      |

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 39  | l2    | 0.71         | 0/1946        | 0.86        | 2/2614 (0.1%) |
| 40  | L3    | 0.74         | 1/3146 (0.0%) | 0.82        | 1/4228 (0.0%) |
| 40  | l3    | 0.88         | 1/3146 (0.0%) | 0.89        | 2/4228 (0.0%) |
| 41  | L4    | 0.84         | 1/2800 (0.0%) | 0.94        | 7/3790 (0.2%) |
| 41  | l4    | 0.74         | 1/2800 (0.0%) | 0.90        | 6/3790 (0.2%) |
| 42  | L5    | 0.57         | 0/2425        | 0.69        | 1/3271 (0.0%) |
| 42  | l5    | 0.73         | 0/2408        | 0.82        | 1/3248 (0.0%) |
| 43  | L6    | 0.76         | 0/1260        | 0.84        | 0/1694        |
| 43  | l6    | 0.78         | 0/1269        | 0.84        | 1/1705 (0.1%) |
| 44  | L7    | 0.78         | 1/1821 (0.1%) | 0.90        | 2/2451 (0.1%) |
| 44  | l7    | 0.85         | 1/1828 (0.1%) | 0.90        | 4/2461 (0.2%) |
| 45  | L8    | 0.55         | 0/1836        | 0.70        | 1/2481 (0.0%) |
| 45  | l8    | 0.51         | 0/1795        | 0.65        | 1/2429 (0.0%) |
| 46  | L9    | 0.65         | 0/1539        | 0.77        | 1/2073 (0.0%) |
| 46  | l9    | 0.77         | 0/1539        | 0.85        | 0/2073        |
| 47  | M0    | 0.71         | 0/1741        | 0.84        | 3/2335 (0.1%) |
| 47  | m0    | 0.75         | 0/1758        | 0.87        | 2/2358 (0.1%) |
| 48  | M1    | 0.54         | 0/1374        | 0.73        | 1/1842 (0.1%) |
| 48  | m1    | 0.65         | 0/1374        | 0.82        | 2/1842 (0.1%) |
| 49  | M3    | 0.75         | 0/1568        | 0.86        | 0/2106        |
| 49  | m3    | 0.69         | 0/1573        | 0.85        | 3/2113 (0.1%) |
| 50  | M4    | 0.73         | 0/1068        | 0.80        | 1/1438 (0.1%) |
| 50  | m4    | 0.82         | 0/1074        | 0.85        | 0/1446        |
| 51  | M5    | 0.77         | 0/1757        | 0.85        | 0/2354        |
| 51  | m5    | 0.66         | 0/1757        | 0.79        | 0/2354        |
| 52  | M6    | 0.86         | 1/1585 (0.1%) | 0.92        | 3/2128 (0.1%) |
| 52  | m6    | 1.02         | 5/1585 (0.3%) | 0.98        | 7/2128 (0.3%) |
| 53  | M7    | 0.80         | 0/1443        | 0.85        | 2/1944 (0.1%) |
| 53  | m7    | 0.89         | 0/1250        | 0.89        | 0/1683        |
| 54  | M8    | 0.79         | 0/1465        | 0.92        | 3/1965 (0.2%) |
| 54  | m8    | 0.73         | 0/1465        | 0.95        | 2/1965 (0.1%) |
| 55  | M9    | 0.57         | 0/1538        | 0.69        | 0/2050        |
| 55  | m9    | 0.61         | 0/1538        | 0.70        | 0/2050        |
| 56  | N0    | 0.78         | 0/1481        | 0.87        | 4/1990 (0.2%) |
| 56  | n0    | 0.87         | 0/1481        | 0.91        | 2/1990 (0.1%) |
| 57  | N1    | 0.78         | 0/1300        | 0.82        | 0/1743        |
| 57  | n1    | 0.85         | 1/1300 (0.1%) | 0.86        | 1/1743 (0.1%) |
| 58  | N2    | 0.42         | 0/812         | 0.62        | 0/1099        |
| 58  | n2    | 0.51         | 0/794         | 0.65        | 0/1076        |
| 59  | N3    | 0.70         | 0/1018        | 0.81        | 0/1369        |
| 59  | n3    | 0.87         | 0/1018        | 0.98        | 1/1369 (0.1%) |
| 60  | N4    | 0.56         | 0/712         | 0.68        | 0/958         |
| 60  | n4    | 0.69         | 0/1052        | 0.75        | 0/1398        |

| Mol | Chain | Bond lengths |                   | Bond angles |                    |
|-----|-------|--------------|-------------------|-------------|--------------------|
|     |       | RMSZ         | # Z  >5           | RMSZ        | # Z  >5            |
| 61  | N5    | 0.63         | 0/979             | 0.80        | 2/1321 (0.2%)      |
| 61  | n5    | 0.65         | 0/974             | 0.77        | 0/1314             |
| 62  | N6    | 0.68         | 0/1004            | 0.90        | 1/1341 (0.1%)      |
| 62  | n6    | 0.71         | 1/1004 (0.1%)     | 0.84        | 0/1341             |
| 63  | N7    | 0.52         | 0/1118            | 0.66        | 0/1497             |
| 63  | n7    | 0.46         | 0/1118            | 0.63        | 0/1497             |
| 64  | N8    | 0.82         | 0/1204            | 0.92        | 2/1612 (0.1%)      |
| 64  | n8    | 0.79         | 0/1204            | 0.90        | 0/1612             |
| 65  | N9    | 0.67         | 0/473             | 0.83        | 2/629 (0.3%)       |
| 65  | n9    | 0.80         | 0/473             | 0.97        | 0/629              |
| 66  | O0    | 0.48         | 0/751             | 0.66        | 0/1008             |
| 66  | o0    | 0.49         | 0/775             | 0.65        | 0/1040             |
| 67  | O1    | 0.60         | 0/890             | 0.72        | 0/1196             |
| 67  | o1    | 0.76         | 0/897             | 0.86        | 0/1205             |
| 68  | O2    | 0.85         | 0/1041            | 0.89        | 2/1394 (0.1%)      |
| 68  | o2    | 0.82         | 0/1041            | 0.94        | 2/1394 (0.1%)      |
| 69  | O3    | 0.95         | 0/868             | 0.91        | 1/1168 (0.1%)      |
| 69  | o3    | 0.92         | 0/868             | 0.84        | 0/1168             |
| 70  | O4    | 0.58         | 0/890             | 0.82        | 4/1189 (0.3%)      |
| 70  | o4    | 0.59         | 0/890             | 0.78        | 0/1189             |
| 71  | O5    | 0.70         | 0/978             | 0.81        | 1/1301 (0.1%)      |
| 71  | o5    | 0.59         | 0/974             | 0.72        | 0/1297             |
| 72  | O6    | 0.64         | 0/778             | 0.79        | 0/1034             |
| 72  | o6    | 0.54         | 0/777             | 0.73        | 0/1033             |
| 73  | O7    | 0.78         | 0/696             | 0.90        | 1/923 (0.1%)       |
| 73  | o7    | 0.75         | 0/696             | 0.85        | 1/923 (0.1%)       |
| 74  | O8    | 0.51         | 0/618             | 0.64        | 0/826              |
| 74  | o8    | 0.42         | 0/614             | 0.61        | 0/822              |
| 75  | O9    | 0.83         | 1/443 (0.2%)      | 0.90        | 0/588              |
| 75  | o9    | 0.76         | 0/443             | 0.83        | 0/588              |
| 76  | Q0    | 0.73         | 0/423             | 0.84        | 0/562              |
| 76  | q0    | 0.95         | 0/423             | 1.03        | 1/562 (0.2%)       |
| 77  | Q1    | 0.72         | 0/234             | 0.96        | 1/300 (0.3%)       |
| 77  | q1    | 0.82         | 0/234             | 1.05        | 2/300 (0.7%)       |
| 78  | Q2    | 0.93         | 1/860 (0.1%)      | 0.85        | 1/1136 (0.1%)      |
| 78  | q2    | 0.82         | 1/860 (0.1%)      | 0.83        | 0/1136             |
| 79  | Q3    | 0.74         | 0/701             | 0.85        | 0/934              |
| 79  | q3    | 0.72         | 0/701             | 0.81        | 0/934              |
| 80  | e0    | 0.56         | 0/499             | 0.74        | 0/665              |
| 81  | sM    | 0.50         | 0/684             | 0.69        | 1/925 (0.1%)       |
| 83  | p0    | 0.46         | 0/1092            | 0.61        | 0/1474             |
| All | All   | 0.90         | 376/430075 (0.1%) | 1.30        | 4764/631366 (0.8%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 7   | s5    | 0                   | 2                   |
| 9   | S7    | 0                   | 1                   |
| 10  | S8    | 0                   | 1                   |
| 16  | C4    | 0                   | 2                   |
| 17  | c5    | 0                   | 1                   |
| 18  | c6    | 0                   | 1                   |
| 19  | C7    | 0                   | 2                   |
| 22  | d0    | 0                   | 1                   |
| 27  | D5    | 0                   | 2                   |
| 28  | D6    | 0                   | 1                   |
| 33  | E1    | 0                   | 1                   |
| 39  | l2    | 0                   | 1                   |
| 42  | l5    | 0                   | 2                   |
| 43  | L6    | 0                   | 1                   |
| 43  | l6    | 0                   | 1                   |
| 44  | l7    | 0                   | 2                   |
| 45  | L8    | 0                   | 1                   |
| 48  | M1    | 0                   | 2                   |
| 51  | M5    | 0                   | 1                   |
| 52  | M6    | 0                   | 1                   |
| 52  | m6    | 0                   | 1                   |
| 53  | M7    | 0                   | 1                   |
| 55  | m9    | 0                   | 1                   |
| 56  | N0    | 0                   | 2                   |
| 56  | n0    | 0                   | 2                   |
| 57  | N1    | 0                   | 1                   |
| 62  | n6    | 0                   | 1                   |
| 64  | N8    | 0                   | 1                   |
| 64  | n8    | 0                   | 2                   |
| 65  | N9    | 0                   | 1                   |
| 67  | O1    | 0                   | 1                   |
| 67  | o1    | 0                   | 2                   |
| All | All   | 0                   | 43                  |

The worst 5 of 376 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 78  | Q2    | 17   | CYS  | CB-SG | 15.91  | 2.09        | 1.82     |
| 36  | 5     | 1152 | G    | N9-C4 | -12.55 | 1.27        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 78  | q2    | 17   | CYS  | CB-SG | 11.87 | 2.02        | 1.82     |
| 36  | 1     | 3181 | C    | N3-C4 | -9.25 | 1.27        | 1.33     |
| 36  | 5     | 2138 | A    | N7-C5 | -8.87 | 1.33        | 1.39     |

The worst 5 of 4764 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 36  | 5     | 1152 | G    | N3-C4-C5  | 24.25  | 140.73      | 128.60   |
| 36  | 5     | 1152 | G    | N3-C4-N9  | -22.33 | 112.60      | 126.00   |
| 36  | 5     | 1152 | G    | C2-N3-C4  | -20.90 | 101.45      | 111.90   |
| 36  | 1     | 2945 | G    | O5'-P-OP2 | -17.25 | 90.00       | 110.70   |
| 36  | 1     | 1308 | A    | O5'-P-OP2 | -17.00 | 90.30       | 110.70   |

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 16  | C4    | 123 | SER  | Peptide |
| 16  | C4    | 124 | ASP  | Peptide |
| 19  | C7    | 22  | PRO  | Peptide |
| 9   | S7    | 131 | PHE  | Peptide |
| 10  | S8    | 147 | ALA  | Peptide |

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 2     | 37283 | 0        | 18757    | 928     | 0            |
| 1   | 6     | 38238 | 0        | 19240    | 830     | 0            |
| 2   | S0    | 1577  | 0        | 1567     | 168     | 0            |
| 2   | s0    | 1583  | 0        | 1578     | 0       | 0            |
| 3   | S1    | 1709  | 0        | 1784     | 163     | 0            |
| 3   | s1    | 1722  | 0        | 1793     | 0       | 0            |
| 4   | S2    | 1635  | 0        | 1723     | 128     | 0            |
| 4   | s2    | 1635  | 0        | 1723     | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | S3    | 1734  | 0        | 1817     | 125     | 0            |
| 5   | s3    | 1734  | 0        | 1817     | 0       | 0            |
| 6   | S4    | 2068  | 0        | 2154     | 150     | 0            |
| 6   | s4    | 2068  | 0        | 2154     | 0       | 0            |
| 7   | S5    | 1609  | 0        | 1675     | 151     | 0            |
| 7   | s5    | 1609  | 0        | 1675     | 0       | 0            |
| 8   | S6    | 1799  | 0        | 1879     | 118     | 0            |
| 8   | s6    | 1755  | 0        | 1846     | 0       | 0            |
| 9   | S7    | 1481  | 0        | 1572     | 117     | 0            |
| 9   | s7    | 1491  | 0        | 1578     | 0       | 0            |
| 10  | S8    | 1489  | 0        | 1525     | 117     | 0            |
| 10  | s8    | 1489  | 0        | 1525     | 0       | 0            |
| 11  | S9    | 1494  | 0        | 1573     | 146     | 0            |
| 11  | s9    | 1494  | 0        | 1573     | 0       | 0            |
| 12  | C0    | 773   | 0        | 729      | 62      | 0            |
| 12  | c0    | 762   | 0        | 699      | 0       | 0            |
| 13  | C1    | 1214  | 0        | 1259     | 89      | 0            |
| 13  | c1    | 1168  | 0        | 1231     | 0       | 0            |
| 14  | C2    | 892   | 0        | 891      | 54      | 0            |
| 14  | c2    | 892   | 0        | 891      | 0       | 0            |
| 15  | C3    | 1192  | 0        | 1255     | 93      | 0            |
| 15  | c3    | 1192  | 0        | 1255     | 0       | 0            |
| 16  | C4    | 891   | 0        | 883      | 97      | 0            |
| 16  | c4    | 949   | 0        | 985      | 0       | 0            |
| 17  | C5    | 977   | 0        | 1002     | 97      | 0            |
| 17  | c5    | 1039  | 0        | 1050     | 0       | 0            |
| 18  | C6    | 1105  | 0        | 1166     | 116     | 0            |
| 18  | c6    | 1111  | 0        | 1171     | 0       | 0            |
| 19  | C7    | 926   | 0        | 930      | 82      | 0            |
| 19  | c7    | 906   | 0        | 909      | 0       | 0            |
| 20  | C8    | 1192  | 0        | 1222     | 111     | 0            |
| 20  | c8    | 1192  | 0        | 1222     | 0       | 0            |
| 21  | C9    | 1112  | 0        | 1124     | 87      | 0            |
| 21  | c9    | 1112  | 0        | 1124     | 0       | 0            |
| 22  | D0    | 855   | 0        | 917      | 83      | 0            |
| 22  | d0    | 882   | 0        | 939      | 0       | 0            |
| 23  | D1    | 684   | 0        | 672      | 57      | 0            |
| 23  | d1    | 684   | 0        | 672      | 0       | 0            |
| 24  | D2    | 1021  | 0        | 1060     | 74      | 0            |
| 24  | d2    | 1021  | 0        | 1060     | 0       | 0            |
| 25  | D3    | 1121  | 0        | 1196     | 89      | 0            |
| 25  | d3    | 1121  | 0        | 1196     | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 26  | D4    | 1073  | 0        | 1132     | 87      | 0            |
| 26  | d4    | 1073  | 0        | 1132     | 0       | 0            |
| 27  | D5    | 563   | 0        | 603      | 64      | 0            |
| 27  | d5    | 558   | 0        | 598      | 0       | 0            |
| 28  | D6    | 769   | 0        | 814      | 94      | 0            |
| 28  | d6    | 769   | 0        | 814      | 0       | 0            |
| 29  | D7    | 610   | 0        | 630      | 39      | 0            |
| 29  | d7    | 610   | 0        | 631      | 0       | 0            |
| 30  | D8    | 497   | 0        | 535      | 40      | 0            |
| 30  | d8    | 497   | 0        | 535      | 0       | 0            |
| 31  | D9    | 442   | 0        | 428      | 25      | 0            |
| 31  | d9    | 442   | 0        | 428      | 0       | 0            |
| 32  | E0    | 475   | 0        | 525      | 37      | 0            |
| 33  | E1    | 566   | 0        | 601      | 58      | 0            |
| 33  | e1    | 608   | 0        | 657      | 0       | 0            |
| 34  | SR    | 2441  | 0        | 2397     | 155     | 0            |
| 34  | sR    | 2442  | 0        | 2392     | 0       | 0            |
| 35  | SM    | 1104  | 0        | 996      | 74      | 0            |
| 36  | 1     | 67355 | 0        | 33845    | 1266    | 0            |
| 36  | 5     | 67376 | 0        | 33851    | 1268    | 0            |
| 37  | 3     | 2579  | 0        | 1304     | 51      | 0            |
| 37  | 7     | 2579  | 0        | 1303     | 52      | 0            |
| 38  | 4     | 3353  | 0        | 1695     | 77      | 0            |
| 38  | 8     | 3353  | 0        | 1695     | 71      | 0            |
| 39  | L2    | 1914  | 0        | 1981     | 166     | 0            |
| 39  | l2    | 1912  | 0        | 1976     | 0       | 0            |
| 40  | L3    | 3075  | 0        | 3142     | 242     | 0            |
| 40  | l3    | 3075  | 0        | 3142     | 0       | 0            |
| 41  | L4    | 2748  | 0        | 2859     | 206     | 0            |
| 41  | l4    | 2748  | 0        | 2859     | 0       | 0            |
| 42  | L5    | 2375  | 0        | 2325     | 210     | 0            |
| 42  | l5    | 2359  | 0        | 2311     | 0       | 0            |
| 43  | L6    | 1239  | 0        | 1326     | 62      | 0            |
| 43  | l6    | 1248  | 0        | 1339     | 0       | 0            |
| 44  | L7    | 1784  | 0        | 1862     | 124     | 0            |
| 44  | l7    | 1791  | 0        | 1869     | 0       | 0            |
| 45  | L8    | 1804  | 0        | 1877     | 129     | 0            |
| 45  | l8    | 1763  | 0        | 1819     | 0       | 0            |
| 46  | L9    | 1518  | 0        | 1587     | 121     | 0            |
| 46  | l9    | 1518  | 0        | 1587     | 0       | 0            |
| 47  | M0    | 1705  | 0        | 1736     | 127     | 0            |
| 47  | m0    | 1722  | 0        | 1755     | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 48  | M1    | 1353  | 0        | 1383     | 95      | 0            |
| 48  | m1    | 1353  | 0        | 1383     | 0       | 0            |
| 49  | M3    | 1543  | 0        | 1608     | 136     | 0            |
| 49  | m3    | 1548  | 0        | 1613     | 0       | 0            |
| 50  | M4    | 1053  | 0        | 1149     | 63      | 0            |
| 50  | m4    | 1059  | 0        | 1154     | 0       | 0            |
| 51  | M5    | 1720  | 0        | 1779     | 130     | 0            |
| 51  | m5    | 1720  | 0        | 1779     | 0       | 0            |
| 52  | M6    | 1555  | 0        | 1659     | 109     | 0            |
| 52  | m6    | 1555  | 0        | 1659     | 0       | 0            |
| 53  | M7    | 1420  | 0        | 1437     | 115     | 0            |
| 53  | m7    | 1227  | 0        | 1236     | 0       | 0            |
| 54  | M8    | 1441  | 0        | 1543     | 92      | 0            |
| 54  | m8    | 1441  | 0        | 1543     | 0       | 0            |
| 55  | M9    | 1521  | 0        | 1617     | 99      | 0            |
| 55  | m9    | 1521  | 0        | 1617     | 0       | 0            |
| 56  | N0    | 1445  | 0        | 1487     | 94      | 0            |
| 56  | n0    | 1445  | 0        | 1487     | 0       | 0            |
| 57  | N1    | 1276  | 0        | 1323     | 84      | 0            |
| 57  | n1    | 1276  | 0        | 1323     | 0       | 0            |
| 58  | N2    | 796   | 0        | 812      | 38      | 0            |
| 58  | n2    | 778   | 0        | 791      | 0       | 0            |
| 59  | N3    | 1003  | 0        | 1048     | 70      | 0            |
| 59  | n3    | 1003  | 0        | 1048     | 0       | 0            |
| 60  | N4    | 699   | 0        | 640      | 27      | 0            |
| 60  | n4    | 1038  | 0        | 1071     | 0       | 0            |
| 61  | N5    | 964   | 0        | 1025     | 63      | 0            |
| 61  | n5    | 959   | 0        | 1023     | 0       | 0            |
| 62  | N6    | 993   | 0        | 1081     | 65      | 0            |
| 62  | n6    | 993   | 0        | 1081     | 0       | 0            |
| 63  | N7    | 1092  | 0        | 1155     | 86      | 0            |
| 63  | n7    | 1092  | 0        | 1155     | 0       | 0            |
| 64  | N8    | 1173  | 0        | 1214     | 86      | 0            |
| 64  | n8    | 1173  | 0        | 1215     | 0       | 0            |
| 65  | N9    | 462   | 0        | 491      | 35      | 0            |
| 65  | n9    | 462   | 0        | 491      | 0       | 0            |
| 66  | O0    | 743   | 0        | 797      | 53      | 0            |
| 66  | o0    | 767   | 0        | 816      | 0       | 0            |
| 67  | O1    | 876   | 0        | 912      | 52      | 0            |
| 67  | o1    | 883   | 0        | 918      | 0       | 0            |
| 68  | O2    | 1020  | 0        | 1090     | 82      | 0            |
| 68  | o2    | 1020  | 0        | 1090     | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 69  | O3    | 850   | 0        | 880      | 67      | 0            |
| 69  | o3    | 850   | 0        | 880      | 0       | 0            |
| 70  | O4    | 880   | 0        | 945      | 72      | 0            |
| 70  | o4    | 880   | 0        | 945      | 0       | 0            |
| 71  | O5    | 969   | 0        | 1078     | 75      | 0            |
| 71  | o5    | 965   | 0        | 1067     | 0       | 0            |
| 72  | O6    | 771   | 0        | 849      | 64      | 0            |
| 72  | o6    | 770   | 0        | 846      | 0       | 0            |
| 73  | O7    | 681   | 0        | 683      | 52      | 0            |
| 73  | o7    | 681   | 0        | 683      | 0       | 0            |
| 74  | O8    | 612   | 0        | 682      | 44      | 0            |
| 74  | o8    | 608   | 0        | 671      | 0       | 0            |
| 75  | O9    | 436   | 0        | 475      | 36      | 0            |
| 75  | o9    | 436   | 0        | 475      | 0       | 0            |
| 76  | Q0    | 417   | 0        | 455      | 25      | 0            |
| 76  | q0    | 417   | 0        | 455      | 0       | 0            |
| 77  | Q1    | 233   | 0        | 284      | 27      | 0            |
| 77  | q1    | 233   | 0        | 284      | 0       | 0            |
| 78  | Q2    | 847   | 0        | 916      | 59      | 0            |
| 78  | q2    | 847   | 0        | 916      | 0       | 0            |
| 79  | Q3    | 694   | 0        | 734      | 58      | 0            |
| 79  | q3    | 694   | 0        | 734      | 0       | 0            |
| 80  | e0    | 491   | 0        | 542      | 0       | 0            |
| 81  | sM    | 681   | 0        | 609      | 0       | 0            |
| 82  | m2    | 750   | 0        | 179      | 0       | 0            |
| 83  | p0    | 1077  | 0        | 1041     | 0       | 0            |
| 84  | p1    | 235   | 0        | 50       | 0       | 0            |
| 85  | p2    | 230   | 0        | 51       | 0       | 0            |
| 86  | 1     | 477   | 0        | 0        | 0       | 0            |
| 86  | 2     | 123   | 0        | 0        | 0       | 0            |
| 86  | 3     | 14    | 0        | 0        | 0       | 0            |
| 86  | 4     | 21    | 0        | 0        | 0       | 0            |
| 86  | 5     | 506   | 0        | 0        | 0       | 0            |
| 86  | 6     | 149   | 0        | 0        | 0       | 0            |
| 86  | 7     | 16    | 0        | 0        | 0       | 0            |
| 86  | 8     | 14    | 0        | 0        | 0       | 0            |
| 86  | D0    | 1     | 0        | 0        | 0       | 0            |
| 86  | D3    | 1     | 0        | 0        | 0       | 0            |
| 86  | D4    | 1     | 0        | 0        | 0       | 0            |
| 86  | L2    | 1     | 0        | 0        | 0       | 0            |
| 86  | L3    | 2     | 0        | 0        | 0       | 0            |
| 86  | L4    | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 86  | L5    | 2     | 0        | 0        | 0       | 0            |
| 86  | L7    | 2     | 0        | 0        | 0       | 0            |
| 86  | L8    | 1     | 0        | 0        | 0       | 0            |
| 86  | M0    | 2     | 0        | 0        | 0       | 0            |
| 86  | M1    | 1     | 0        | 0        | 0       | 0            |
| 86  | M3    | 3     | 0        | 0        | 0       | 0            |
| 86  | M5    | 1     | 0        | 0        | 0       | 0            |
| 86  | M6    | 1     | 0        | 0        | 0       | 0            |
| 86  | M7    | 6     | 0        | 0        | 0       | 0            |
| 86  | M8    | 1     | 0        | 0        | 0       | 0            |
| 86  | M9    | 1     | 0        | 0        | 0       | 0            |
| 86  | N0    | 1     | 0        | 0        | 0       | 0            |
| 86  | N3    | 3     | 0        | 0        | 0       | 0            |
| 86  | N5    | 1     | 0        | 0        | 0       | 0            |
| 86  | N8    | 3     | 0        | 0        | 0       | 0            |
| 86  | O4    | 1     | 0        | 0        | 0       | 0            |
| 86  | O7    | 1     | 0        | 0        | 0       | 0            |
| 86  | O8    | 1     | 0        | 0        | 0       | 0            |
| 86  | Q2    | 1     | 0        | 0        | 0       | 0            |
| 86  | S2    | 1     | 0        | 0        | 0       | 0            |
| 86  | S8    | 1     | 0        | 0        | 0       | 0            |
| 86  | SM    | 1     | 0        | 0        | 0       | 0            |
| 86  | c1    | 1     | 0        | 0        | 0       | 0            |
| 86  | c7    | 1     | 0        | 0        | 0       | 0            |
| 86  | d3    | 2     | 0        | 0        | 0       | 0            |
| 86  | d4    | 1     | 0        | 0        | 0       | 0            |
| 86  | l2    | 2     | 0        | 0        | 0       | 0            |
| 86  | l3    | 2     | 0        | 0        | 0       | 0            |
| 86  | l4    | 1     | 0        | 0        | 0       | 0            |
| 86  | l5    | 2     | 0        | 0        | 0       | 0            |
| 86  | l7    | 2     | 0        | 0        | 0       | 0            |
| 86  | l9    | 1     | 0        | 0        | 0       | 0            |
| 86  | m1    | 1     | 0        | 0        | 0       | 0            |
| 86  | m5    | 3     | 0        | 0        | 0       | 0            |
| 86  | m6    | 1     | 0        | 0        | 0       | 0            |
| 86  | m7    | 5     | 0        | 0        | 0       | 0            |
| 86  | n0    | 1     | 0        | 0        | 0       | 0            |
| 86  | n3    | 2     | 0        | 0        | 0       | 0            |
| 86  | n6    | 1     | 0        | 0        | 0       | 0            |
| 86  | n8    | 5     | 0        | 0        | 0       | 0            |
| 86  | o1    | 2     | 0        | 0        | 0       | 0            |
| 86  | o3    | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 86  | o4    | 1     | 0        | 0        | 0       | 0            |
| 86  | q0    | 1     | 0        | 0        | 0       | 0            |
| 86  | q1    | 1     | 0        | 0        | 0       | 0            |
| 86  | q3    | 1     | 0        | 0        | 0       | 0            |
| 86  | s1    | 1     | 0        | 0        | 0       | 0            |
| 86  | s4    | 1     | 0        | 0        | 0       | 0            |
| 86  | s8    | 2     | 0        | 0        | 0       | 0            |
| 86  | sM    | 2     | 0        | 0        | 0       | 0            |
| 87  | 1     | 2436  | 0        | 0        | 267     | 0            |
| 87  | 2     | 1106  | 0        | 0        | 125     | 0            |
| 87  | 3     | 84    | 0        | 0        | 5       | 0            |
| 87  | 4     | 91    | 0        | 0        | 6       | 0            |
| 87  | 5     | 2478  | 0        | 0        | 273     | 0            |
| 87  | 6     | 1106  | 0        | 0        | 114     | 0            |
| 87  | 7     | 77    | 0        | 0        | 6       | 0            |
| 87  | 8     | 112   | 0        | 0        | 16      | 0            |
| 87  | C3    | 7     | 0        | 0        | 2       | 0            |
| 87  | C5    | 7     | 0        | 0        | 4       | 0            |
| 87  | C8    | 7     | 0        | 0        | 0       | 0            |
| 87  | D3    | 7     | 0        | 0        | 0       | 0            |
| 87  | D9    | 7     | 0        | 0        | 1       | 0            |
| 87  | L3    | 21    | 0        | 0        | 3       | 0            |
| 87  | L4    | 7     | 0        | 0        | 3       | 0            |
| 87  | M0    | 7     | 0        | 0        | 0       | 0            |
| 87  | M5    | 7     | 0        | 0        | 1       | 0            |
| 87  | M6    | 7     | 0        | 0        | 0       | 0            |
| 87  | M7    | 14    | 0        | 0        | 3       | 0            |
| 87  | M8    | 7     | 0        | 0        | 0       | 0            |
| 87  | M9    | 7     | 0        | 0        | 1       | 0            |
| 87  | N1    | 7     | 0        | 0        | 0       | 0            |
| 87  | N9    | 7     | 0        | 0        | 0       | 0            |
| 87  | O2    | 7     | 0        | 0        | 1       | 0            |
| 87  | O3    | 7     | 0        | 0        | 1       | 0            |
| 87  | O7    | 14    | 0        | 0        | 7       | 0            |
| 87  | O9    | 7     | 0        | 0        | 3       | 0            |
| 87  | Q2    | 7     | 0        | 0        | 3       | 0            |
| 87  | S8    | 7     | 0        | 0        | 0       | 0            |
| 87  | SR    | 7     | 0        | 0        | 0       | 0            |
| 87  | c1    | 7     | 0        | 0        | 0       | 0            |
| 87  | c3    | 7     | 0        | 0        | 0       | 0            |
| 87  | c5    | 7     | 0        | 0        | 0       | 0            |
| 87  | c8    | 7     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 87  | d4    | 7     | 0        | 0        | 0       | 0            |
| 87  | d9    | 7     | 0        | 0        | 0       | 0            |
| 87  | l3    | 14    | 0        | 0        | 0       | 0            |
| 87  | l4    | 14    | 0        | 0        | 0       | 0            |
| 87  | l5    | 21    | 0        | 0        | 0       | 0            |
| 87  | l9    | 7     | 0        | 0        | 0       | 0            |
| 87  | m0    | 14    | 0        | 0        | 0       | 0            |
| 87  | m1    | 7     | 0        | 0        | 0       | 0            |
| 87  | m4    | 7     | 0        | 0        | 0       | 0            |
| 87  | m5    | 7     | 0        | 0        | 0       | 0            |
| 87  | m6    | 7     | 0        | 0        | 0       | 0            |
| 87  | m7    | 7     | 0        | 0        | 0       | 0            |
| 87  | m8    | 7     | 0        | 0        | 0       | 0            |
| 87  | m9    | 7     | 0        | 0        | 0       | 0            |
| 87  | n3    | 7     | 0        | 0        | 0       | 0            |
| 87  | n6    | 7     | 0        | 0        | 0       | 0            |
| 87  | n9    | 7     | 0        | 0        | 0       | 0            |
| 87  | o2    | 7     | 0        | 0        | 0       | 0            |
| 87  | o3    | 7     | 0        | 0        | 0       | 0            |
| 87  | o7    | 14    | 0        | 0        | 0       | 0            |
| 87  | q2    | 7     | 0        | 0        | 0       | 0            |
| 87  | s1    | 14    | 0        | 0        | 0       | 0            |
| 87  | s4    | 7     | 0        | 0        | 0       | 0            |
| 87  | s8    | 7     | 0        | 0        | 0       | 0            |
| 87  | s9    | 7     | 0        | 0        | 0       | 0            |
| 87  | sR    | 7     | 0        | 0        | 0       | 0            |
| 88  | D6    | 1     | 0        | 0        | 0       | 0            |
| 88  | D7    | 1     | 0        | 0        | 0       | 0            |
| 88  | D9    | 1     | 0        | 0        | 0       | 0            |
| 88  | E1    | 1     | 0        | 0        | 0       | 0            |
| 88  | O7    | 1     | 0        | 0        | 0       | 0            |
| 88  | Q0    | 1     | 0        | 0        | 0       | 0            |
| 88  | Q2    | 1     | 0        | 0        | 3       | 0            |
| 88  | Q3    | 1     | 0        | 0        | 0       | 0            |
| 88  | d6    | 1     | 0        | 0        | 0       | 0            |
| 88  | d7    | 1     | 0        | 0        | 0       | 0            |
| 88  | d9    | 1     | 0        | 0        | 0       | 0            |
| 88  | e1    | 1     | 0        | 0        | 0       | 0            |
| 88  | o7    | 1     | 0        | 0        | 0       | 0            |
| 88  | q0    | 1     | 0        | 0        | 0       | 0            |
| 88  | q2    | 1     | 0        | 0        | 0       | 0            |
| 88  | q3    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 89  | 1     | 21     | 0        | 0        | 0       | 0            |
| 89  | 5     | 21     | 0        | 0        | 1       | 0            |
| All | All   | 411211 | 0        | 297283   | 9909    | 0            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 9909 close contacts within the same asymmetric unit are listed below.

| Atom-1             | Atom-2            | Distance(Å) | Clash(Å) |
|--------------------|-------------------|-------------|----------|
| 78:Q2:17:CYS:CB    | 78:Q2:17:CYS:SG   | 2.09        | 1.48     |
| 78:Q2:17:CYS:CB    | 88:Q2:501:ZN:ZN   | 1.11        | 1.28     |
| 36:1:1481:A:O2'    | 36:1:1858:A:N3    | 1.84        | 1.10     |
| 42:L5:152:ARG:HH11 | 42:L5:152:ARG:HG3 | 1.87        | 1.10     |
| 40:L3:41:VAL:HA    | 40:L3:185:GLY:HA3 | 1.36        | 1.05     |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2   | S0    | 204/251 (81%) | 152 (74%) | 31 (15%) | 21 (10%) | 1           | 4  |
| 2   | s0    | 204/251 (81%) | 153 (75%) | 26 (13%) | 25 (12%) | 1           | 2  |
| 3   | S1    | 212/254 (84%) | 146 (69%) | 39 (18%) | 27 (13%) | 0           | 2  |
| 3   | s1    | 214/254 (84%) | 177 (83%) | 26 (12%) | 11 (5%)  | 3           | 18 |
| 4   | S2    | 215/253 (85%) | 187 (87%) | 17 (8%)  | 11 (5%)  | 3           | 18 |
| 4   | s2    | 215/253 (85%) | 186 (86%) | 16 (7%)  | 13 (6%)  | 2           | 14 |
| 5   | S3    | 221/239 (92%) | 179 (81%) | 29 (13%) | 13 (6%)  | 2           | 14 |
| 5   | s3    | 221/239 (92%) | 183 (83%) | 19 (9%)  | 19 (9%)  | 1           | 5  |
| 6   | S4    | 258/260 (99%) | 206 (80%) | 41 (16%) | 11 (4%)  | 4           | 23 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 6   | s4    | 258/260 (99%) | 216 (84%) | 24 (9%)  | 18 (7%)  | 2           | 9  |
| 7   | S5    | 204/224 (91%) | 158 (78%) | 32 (16%) | 14 (7%)  | 2           | 9  |
| 7   | s5    | 204/224 (91%) | 164 (80%) | 25 (12%) | 15 (7%)  | 2           | 8  |
| 8   | S6    | 224/236 (95%) | 194 (87%) | 17 (8%)  | 13 (6%)  | 3           | 15 |
| 8   | s6    | 216/236 (92%) | 189 (88%) | 15 (7%)  | 12 (6%)  | 3           | 16 |
| 9   | S7    | 182/189 (96%) | 137 (75%) | 25 (14%) | 20 (11%) | 1           | 3  |
| 9   | s7    | 184/189 (97%) | 148 (80%) | 21 (11%) | 15 (8%)  | 1           | 6  |
| 10  | S8    | 184/200 (92%) | 154 (84%) | 21 (11%) | 9 (5%)   | 3           | 20 |
| 10  | s8    | 184/200 (92%) | 163 (89%) | 16 (9%)  | 5 (3%)   | 8           | 38 |
| 11  | S9    | 183/196 (93%) | 151 (82%) | 23 (13%) | 9 (5%)   | 3           | 20 |
| 11  | s9    | 183/196 (93%) | 140 (76%) | 34 (19%) | 9 (5%)   | 3           | 20 |
| 12  | C0    | 94/105 (90%)  | 68 (72%)  | 15 (16%) | 11 (12%) | 1           | 3  |
| 12  | c0    | 92/105 (88%)  | 64 (70%)  | 14 (15%) | 14 (15%) | 0           | 1  |
| 13  | C1    | 153/155 (99%) | 126 (82%) | 16 (10%) | 11 (7%)  | 2           | 8  |
| 13  | c1    | 144/155 (93%) | 118 (82%) | 17 (12%) | 9 (6%)   | 2           | 12 |
| 14  | C2    | 122/142 (86%) | 70 (57%)  | 25 (20%) | 27 (22%) | 0           | 0  |
| 14  | c2    | 122/142 (86%) | 68 (56%)  | 32 (26%) | 22 (18%) | 0           | 1  |
| 15  | C3    | 148/150 (99%) | 123 (83%) | 18 (12%) | 7 (5%)   | 4           | 21 |
| 15  | c3    | 148/150 (99%) | 120 (81%) | 17 (12%) | 11 (7%)  | 2           | 8  |
| 16  | C4    | 125/136 (92%) | 94 (75%)  | 15 (12%) | 16 (13%) | 0           | 2  |
| 16  | c4    | 126/136 (93%) | 101 (80%) | 16 (13%) | 9 (7%)   | 2           | 9  |
| 17  | C5    | 122/141 (86%) | 88 (72%)  | 23 (19%) | 11 (9%)  | 1           | 5  |
| 17  | c5    | 133/141 (94%) | 92 (69%)  | 22 (16%) | 19 (14%) | 0           | 1  |
| 18  | C6    | 139/142 (98%) | 116 (84%) | 16 (12%) | 7 (5%)   | 3           | 19 |
| 18  | c6    | 140/142 (99%) | 116 (83%) | 16 (11%) | 8 (6%)   | 3           | 16 |
| 19  | C7    | 116/136 (85%) | 91 (78%)  | 13 (11%) | 12 (10%) | 1           | 4  |
| 19  | c7    | 113/136 (83%) | 87 (77%)  | 18 (16%) | 8 (7%)   | 2           | 9  |
| 20  | C8    | 143/145 (99%) | 115 (80%) | 16 (11%) | 12 (8%)  | 1           | 6  |
| 20  | c8    | 143/145 (99%) | 114 (80%) | 20 (14%) | 9 (6%)   | 2           | 12 |
| 21  | C9    | 141/143 (99%) | 115 (82%) | 22 (16%) | 4 (3%)   | 8           | 37 |
| 21  | c9    | 141/143 (99%) | 119 (84%) | 16 (11%) | 6 (4%)   | 4           | 23 |

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| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|----------|-------------|----|
| 22  | D0    | 105/120 (88%)  | 88 (84%)  | 13 (12%) | 4 (4%)   | 5           | 27 |
| 22  | d0    | 108/120 (90%)  | 82 (76%)  | 16 (15%) | 10 (9%)  | 1           | 5  |
| 23  | D1    | 85/87 (98%)    | 61 (72%)  | 16 (19%) | 8 (9%)   | 1           | 5  |
| 23  | d1    | 85/87 (98%)    | 72 (85%)  | 8 (9%)   | 5 (6%)   | 2           | 14 |
| 24  | D2    | 127/129 (98%)  | 106 (84%) | 19 (15%) | 2 (2%)   | 14          | 56 |
| 24  | d2    | 127/129 (98%)  | 114 (90%) | 12 (9%)  | 1 (1%)   | 27          | 76 |
| 25  | D3    | 142/144 (99%)  | 113 (80%) | 19 (13%) | 10 (7%)  | 2           | 9  |
| 25  | d3    | 142/144 (99%)  | 123 (87%) | 16 (11%) | 3 (2%)   | 11          | 47 |
| 26  | D4    | 132/134 (98%)  | 103 (78%) | 20 (15%) | 9 (7%)   | 2           | 10 |
| 26  | d4    | 132/134 (98%)  | 103 (78%) | 21 (16%) | 8 (6%)   | 2           | 14 |
| 27  | D5    | 68/107 (64%)   | 47 (69%)  | 9 (13%)  | 12 (18%) | 0           | 1  |
| 27  | d5    | 67/107 (63%)   | 52 (78%)  | 9 (13%)  | 6 (9%)   | 1           | 5  |
| 28  | D6    | 95/97 (98%)    | 59 (62%)  | 18 (19%) | 18 (19%) | 0           | 0  |
| 28  | d6    | 95/97 (98%)    | 74 (78%)  | 12 (13%) | 9 (10%)  | 1           | 4  |
| 29  | D7    | 79/81 (98%)    | 66 (84%)  | 8 (10%)  | 5 (6%)   | 2           | 12 |
| 29  | d7    | 79/81 (98%)    | 60 (76%)  | 12 (15%) | 7 (9%)   | 1           | 5  |
| 30  | D8    | 61/66 (92%)    | 51 (84%)  | 6 (10%)  | 4 (7%)   | 2           | 10 |
| 30  | d8    | 61/66 (92%)    | 42 (69%)  | 15 (25%) | 4 (7%)   | 2           | 10 |
| 31  | D9    | 51/55 (93%)    | 41 (80%)  | 8 (16%)  | 2 (4%)   | 5           | 26 |
| 31  | d9    | 51/55 (93%)    | 41 (80%)  | 6 (12%)  | 4 (8%)   | 1           | 7  |
| 32  | E0    | 58/60 (97%)    | 44 (76%)  | 12 (21%) | 2 (3%)   | 6           | 31 |
| 33  | E1    | 69/76 (91%)    | 36 (52%)  | 17 (25%) | 16 (23%) | 0           | 0  |
| 33  | e1    | 74/76 (97%)    | 36 (49%)  | 17 (23%) | 21 (28%) | 0           | 0  |
| 34  | SR    | 316/318 (99%)  | 271 (86%) | 35 (11%) | 10 (3%)  | 6           | 33 |
| 34  | sR    | 316/318 (99%)  | 270 (85%) | 36 (11%) | 10 (3%)  | 6           | 33 |
| 35  | SM    | 155/273 (57%)  | 113 (73%) | 23 (15%) | 19 (12%) | 1           | 2  |
| 39  | L2    | 250/253 (99%)  | 223 (89%) | 21 (8%)  | 6 (2%)   | 9           | 42 |
| 39  | l2    | 250/253 (99%)  | 210 (84%) | 30 (12%) | 10 (4%)  | 5           | 25 |
| 40  | L3    | 384/386 (100%) | 326 (85%) | 45 (12%) | 13 (3%)  | 6           | 31 |
| 40  | l3    | 384/386 (100%) | 340 (88%) | 32 (8%)  | 12 (3%)  | 7           | 34 |
| 41  | L4    | 359/361 (99%)  | 299 (83%) | 43 (12%) | 17 (5%)  | 4           | 21 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 41  | l4    | 359/361 (99%) | 300 (84%) | 39 (11%) | 20 (6%)  | 3           | 16 |
| 42  | L5    | 294/296 (99%) | 242 (82%) | 31 (10%) | 21 (7%)  | 2           | 9  |
| 42  | l5    | 292/296 (99%) | 255 (87%) | 30 (10%) | 7 (2%)   | 9           | 42 |
| 43  | L6    | 152/175 (87%) | 132 (87%) | 16 (10%) | 4 (3%)   | 8           | 39 |
| 43  | l6    | 153/175 (87%) | 129 (84%) | 20 (13%) | 4 (3%)   | 8           | 39 |
| 44  | L7    | 220/243 (90%) | 198 (90%) | 12 (6%)  | 10 (4%)  | 4           | 22 |
| 44  | l7    | 221/243 (91%) | 195 (88%) | 20 (9%)  | 6 (3%)   | 8           | 38 |
| 45  | L8    | 231/255 (91%) | 188 (81%) | 35 (15%) | 8 (4%)   | 6           | 30 |
| 45  | l8    | 229/255 (90%) | 188 (82%) | 21 (9%)  | 20 (9%)  | 1           | 5  |
| 46  | L9    | 189/191 (99%) | 167 (88%) | 15 (8%)  | 7 (4%)   | 5           | 28 |
| 46  | l9    | 189/191 (99%) | 171 (90%) | 15 (8%)  | 3 (2%)   | 14          | 56 |
| 47  | M0    | 207/220 (94%) | 178 (86%) | 18 (9%)  | 11 (5%)  | 3           | 18 |
| 47  | m0    | 209/220 (95%) | 167 (80%) | 27 (13%) | 15 (7%)  | 2           | 8  |
| 48  | M1    | 167/173 (96%) | 131 (78%) | 21 (13%) | 15 (9%)  | 1           | 5  |
| 48  | m1    | 167/173 (96%) | 139 (83%) | 16 (10%) | 12 (7%)  | 2           | 8  |
| 49  | M3    | 191/198 (96%) | 164 (86%) | 16 (8%)  | 11 (6%)  | 3           | 15 |
| 49  | m3    | 192/198 (97%) | 159 (83%) | 17 (9%)  | 16 (8%)  | 1           | 6  |
| 50  | M4    | 134/137 (98%) | 117 (87%) | 12 (9%)  | 5 (4%)   | 5           | 28 |
| 50  | m4    | 135/137 (98%) | 122 (90%) | 10 (7%)  | 3 (2%)   | 10          | 45 |
| 51  | M5    | 201/203 (99%) | 181 (90%) | 12 (6%)  | 8 (4%)   | 5           | 25 |
| 51  | m5    | 201/203 (99%) | 179 (89%) | 16 (8%)  | 6 (3%)   | 7           | 34 |
| 52  | M6    | 195/198 (98%) | 181 (93%) | 11 (6%)  | 3 (2%)   | 15          | 58 |
| 52  | m6    | 195/198 (98%) | 179 (92%) | 8 (4%)   | 8 (4%)   | 4           | 24 |
| 53  | M7    | 181/183 (99%) | 152 (84%) | 22 (12%) | 7 (4%)   | 5           | 26 |
| 53  | m7    | 153/183 (84%) | 138 (90%) | 13 (8%)  | 2 (1%)   | 18          | 62 |
| 54  | M8    | 183/185 (99%) | 165 (90%) | 14 (8%)  | 4 (2%)   | 10          | 45 |
| 54  | m8    | 183/185 (99%) | 155 (85%) | 22 (12%) | 6 (3%)   | 6           | 32 |
| 55  | M9    | 186/188 (99%) | 172 (92%) | 13 (7%)  | 1 (0%)   | 38          | 84 |
| 55  | m9    | 186/188 (99%) | 172 (92%) | 13 (7%)  | 1 (0%)   | 38          | 84 |
| 56  | N0    | 170/172 (99%) | 150 (88%) | 15 (9%)  | 5 (3%)   | 7           | 35 |
| 56  | n0    | 170/172 (99%) | 158 (93%) | 11 (6%)  | 1 (1%)   | 33          | 81 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 57  | N1    | 157/159 (99%) | 133 (85%) | 18 (12%) | 6 (4%)   | 5           | 27 |
| 57  | n1    | 157/159 (99%) | 141 (90%) | 12 (8%)  | 4 (2%)   | 9           | 40 |
| 58  | N2    | 98/120 (82%)  | 76 (78%)  | 17 (17%) | 5 (5%)   | 3           | 18 |
| 58  | n2    | 96/120 (80%)  | 77 (80%)  | 13 (14%) | 6 (6%)   | 2           | 12 |
| 59  | N3    | 134/136 (98%) | 124 (92%) | 9 (7%)   | 1 (1%)   | 30          | 78 |
| 59  | n3    | 134/136 (98%) | 121 (90%) | 11 (8%)  | 2 (2%)   | 15          | 58 |
| 60  | N4    | 96/155 (62%)  | 74 (77%)  | 13 (14%) | 9 (9%)   | 1           | 5  |
| 60  | n4    | 133/155 (86%) | 107 (80%) | 17 (13%) | 9 (7%)   | 2           | 10 |
| 61  | N5    | 119/141 (84%) | 106 (89%) | 12 (10%) | 1 (1%)   | 27          | 76 |
| 61  | n5    | 118/141 (84%) | 98 (83%)  | 11 (9%)  | 9 (8%)   | 2           | 7  |
| 62  | N6    | 124/126 (98%) | 110 (89%) | 8 (6%)   | 6 (5%)   | 4           | 20 |
| 62  | n6    | 124/126 (98%) | 113 (91%) | 7 (6%)   | 4 (3%)   | 6           | 33 |
| 63  | N7    | 133/135 (98%) | 109 (82%) | 18 (14%) | 6 (4%)   | 4           | 22 |
| 63  | n7    | 133/135 (98%) | 104 (78%) | 18 (14%) | 11 (8%)  | 1           | 6  |
| 64  | N8    | 146/148 (99%) | 121 (83%) | 15 (10%) | 10 (7%)  | 2           | 10 |
| 64  | n8    | 146/148 (99%) | 119 (82%) | 22 (15%) | 5 (3%)   | 6           | 31 |
| 65  | N9    | 56/58 (97%)   | 48 (86%)  | 6 (11%)  | 2 (4%)   | 5           | 29 |
| 65  | n9    | 56/58 (97%)   | 40 (71%)  | 12 (21%) | 4 (7%)   | 2           | 9  |
| 66  | O0    | 95/104 (91%)  | 89 (94%)  | 4 (4%)   | 2 (2%)   | 11          | 47 |
| 66  | o0    | 98/104 (94%)  | 88 (90%)  | 6 (6%)   | 4 (4%)   | 4           | 24 |
| 67  | O1    | 107/112 (96%) | 95 (89%)  | 7 (6%)   | 5 (5%)   | 4           | 21 |
| 67  | o1    | 107/112 (96%) | 90 (84%)  | 12 (11%) | 5 (5%)   | 4           | 21 |
| 68  | O2    | 125/129 (97%) | 112 (90%) | 10 (8%)  | 3 (2%)   | 9           | 42 |
| 68  | o2    | 125/129 (97%) | 106 (85%) | 13 (10%) | 6 (5%)   | 4           | 20 |
| 69  | O3    | 104/106 (98%) | 94 (90%)  | 7 (7%)   | 3 (3%)   | 7           | 35 |
| 69  | o3    | 104/106 (98%) | 92 (88%)  | 8 (8%)   | 4 (4%)   | 5           | 27 |
| 70  | O4    | 110/119 (92%) | 97 (88%)  | 12 (11%) | 1 (1%)   | 25          | 73 |
| 70  | o4    | 110/119 (92%) | 93 (84%)  | 11 (10%) | 6 (6%)   | 3           | 16 |
| 71  | O5    | 117/119 (98%) | 104 (89%) | 12 (10%) | 1 (1%)   | 25          | 73 |
| 71  | o5    | 117/119 (98%) | 102 (87%) | 13 (11%) | 2 (2%)   | 14          | 54 |
| 72  | O6    | 97/99 (98%)   | 77 (79%)  | 15 (16%) | 5 (5%)   | 3           | 18 |

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| Mol | Chain | Analysed          | Favoured    | Allowed    | Outliers  | Percentiles |     |
|-----|-------|-------------------|-------------|------------|-----------|-------------|-----|
| 72  | o6    | 97/99 (98%)       | 77 (79%)    | 13 (13%)   | 7 (7%)    | 2           | 8   |
| 73  | O7    | 85/87 (98%)       | 74 (87%)    | 8 (9%)     | 3 (4%)    | 6           | 30  |
| 73  | o7    | 85/87 (98%)       | 75 (88%)    | 8 (9%)     | 2 (2%)    | 9           | 42  |
| 74  | O8    | 75/77 (97%)       | 62 (83%)    | 11 (15%)   | 2 (3%)    | 8           | 38  |
| 74  | o8    | 75/77 (97%)       | 60 (80%)    | 11 (15%)   | 4 (5%)    | 3           | 18  |
| 75  | O9    | 48/50 (96%)       | 39 (81%)    | 8 (17%)    | 1 (2%)    | 11          | 47  |
| 75  | o9    | 48/50 (96%)       | 41 (85%)    | 6 (12%)    | 1 (2%)    | 11          | 47  |
| 76  | Q0    | 50/52 (96%)       | 46 (92%)    | 2 (4%)     | 2 (4%)    | 5           | 25  |
| 76  | q0    | 50/52 (96%)       | 47 (94%)    | 2 (4%)     | 1 (2%)    | 11          | 48  |
| 77  | Q1    | 23/25 (92%)       | 22 (96%)    | 1 (4%)     | 0         | 100         | 100 |
| 77  | q1    | 23/25 (92%)       | 21 (91%)    | 1 (4%)     | 1 (4%)    | 4           | 23  |
| 78  | Q2    | 103/105 (98%)     | 84 (82%)    | 13 (13%)   | 6 (6%)    | 3           | 15  |
| 78  | q2    | 103/105 (98%)     | 92 (89%)    | 10 (10%)   | 1 (1%)    | 22          | 70  |
| 79  | Q3    | 89/91 (98%)       | 77 (86%)    | 8 (9%)     | 4 (4%)    | 4           | 22  |
| 79  | q3    | 89/91 (98%)       | 82 (92%)    | 6 (7%)     | 1 (1%)    | 21          | 67  |
| 80  | e0    | 60/62 (97%)       | 43 (72%)    | 11 (18%)   | 6 (10%)   | 1           | 4   |
| 81  | sM    | 98/273 (36%)      | 62 (63%)    | 22 (22%)   | 14 (14%)  | 0           | 1   |
| 83  | p0    | 139/311 (45%)     | 120 (86%)   | 15 (11%)   | 4 (3%)    | 7           | 35  |
| All | All   | 22333/24141 (92%) | 18562 (83%) | 2524 (11%) | 1247 (6%) | 3           | 16  |

5 of 1247 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S0    | 4   | PRO  |
| 2   | S0    | 39  | ASN  |
| 2   | S0    | 66  | ALA  |
| 2   | S0    | 158 | VAL  |
| 2   | S0    | 191 | ARG  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2   | S0    | 164/209 (78%)  | 133 (81%) | 31 (19%) | 2           | 12 |
| 2   | s0    | 165/209 (79%)  | 131 (79%) | 34 (21%) | 2           | 9  |
| 3   | S1    | 191/223 (86%)  | 155 (81%) | 36 (19%) | 2           | 12 |
| 3   | s1    | 192/223 (86%)  | 163 (85%) | 29 (15%) | 4           | 20 |
| 4   | S2    | 176/204 (86%)  | 142 (81%) | 34 (19%) | 2           | 12 |
| 4   | s2    | 176/204 (86%)  | 133 (76%) | 43 (24%) | 1           | 5  |
| 5   | S3    | 182/194 (94%)  | 145 (80%) | 37 (20%) | 2           | 9  |
| 5   | s3    | 182/194 (94%)  | 151 (83%) | 31 (17%) | 3           | 15 |
| 6   | S4    | 221/221 (100%) | 183 (83%) | 38 (17%) | 3           | 14 |
| 6   | s4    | 221/221 (100%) | 183 (83%) | 38 (17%) | 3           | 14 |
| 7   | S5    | 173/190 (91%)  | 142 (82%) | 31 (18%) | 2           | 13 |
| 7   | s5    | 173/190 (91%)  | 133 (77%) | 40 (23%) | 1           | 6  |
| 8   | S6    | 188/201 (94%)  | 148 (79%) | 40 (21%) | 1           | 8  |
| 8   | s6    | 187/201 (93%)  | 151 (81%) | 36 (19%) | 2           | 12 |
| 9   | S7    | 165/169 (98%)  | 140 (85%) | 25 (15%) | 4           | 20 |
| 9   | s7    | 165/169 (98%)  | 138 (84%) | 27 (16%) | 3           | 16 |
| 10  | S8    | 150/161 (93%)  | 130 (87%) | 20 (13%) | 6           | 25 |
| 10  | s8    | 150/161 (93%)  | 128 (85%) | 22 (15%) | 4           | 21 |
| 11  | S9    | 158/165 (96%)  | 123 (78%) | 35 (22%) | 1           | 7  |
| 11  | s9    | 158/165 (96%)  | 128 (81%) | 30 (19%) | 2           | 12 |
| 12  | C0    | 77/98 (79%)    | 67 (87%)  | 10 (13%) | 6           | 26 |
| 12  | c0    | 73/98 (74%)    | 63 (86%)  | 10 (14%) | 5           | 24 |
| 13  | C1    | 129/136 (95%)  | 107 (83%) | 22 (17%) | 3           | 15 |
| 13  | c1    | 129/136 (95%)  | 106 (82%) | 23 (18%) | 2           | 14 |
| 14  | C2    | 88/118 (75%)   | 66 (75%)  | 22 (25%) | 1           | 4  |
| 14  | c2    | 88/118 (75%)   | 66 (75%)  | 22 (25%) | 1           | 4  |
| 15  | C3    | 127/127 (100%) | 100 (79%) | 27 (21%) | 1           | 8  |
| 15  | c3    | 127/127 (100%) | 103 (81%) | 24 (19%) | 2           | 12 |
| 16  | C4    | 81/104 (78%)   | 60 (74%)  | 21 (26%) | 1           | 4  |
| 16  | c4    | 97/104 (93%)   | 76 (78%)  | 21 (22%) | 1           | 8  |
| 17  | C5    | 101/117 (86%)  | 85 (84%)  | 16 (16%) | 4           | 18 |
| 17  | c5    | 103/117 (88%)  | 84 (82%)  | 19 (18%) | 2           | 13 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 18  | C6    | 117/118 (99%)  | 94 (80%)  | 23 (20%) | 2           | 11 |
| 18  | c6    | 118/118 (100%) | 93 (79%)  | 25 (21%) | 1           | 8  |
| 19  | C7    | 94/124 (76%)   | 72 (77%)  | 22 (23%) | 1           | 5  |
| 19  | c7    | 92/124 (74%)   | 78 (85%)  | 14 (15%) | 4           | 20 |
| 20  | C8    | 128/128 (100%) | 95 (74%)  | 33 (26%) | 1           | 4  |
| 20  | c8    | 128/128 (100%) | 103 (80%) | 25 (20%) | 2           | 11 |
| 21  | C9    | 115/115 (100%) | 92 (80%)  | 23 (20%) | 2           | 10 |
| 21  | c9    | 115/115 (100%) | 93 (81%)  | 22 (19%) | 2           | 12 |
| 22  | D0    | 100/113 (88%)  | 78 (78%)  | 22 (22%) | 1           | 7  |
| 22  | d0    | 103/113 (91%)  | 78 (76%)  | 25 (24%) | 1           | 5  |
| 23  | D1    | 74/74 (100%)   | 61 (82%)  | 13 (18%) | 3           | 14 |
| 23  | d1    | 74/74 (100%)   | 56 (76%)  | 18 (24%) | 1           | 5  |
| 24  | D2    | 110/110 (100%) | 94 (86%)  | 16 (14%) | 5           | 22 |
| 24  | d2    | 110/110 (100%) | 93 (84%)  | 17 (16%) | 4           | 19 |
| 25  | D3    | 119/119 (100%) | 98 (82%)  | 21 (18%) | 3           | 14 |
| 25  | d3    | 119/119 (100%) | 104 (87%) | 15 (13%) | 7           | 27 |
| 26  | D4    | 112/112 (100%) | 93 (83%)  | 19 (17%) | 3           | 15 |
| 26  | d4    | 112/112 (100%) | 94 (84%)  | 18 (16%) | 3           | 17 |
| 27  | D5    | 61/88 (69%)    | 46 (75%)  | 15 (25%) | 1           | 4  |
| 27  | d5    | 61/88 (69%)    | 51 (84%)  | 10 (16%) | 3           | 16 |
| 28  | D6    | 83/83 (100%)   | 67 (81%)  | 16 (19%) | 2           | 12 |
| 28  | d6    | 83/83 (100%)   | 73 (88%)  | 10 (12%) | 7           | 30 |
| 29  | D7    | 70/70 (100%)   | 64 (91%)  | 6 (9%)   | 15          | 50 |
| 29  | d7    | 70/70 (100%)   | 60 (86%)  | 10 (14%) | 5           | 22 |
| 30  | D8    | 56/59 (95%)    | 44 (79%)  | 12 (21%) | 1           | 8  |
| 30  | d8    | 56/59 (95%)    | 44 (79%)  | 12 (21%) | 1           | 8  |
| 31  | D9    | 47/48 (98%)    | 39 (83%)  | 8 (17%)  | 3           | 15 |
| 31  | d9    | 47/48 (98%)    | 37 (79%)  | 10 (21%) | 1           | 8  |
| 32  | E0    | 51/51 (100%)   | 41 (80%)  | 10 (20%) | 2           | 11 |
| 33  | E1    | 62/66 (94%)    | 46 (74%)  | 16 (26%) | 1           | 4  |
| 33  | e1    | 66/66 (100%)   | 51 (77%)  | 15 (23%) | 1           | 6  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 34  | SR    | 260/261 (100%) | 222 (85%) | 38 (15%) | 5           | 21 |
| 34  | sR    | 260/261 (100%) | 233 (90%) | 27 (10%) | 10          | 37 |
| 35  | SM    | 97/228 (42%)   | 76 (78%)  | 21 (22%) | 1           | 8  |
| 39  | L2    | 193/195 (99%)  | 150 (78%) | 43 (22%) | 1           | 7  |
| 39  | l2    | 192/195 (98%)  | 152 (79%) | 40 (21%) | 2           | 8  |
| 40  | L3    | 321/322 (100%) | 257 (80%) | 64 (20%) | 2           | 10 |
| 40  | l3    | 320/322 (99%)  | 251 (78%) | 69 (22%) | 1           | 8  |
| 41  | L4    | 288/288 (100%) | 228 (79%) | 60 (21%) | 2           | 8  |
| 41  | l4    | 288/288 (100%) | 229 (80%) | 59 (20%) | 2           | 9  |
| 42  | L5    | 244/244 (100%) | 197 (81%) | 47 (19%) | 2           | 12 |
| 42  | l5    | 243/244 (100%) | 196 (81%) | 47 (19%) | 2           | 12 |
| 43  | L6    | 134/152 (88%)  | 112 (84%) | 22 (16%) | 3           | 16 |
| 43  | l6    | 135/152 (89%)  | 112 (83%) | 23 (17%) | 3           | 15 |
| 44  | L7    | 186/204 (91%)  | 162 (87%) | 24 (13%) | 6           | 26 |
| 44  | l7    | 187/204 (92%)  | 160 (86%) | 27 (14%) | 5           | 22 |
| 45  | L8    | 187/207 (90%)  | 152 (81%) | 35 (19%) | 2           | 12 |
| 45  | l8    | 177/207 (86%)  | 147 (83%) | 30 (17%) | 3           | 15 |
| 46  | L9    | 171/171 (100%) | 134 (78%) | 37 (22%) | 1           | 8  |
| 46  | l9    | 171/171 (100%) | 137 (80%) | 34 (20%) | 2           | 10 |
| 47  | M0    | 177/186 (95%)  | 143 (81%) | 34 (19%) | 2           | 12 |
| 47  | m0    | 179/186 (96%)  | 142 (79%) | 37 (21%) | 2           | 8  |
| 48  | M1    | 147/150 (98%)  | 115 (78%) | 32 (22%) | 1           | 8  |
| 48  | m1    | 147/150 (98%)  | 122 (83%) | 25 (17%) | 3           | 15 |
| 49  | M3    | 154/158 (98%)  | 128 (83%) | 26 (17%) | 3           | 15 |
| 49  | m3    | 154/158 (98%)  | 130 (84%) | 24 (16%) | 4           | 18 |
| 50  | M4    | 107/108 (99%)  | 84 (78%)  | 23 (22%) | 1           | 8  |
| 50  | m4    | 108/108 (100%) | 88 (82%)  | 20 (18%) | 2           | 13 |
| 51  | M5    | 175/175 (100%) | 138 (79%) | 37 (21%) | 1           | 8  |
| 51  | m5    | 175/175 (100%) | 149 (85%) | 26 (15%) | 4           | 20 |
| 52  | M6    | 160/161 (99%)  | 133 (83%) | 27 (17%) | 3           | 15 |
| 52  | m6    | 160/161 (99%)  | 132 (82%) | 28 (18%) | 3           | 14 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 53  | M7    | 140/145 (97%)  | 109 (78%) | 31 (22%) | 1           | 7  |
| 53  | m7    | 125/145 (86%)  | 103 (82%) | 22 (18%) | 3           | 14 |
| 54  | M8    | 150/150 (100%) | 128 (85%) | 22 (15%) | 4           | 21 |
| 54  | m8    | 150/150 (100%) | 118 (79%) | 32 (21%) | 1           | 8  |
| 55  | M9    | 153/153 (100%) | 132 (86%) | 21 (14%) | 5           | 24 |
| 55  | m9    | 153/153 (100%) | 120 (78%) | 33 (22%) | 1           | 8  |
| 56  | N0    | 156/156 (100%) | 121 (78%) | 35 (22%) | 1           | 7  |
| 56  | n0    | 156/156 (100%) | 124 (80%) | 32 (20%) | 2           | 9  |
| 57  | N1    | 136/136 (100%) | 108 (79%) | 28 (21%) | 2           | 9  |
| 57  | n1    | 136/136 (100%) | 108 (79%) | 28 (21%) | 2           | 9  |
| 58  | N2    | 87/106 (82%)   | 74 (85%)  | 13 (15%) | 4           | 20 |
| 58  | n2    | 85/106 (80%)   | 72 (85%)  | 13 (15%) | 4           | 19 |
| 59  | N3    | 104/104 (100%) | 86 (83%)  | 18 (17%) | 3           | 14 |
| 59  | n3    | 104/104 (100%) | 94 (90%)  | 10 (10%) | 12          | 43 |
| 60  | N4    | 57/129 (44%)   | 50 (88%)  | 7 (12%)  | 7           | 28 |
| 60  | n4    | 100/129 (78%)  | 82 (82%)  | 18 (18%) | 2           | 13 |
| 61  | N5    | 104/117 (89%)  | 84 (81%)  | 20 (19%) | 2           | 12 |
| 61  | n5    | 104/117 (89%)  | 83 (80%)  | 21 (20%) | 2           | 10 |
| 62  | N6    | 109/109 (100%) | 83 (76%)  | 26 (24%) | 1           | 5  |
| 62  | n6    | 109/109 (100%) | 82 (75%)  | 27 (25%) | 1           | 4  |
| 63  | N7    | 115/115 (100%) | 94 (82%)  | 21 (18%) | 2           | 13 |
| 63  | n7    | 115/115 (100%) | 93 (81%)  | 22 (19%) | 2           | 12 |
| 64  | N8    | 118/118 (100%) | 96 (81%)  | 22 (19%) | 2           | 13 |
| 64  | n8    | 118/118 (100%) | 93 (79%)  | 25 (21%) | 1           | 8  |
| 65  | N9    | 46/46 (100%)   | 35 (76%)  | 11 (24%) | 1           | 5  |
| 65  | n9    | 46/46 (100%)   | 37 (80%)  | 9 (20%)  | 2           | 11 |
| 66  | O0    | 81/87 (93%)    | 68 (84%)  | 13 (16%) | 3           | 17 |
| 66  | o0    | 84/87 (97%)    | 70 (83%)  | 14 (17%) | 3           | 16 |
| 67  | O1    | 92/96 (96%)    | 71 (77%)  | 21 (23%) | 1           | 6  |
| 67  | o1    | 94/96 (98%)    | 74 (79%)  | 20 (21%) | 1           | 8  |
| 68  | O2    | 109/110 (99%)  | 87 (80%)  | 22 (20%) | 2           | 10 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers   | Percentiles |    |
|-----|-------|-------------------|-------------|------------|-------------|----|
| 68  | o2    | 109/110 (99%)     | 85 (78%)    | 24 (22%)   | 1           | 7  |
| 69  | O3    | 90/90 (100%)      | 81 (90%)    | 9 (10%)    | 11          | 39 |
| 69  | o3    | 90/90 (100%)      | 77 (86%)    | 13 (14%)   | 5           | 22 |
| 70  | O4    | 95/101 (94%)      | 74 (78%)    | 21 (22%)   | 1           | 7  |
| 70  | o4    | 95/101 (94%)      | 75 (79%)    | 20 (21%)   | 1           | 8  |
| 71  | O5    | 104/104 (100%)    | 80 (77%)    | 24 (23%)   | 1           | 6  |
| 71  | o5    | 103/104 (99%)     | 80 (78%)    | 23 (22%)   | 1           | 7  |
| 72  | O6    | 81/81 (100%)      | 65 (80%)    | 16 (20%)   | 2           | 11 |
| 72  | o6    | 80/81 (99%)       | 56 (70%)    | 24 (30%)   | 0           | 2  |
| 73  | O7    | 70/70 (100%)      | 58 (83%)    | 12 (17%)   | 3           | 15 |
| 73  | o7    | 70/70 (100%)      | 58 (83%)    | 12 (17%)   | 3           | 15 |
| 74  | O8    | 68/68 (100%)      | 52 (76%)    | 16 (24%)   | 1           | 5  |
| 74  | o8    | 67/68 (98%)       | 53 (79%)    | 14 (21%)   | 1           | 8  |
| 75  | O9    | 45/45 (100%)      | 40 (89%)    | 5 (11%)    | 9           | 34 |
| 75  | o9    | 45/45 (100%)      | 36 (80%)    | 9 (20%)    | 2           | 10 |
| 76  | Q0    | 47/47 (100%)      | 35 (74%)    | 12 (26%)   | 1           | 4  |
| 76  | q0    | 47/47 (100%)      | 35 (74%)    | 12 (26%)   | 1           | 4  |
| 77  | Q1    | 23/23 (100%)      | 15 (65%)    | 8 (35%)    | 0           | 1  |
| 77  | q1    | 23/23 (100%)      | 14 (61%)    | 9 (39%)    | 0           | 1  |
| 78  | Q2    | 90/90 (100%)      | 67 (74%)    | 23 (26%)   | 1           | 4  |
| 78  | q2    | 90/90 (100%)      | 73 (81%)    | 17 (19%)   | 2           | 12 |
| 79  | Q3    | 71/71 (100%)      | 56 (79%)    | 15 (21%)   | 1           | 8  |
| 79  | q3    | 71/71 (100%)      | 63 (89%)    | 8 (11%)    | 9           | 33 |
| 80  | e0    | 53/53 (100%)      | 42 (79%)    | 11 (21%)   | 2           | 8  |
| 81  | sM    | 54/228 (24%)      | 40 (74%)    | 14 (26%)   | 1           | 4  |
| 83  | p0    | 105/253 (42%)     | 80 (76%)    | 25 (24%)   | 1           | 5  |
| All | All   | 18729/20239 (92%) | 15175 (81%) | 3554 (19%) | 2           | 12 |

5 of 3554 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 68  | O2    | 61  | LYS  |
| 7   | s5    | 170 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 64  | n8    | 46  | ASP  |
| 71  | O5    | 28  | LEU  |
| 2   | s0    | 119 | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | L5    | 40  | HIS  |
| 74  | O8    | 32  | ASN  |
| 59  | n3    | 33  | ASN  |
| 42  | L5    | 264 | GLN  |
| 78  | Q2    | 23  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|----------|-------------------|-----------------|
| 1   | 2     | 0/1800   | -                 | -               |
| 1   | 6     | 0/1800   | -                 | -               |
| 36  | 1     | 0/3396   | -                 | -               |
| 36  | 5     | 0/3396   | -                 | -               |
| 37  | 3     | 0/121    | -                 | -               |
| 37  | 7     | 0/121    | -                 | -               |
| 38  | 4     | 0/158    | -                 | -               |
| 38  | 8     | 0/158    | -                 | -               |
| All | All   | 0/10950  | -                 | -               |

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2563 ligands modelled in this entry, 1428 are monoatomic - leaving 1135 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 | $\# Z  > 2$ |
| 87  | OHX  | 1     | 3870 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3871 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3872 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3873 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3874 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3875 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3876 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3877 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3878 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3879 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3880 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3881 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3882 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3883 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3884 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3885 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3886 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3887 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3888 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3889 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3890 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3891 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3892 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3893 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3894 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3895 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3896 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3897 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3898 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3899 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |
| 87  | OHX  | 1     | 3900 | -    | 0,6,6        | 0.00 | -           | 0,15,15     | 0.00 | -           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 1     | 3901 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3902 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3903 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3904 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3905 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3906 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3907 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3908 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3909 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3910 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3911 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3912 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3913 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3914 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3915 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3916 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3917 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3918 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3919 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3920 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3921 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3922 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3923 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3924 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3925 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3926 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3927 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3928 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3929 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3930 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3931 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3932 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3933 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3934 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3935 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3936 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3937 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3938 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3939 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3940 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3941 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3942 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3943 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 1     | 3944 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3945 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3946 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3947 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3948 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3949 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3950 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3951 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3952 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3953 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3954 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3955 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3956 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3957 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3958 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3959 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3960 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3961 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3962 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3963 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3964 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3965 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3966 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3967 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3968 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3969 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3970 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3971 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3972 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3973 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3974 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3975 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3976 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3977 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3978 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3979 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3980 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3981 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3982 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3983 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3984 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3985 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3986 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 1     | 3987 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3988 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3989 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3990 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3991 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3992 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3993 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3994 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3995 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3996 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3997 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3998 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 3999 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4000 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4001 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4002 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4003 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4004 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4005 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4006 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4007 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4008 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4009 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4010 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4011 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4012 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4013 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4014 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4015 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4016 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4017 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4018 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4019 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4020 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4021 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4022 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4023 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4024 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4025 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4026 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4027 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4028 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4029 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 1     | 4030 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4031 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4032 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4033 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4034 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4035 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4036 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4037 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4038 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4039 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4040 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4041 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4042 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4043 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4044 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4045 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4046 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4047 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4048 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4049 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4050 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4051 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4052 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4053 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4054 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4055 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4056 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4057 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4058 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4059 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4060 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4061 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4062 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4063 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4064 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4065 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4066 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4067 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4068 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4069 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4070 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4071 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4072 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 1     | 4073 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4074 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4075 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4076 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4077 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4078 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4079 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4080 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4081 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4082 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4083 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4084 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4085 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4086 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4087 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4088 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4089 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4090 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4091 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4092 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4093 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4094 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4095 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4096 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4097 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4098 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4099 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4100 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4101 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4102 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4103 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4104 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4105 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4106 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4107 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4108 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4109 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4110 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4111 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4112 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4113 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4114 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4115 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 1     | 4116 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4117 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4118 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4119 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4120 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4121 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4122 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4123 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4124 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4125 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4126 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4127 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4128 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4129 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4130 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4131 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4132 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4133 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4134 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4135 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4136 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4137 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4138 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4139 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4140 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4141 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4142 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4143 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4144 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4145 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4146 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4147 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4148 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4149 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4150 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4151 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4152 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4153 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4154 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4155 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4156 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4157 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4158 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 1     | 4159 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4160 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4161 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4162 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4163 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4164 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4165 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4166 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4167 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4168 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4169 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4170 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4171 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4172 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4173 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4174 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4175 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4176 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4177 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4178 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4179 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4180 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4181 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4182 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4183 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4184 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4185 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4186 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4187 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4188 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4189 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4190 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4191 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4192 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4193 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4194 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4195 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4196 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4197 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4198 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4199 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4200 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4201 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 1     | 4202 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4203 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4204 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4205 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4206 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4207 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4208 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4209 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4210 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4211 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4212 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4213 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4214 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4215 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4216 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 1     | 4217 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 89  | 3KD  | 1     | 4218 | -    | 25,25,25     | 0.75 | 0        | 39,39,39    | 1.90 | 6 (15%)  |
| 87  | OHX  | 2     | 2021 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2022 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2023 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2024 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2025 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2026 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2027 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2028 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2029 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2030 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2031 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2032 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2033 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2034 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2035 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2036 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2037 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2038 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2039 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2040 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2041 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2042 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2043 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2044 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2045 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2046 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 2     | 2047 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2048 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2049 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2050 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2051 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2052 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2053 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2054 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2055 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2056 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2057 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2058 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2059 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2060 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2061 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2062 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2063 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2064 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2065 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2066 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2067 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2068 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2069 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2070 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2071 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2072 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2073 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2074 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2075 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2076 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2077 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2078 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2079 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2080 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2081 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2082 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2083 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2084 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2085 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2086 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2087 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2088 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2089 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 2     | 2090 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2091 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2092 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2093 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2094 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2095 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2096 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2097 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2098 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2099 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2100 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2101 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2102 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2103 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2104 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2105 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2106 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2107 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2108 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2109 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2110 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2111 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2112 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2113 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2114 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2115 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2116 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2117 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2118 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2119 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2120 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2121 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2122 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2123 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2124 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2125 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2126 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2127 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2128 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2129 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2130 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2131 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2132 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 2     | 2133 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2134 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2135 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2136 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2137 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2138 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2139 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2140 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2141 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2142 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2143 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2144 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2145 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2146 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2147 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2148 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2149 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2150 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2151 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2152 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2153 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2154 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2155 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2156 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2157 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2158 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2159 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2160 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2161 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2162 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2163 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2164 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2165 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2166 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2167 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2168 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2169 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2170 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2171 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2172 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2173 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2174 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2175 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 2     | 2176 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2177 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 2     | 2178 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 3     | 215  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 3     | 216  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 3     | 217  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 3     | 218  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 3     | 219  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 3     | 220  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 3     | 221  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 3     | 222  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 3     | 223  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 3     | 224  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 3     | 225  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 3     | 226  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 4     | 221  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 4     | 222  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 4     | 223  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 4     | 224  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 4     | 225  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 4     | 226  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 4     | 227  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 4     | 228  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 4     | 229  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 4     | 230  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 4     | 231  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 4     | 232  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 4     | 233  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3900 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3901 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3902 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3903 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3904 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3905 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3906 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3907 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3908 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3909 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3910 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3911 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3912 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3913 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3914 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 5     | 3915 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3916 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3917 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3918 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3919 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3920 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3921 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3922 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3923 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3924 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3925 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3926 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3927 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3928 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3929 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3930 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3931 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3932 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3933 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3934 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3935 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3936 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3937 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3938 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3939 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3940 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3941 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3942 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3943 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3944 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3945 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3946 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3947 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3948 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3949 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3950 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3951 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3952 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3953 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3954 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3955 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3956 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3957 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 5     | 3958 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3959 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3960 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3961 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3962 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3963 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3964 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3965 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3966 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3967 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3968 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3969 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3970 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3971 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3972 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3973 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3974 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3975 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3976 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3977 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3978 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3979 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3980 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3981 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3982 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3983 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3984 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3985 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3986 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3987 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3988 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3989 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3990 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3991 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3992 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3993 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3994 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3995 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3996 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3997 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3998 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 3999 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4000 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 5     | 4001 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4002 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4003 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4004 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4005 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4006 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4007 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4008 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4009 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4010 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4011 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4012 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4013 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4014 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4015 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4016 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4017 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4018 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4019 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4020 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4021 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4022 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4023 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4024 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4025 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4026 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4027 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4028 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4029 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4030 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4031 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4032 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4033 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4034 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4035 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4036 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4037 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4038 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4039 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4040 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4041 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4042 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4043 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 5     | 4044 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4045 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4046 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4047 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4048 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4049 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4050 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4051 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4052 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4053 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4054 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4055 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4056 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4057 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4058 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4059 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4060 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4061 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4062 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4063 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4064 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4065 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4066 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4067 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4068 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4069 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4070 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4071 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4072 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4073 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4074 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4075 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4076 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4077 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4078 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4079 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4080 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4081 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4082 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4083 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4084 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4085 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4086 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 5     | 4087 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4088 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4089 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4090 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4091 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4092 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4093 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4094 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4095 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4096 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4097 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4098 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4099 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4100 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4101 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4102 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4103 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4104 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4105 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4106 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4107 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4108 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4109 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4110 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4111 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4112 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4113 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4114 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4115 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4116 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4117 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4118 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4119 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4120 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4121 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4122 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4123 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4124 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4125 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4126 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4127 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4128 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4129 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 5     | 4130 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4131 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4132 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4133 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4134 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4135 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4136 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4137 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4138 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4139 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4140 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4141 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4142 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4143 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4144 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4145 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4146 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4147 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4148 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4149 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4150 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4151 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4152 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4153 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4154 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4155 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4156 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4157 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4158 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4159 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4160 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4161 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4162 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4163 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4164 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4165 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4166 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4167 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4168 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4169 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4170 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4171 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4172 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 5     | 4173 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4174 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4175 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4176 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4177 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4178 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4179 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4180 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4181 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4182 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4183 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4184 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4185 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4186 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4187 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4188 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4189 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4190 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4191 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4192 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4193 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4194 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4195 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4196 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4197 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4198 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4199 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4200 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4201 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4202 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4203 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4204 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4205 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4206 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4207 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4208 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4209 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4210 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4211 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4212 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4213 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4214 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4215 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 5     | 4216 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4217 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4218 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4219 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4220 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4221 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4222 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4223 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4224 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4225 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4226 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4227 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4228 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4229 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4230 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4231 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4232 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4233 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4234 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4235 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4236 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4237 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4238 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4239 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4240 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4241 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4242 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4243 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4244 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4245 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4246 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4247 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4248 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4249 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4250 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4251 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4252 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 5     | 4253 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 89  | 3KD  | 5     | 4254 | -    | 25,25,25     | 0.99 | 2 (8%)   | 39,39,39    | 1.67 | 5 (12%)  |
| 87  | OHX  | 6     | 2050 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2051 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2052 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2053 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 6     | 2054 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2055 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2056 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2057 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2058 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2059 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2060 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2061 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2062 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2063 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2064 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2065 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2066 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2067 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2068 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2069 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2070 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2071 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2072 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2073 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2074 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2075 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2076 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2077 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2078 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2079 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2080 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2081 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2082 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2083 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2084 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2085 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2086 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2087 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2088 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2089 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2090 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2091 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2092 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2093 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2094 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2095 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2096 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 6     | 2097 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2098 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2099 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2100 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2101 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2102 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2103 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2104 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2105 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2106 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2107 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2108 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2109 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2110 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2111 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2112 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2113 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2114 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2115 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2116 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2117 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2118 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2119 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2120 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2121 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2122 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2123 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2124 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2125 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2126 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2127 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2128 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2129 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2130 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2131 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2132 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2133 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2134 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2135 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2136 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2137 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2138 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2139 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 6     | 2140 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2141 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2142 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2143 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2144 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2145 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2146 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2147 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2148 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2149 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2150 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2151 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2152 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2153 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2154 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2155 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2156 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2157 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2158 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2159 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2160 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2161 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2162 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2163 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2164 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2165 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2166 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2167 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2168 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2169 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2170 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2171 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2172 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2173 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2174 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2175 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2176 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2177 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2178 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2179 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2180 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2181 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2182 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 6     | 2183 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2184 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2185 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2186 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2187 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2188 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2189 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2190 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2191 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2192 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2193 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2194 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2195 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2196 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2197 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2198 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2199 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2200 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2201 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2202 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2203 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2204 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2205 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2206 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 6     | 2207 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 7     | 217  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 7     | 218  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 7     | 219  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 7     | 220  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 7     | 221  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 7     | 222  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 7     | 223  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 7     | 224  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 7     | 225  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 7     | 226  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 7     | 227  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 8     | 215  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 8     | 216  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 8     | 217  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 8     | 218  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 8     | 219  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 8     | 220  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 8     | 221  | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | 8     | 222 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 8     | 223 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 8     | 224 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 8     | 225 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 8     | 226 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 8     | 227 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 8     | 228 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 8     | 229 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | 8     | 230 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | C3    | 201 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | C5    | 201 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | C8    | 201 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | D3    | 202 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | D9    | 102 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | L3    | 403 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | L3    | 404 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | L3    | 405 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | L4    | 403 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | M0    | 303 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | M5    | 302 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | M6    | 202 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | M7    | 207 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | M7    | 208 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | M8    | 202 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | M9    | 202 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | N1    | 201 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | N9    | 101 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | O2    | 201 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | O3    | 201 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | O7    | 103 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | O7    | 104 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | O9    | 101 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | Q2    | 503 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | S8    | 302 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | SR    | 401 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | c1    | 202 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | c3    | 201 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | c5    | 201 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | c8    | 201 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | d4    | 202 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | d9    | 102 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | l3    | 403 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | l3    | 404 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | OHX  | l4    | 402 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | l4    | 403 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | l5    | 303 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | l5    | 304 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | l5    | 305 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | l9    | 202 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | m0    | 301 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | m0    | 302 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | m1    | 202 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | m4    | 201 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | m5    | 304 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | m6    | 202 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | m7    | 206 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | m8    | 201 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | m9    | 201 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | n3    | 203 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | n6    | 202 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | n9    | 101 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | o2    | 201 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | o3    | 203 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | o7    | 502 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | o7    | 503 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | q2    | 502 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | s1    | 302 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | s1    | 303 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | s4    | 302 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | s8    | 303 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | s9    | 201 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |
| 87  | OHX  | sR    | 401 | -    | 0,6,6        | 0.00 | -        | 0,15,15     | 0.00 | -        |

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   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 1     | 3870 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3871 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3872 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3873 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3874 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3875 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3876 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 1     | 3877 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3878 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3879 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3880 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3881 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3882 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3883 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3884 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3885 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3886 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3887 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3888 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3889 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3890 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3891 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3892 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3893 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3894 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3895 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3896 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3897 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3898 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3899 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3900 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3901 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3902 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3903 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3904 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3905 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3906 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3907 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3908 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3909 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3910 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3911 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3912 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3913 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3914 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3915 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3916 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3917 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3918 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 1     | 3919 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3920 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3921 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3922 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3923 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3924 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3925 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3926 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3927 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3928 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3929 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3930 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3931 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3932 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3933 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3934 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3935 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3936 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3937 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3938 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3939 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3940 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3941 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3942 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3943 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3944 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3945 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3946 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3947 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3948 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3949 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3950 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3951 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3952 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3953 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3954 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3955 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3956 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3957 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3958 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3959 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3960 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 1     | 3961 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3962 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3963 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3964 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3965 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3966 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3967 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3968 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3969 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3970 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3971 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3972 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3973 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3974 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3975 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3976 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3977 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3978 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3979 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3980 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3981 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3982 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3983 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3984 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3985 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3986 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3987 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3988 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3989 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3990 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3991 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3992 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3993 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3994 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3995 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3996 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3997 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3998 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 3999 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4000 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4001 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4002 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 1     | 4003 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4004 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4005 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4006 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4007 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4008 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4009 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4010 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4011 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4012 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4013 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4014 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4015 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4016 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4017 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4018 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4019 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4020 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4021 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4022 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4023 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4024 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4025 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4026 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4027 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4028 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4029 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4030 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4031 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4032 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4033 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4034 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4035 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4036 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4037 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4038 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4039 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4040 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4041 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4042 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4043 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4044 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 1     | 4045 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4046 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4047 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4048 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4049 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4050 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4051 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4052 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4053 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4054 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4055 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4056 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4057 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4058 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4059 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4060 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4061 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4062 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4063 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4064 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4065 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4066 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4067 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4068 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4069 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4070 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4071 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4072 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4073 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4074 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4075 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4076 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4077 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4078 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4079 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4080 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4081 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4082 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4083 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4084 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4085 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4086 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 1     | 4087 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4088 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4089 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4090 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4091 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4092 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4093 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4094 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4095 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4096 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4097 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4098 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4099 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4100 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4101 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4102 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4103 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4104 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4105 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4106 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4107 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4108 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4109 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4110 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4111 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4112 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4113 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4114 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4115 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4116 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4117 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4118 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4119 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4120 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4121 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4122 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4123 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4124 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4125 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4126 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4127 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4128 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 1     | 4129 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4130 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4131 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4132 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4133 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4134 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4135 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4136 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4137 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4138 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4139 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4140 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4141 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4142 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4143 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4144 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4145 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4146 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4147 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4148 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4149 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4150 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4151 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4152 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4153 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4154 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4155 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4156 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4157 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4158 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4159 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4160 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4161 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4162 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4163 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4164 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4165 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4166 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4167 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4168 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4169 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4170 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 1     | 4171 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4172 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4173 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4174 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4175 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4176 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4177 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4178 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4179 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4180 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4181 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4182 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4183 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4184 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4185 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4186 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4187 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4188 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4189 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4190 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4191 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4192 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4193 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4194 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4195 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4196 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4197 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4198 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4199 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4200 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4201 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4202 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4203 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4204 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4205 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4206 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4207 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4208 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4209 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4210 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4211 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 1     | 4212 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 87  | OHX  | 1     | 4213 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 1     | 4214 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 1     | 4215 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 1     | 4216 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 1     | 4217 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 89  | 3KD  | 1     | 4218 | -    | -       | 0/0/43/43 | 0/5/5/5 |
| 87  | OHX  | 2     | 2021 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2022 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2023 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2024 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2025 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2026 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2027 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2028 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2029 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2030 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2031 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2032 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2033 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2034 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2035 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2036 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2037 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2038 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2039 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2040 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2041 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2042 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2043 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2044 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2045 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2046 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2047 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2048 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2049 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2050 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2051 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2052 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2053 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2054 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2055 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 2     | 2056 | -    | -       | 0/0/0/0   | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 2     | 2057 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2058 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2059 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2060 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2061 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2062 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2063 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2064 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2065 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2066 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2067 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2068 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2069 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2070 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2071 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2072 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2073 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2074 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2075 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2076 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2077 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2078 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2079 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2080 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2081 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2082 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2083 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2084 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2085 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2086 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2087 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2088 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2089 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2090 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2091 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2092 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2093 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2094 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2095 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2096 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2097 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2098 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 2     | 2099 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2100 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2101 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2102 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2103 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2104 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2105 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2106 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2107 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2108 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2109 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2110 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2111 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2112 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2113 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2114 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2115 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2116 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2117 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2118 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2119 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2120 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2121 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2122 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2123 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2124 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2125 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2126 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2127 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2128 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2129 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2130 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2131 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2132 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2133 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2134 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2135 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2136 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2137 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2138 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2139 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2140 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 2     | 2141 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2142 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2143 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2144 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2145 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2146 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2147 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2148 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2149 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2150 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2151 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2152 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2153 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2154 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2155 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2156 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2157 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2158 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2159 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2160 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2161 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2162 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2163 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2164 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2165 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2166 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2167 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2168 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2169 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2170 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2171 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2172 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2173 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2174 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2175 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2176 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2177 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 2     | 2178 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 3     | 215  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 3     | 216  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 3     | 217  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 3     | 218  | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 3     | 219  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 3     | 220  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 3     | 221  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 3     | 222  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 3     | 223  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 3     | 224  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 3     | 225  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 3     | 226  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 4     | 221  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 4     | 222  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 4     | 223  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 4     | 224  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 4     | 225  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 4     | 226  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 4     | 227  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 4     | 228  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 4     | 229  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 4     | 230  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 4     | 231  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 4     | 232  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 4     | 233  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3900 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3901 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3902 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3903 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3904 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3905 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3906 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3907 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3908 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3909 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3910 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3911 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3912 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3913 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3914 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3915 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3916 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3917 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3918 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3919 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3920 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 5     | 3921 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3922 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3923 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3924 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3925 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3926 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3927 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3928 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3929 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3930 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3931 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3932 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3933 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3934 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3935 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3936 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3937 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3938 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3939 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3940 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3941 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3942 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3943 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3944 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3945 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3946 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3947 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3948 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3949 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3950 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3951 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3952 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3953 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3954 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3955 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3956 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3957 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3958 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3959 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3960 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3961 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3962 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 5     | 3963 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3964 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3965 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3966 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3967 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3968 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3969 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3970 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3971 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3972 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3973 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3974 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3975 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3976 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3977 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3978 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3979 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3980 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3981 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3982 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3983 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3984 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3985 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3986 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3987 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3988 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3989 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3990 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3991 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3992 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3993 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3994 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3995 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3996 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3997 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3998 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 3999 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4000 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4001 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4002 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4003 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4004 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 5     | 4005 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4006 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4007 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4008 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4009 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4010 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4011 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4012 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4013 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4014 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4015 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4016 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4017 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4018 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4019 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4020 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4021 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4022 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4023 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4024 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4025 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4026 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4027 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4028 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4029 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4030 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4031 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4032 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4033 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4034 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4035 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4036 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4037 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4038 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4039 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4040 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4041 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4042 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4043 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4044 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4045 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4046 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 5     | 4047 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4048 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4049 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4050 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4051 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4052 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4053 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4054 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4055 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4056 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4057 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4058 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4059 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4060 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4061 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4062 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4063 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4064 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4065 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4066 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4067 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4068 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4069 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4070 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4071 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4072 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4073 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4074 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4075 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4076 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4077 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4078 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4079 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4080 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4081 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4082 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4083 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4084 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4085 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4086 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4087 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4088 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 5     | 4089 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4090 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4091 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4092 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4093 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4094 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4095 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4096 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4097 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4098 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4099 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4100 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4101 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4102 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4103 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4104 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4105 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4106 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4107 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4108 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4109 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4110 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4111 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4112 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4113 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4114 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4115 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4116 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4117 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4118 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4119 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4120 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4121 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4122 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4123 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4124 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4125 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4126 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4127 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4128 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4129 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4130 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 5     | 4131 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4132 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4133 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4134 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4135 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4136 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4137 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4138 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4139 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4140 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4141 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4142 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4143 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4144 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4145 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4146 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4147 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4148 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4149 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4150 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4151 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4152 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4153 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4154 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4155 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4156 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4157 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4158 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4159 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4160 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4161 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4162 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4163 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4164 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4165 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4166 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4167 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4168 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4169 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4170 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4171 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4172 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 5     | 4173 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4174 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4175 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4176 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4177 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4178 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4179 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4180 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4181 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4182 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4183 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4184 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4185 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4186 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4187 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4188 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4189 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4190 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4191 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4192 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4193 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4194 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4195 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4196 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4197 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4198 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4199 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4200 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4201 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4202 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4203 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4204 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4205 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4206 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4207 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4208 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4209 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4210 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4211 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4212 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4213 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 5     | 4214 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 87  | OHX  | 5     | 4215 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4216 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4217 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4218 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4219 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4220 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4221 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4222 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4223 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4224 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4225 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4226 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4227 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4228 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4229 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4230 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4231 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4232 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4233 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4234 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4235 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4236 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4237 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4238 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4239 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4240 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4241 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4242 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4243 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4244 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4245 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4246 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4247 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4248 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4249 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4250 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4251 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4252 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 5     | 4253 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 89  | 3KD  | 5     | 4254 | -    | -       | 0/0/43/43 | 0/5/5/5 |
| 87  | OHX  | 6     | 2050 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 87  | OHX  | 6     | 2051 | -    | -       | 0/0/0/0   | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 6     | 2052 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2053 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2054 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2055 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2056 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2057 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2058 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2059 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2060 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2061 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2062 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2063 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2064 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2065 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2066 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2067 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2068 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2069 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2070 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2071 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2072 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2073 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2074 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2075 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2076 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2077 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2078 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2079 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2080 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2081 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2082 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2083 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2084 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2085 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2086 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2087 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2088 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2089 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2090 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2091 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2092 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2093 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 6     | 2094 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2095 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2096 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2097 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2098 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2099 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2100 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2101 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2102 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2103 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2104 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2105 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2106 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2107 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2108 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2109 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2110 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2111 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2112 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2113 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2114 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2115 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2116 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2117 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2118 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2119 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2120 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2121 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2122 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2123 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2124 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2125 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2126 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2127 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2128 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2129 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2130 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2131 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2132 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2133 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2134 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2135 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 6     | 2136 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2137 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2138 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2139 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2140 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2141 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2142 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2143 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2144 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2145 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2146 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2147 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2148 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2149 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2150 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2151 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2152 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2153 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2154 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2155 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2156 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2157 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2158 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2159 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2160 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2161 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2162 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2163 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2164 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2165 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2166 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2167 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2168 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2169 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2170 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2171 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2172 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2173 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2174 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2175 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2176 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2177 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 87  | OHX  | 6     | 2178 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2179 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2180 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2181 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2182 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2183 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2184 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2185 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2186 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2187 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2188 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2189 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2190 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2191 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2192 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2193 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2194 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2195 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2196 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2197 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2198 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2199 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2200 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2201 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2202 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2203 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2204 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2205 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2206 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 6     | 2207 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 7     | 217  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 7     | 218  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 7     | 219  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 7     | 220  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 7     | 221  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 7     | 222  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 7     | 223  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 7     | 224  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 7     | 225  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 7     | 226  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 7     | 227  | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 8     | 215  | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 87  | OHX  | 8     | 216 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 8     | 217 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 8     | 218 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 8     | 219 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 8     | 220 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 8     | 221 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 8     | 222 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 8     | 223 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 8     | 224 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 8     | 225 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 8     | 226 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 8     | 227 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 8     | 228 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 8     | 229 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | 8     | 230 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | C3    | 201 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | C5    | 201 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | C8    | 201 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | D3    | 202 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | D9    | 102 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | L3    | 403 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | L3    | 404 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | L3    | 405 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | L4    | 403 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | M0    | 303 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | M5    | 302 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | M6    | 202 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | M7    | 207 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | M7    | 208 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | M8    | 202 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | M9    | 202 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | N1    | 201 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | N9    | 101 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | O2    | 201 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | O3    | 201 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | O7    | 103 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | O7    | 104 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | O9    | 101 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | Q2    | 503 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | S8    | 302 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | SR    | 401 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | c1    | 202 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 87  | OHX  | c3    | 201 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | c5    | 201 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | c8    | 201 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | d4    | 202 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | d9    | 102 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | l3    | 403 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | l3    | 404 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | l4    | 402 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | l4    | 403 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | l5    | 303 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | l5    | 304 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | l5    | 305 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | l9    | 202 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | m0    | 301 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | m0    | 302 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | m1    | 202 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | m4    | 201 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | m5    | 304 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | m6    | 202 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | m7    | 206 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | m8    | 201 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | m9    | 201 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | n3    | 203 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | n6    | 202 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | n9    | 101 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | o2    | 201 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | o3    | 203 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | o7    | 502 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | o7    | 503 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | q2    | 502 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | s1    | 302 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | s1    | 303 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | s4    | 302 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | s8    | 303 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | s9    | 201 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 87  | OHX  | sR    | 401 | -    | -       | 0/0/0/0  | 0/0/0/0 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 89  | 5     | 4254 | 3KD  | C13-C12 | 3.12  | 1.54        | 1.50     |
| 89  | 5     | 4254 | 3KD  | C8-C9   | -2.17 | 1.47        | 1.51     |



The worst 5 of 11 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 89  | 1     | 4218 | 3KD  | C2-N-C10   | -6.59 | 97.37       | 110.67   |
| 89  | 5     | 4254 | 3KD  | C8-C9-C10  | -6.54 | 102.40      | 110.44   |
| 89  | 1     | 4218 | 3KD  | C8-C9-C10  | -6.34 | 102.64      | 110.44   |
| 89  | 5     | 4254 | 3KD  | C2-N-C10   | -4.31 | 101.97      | 110.67   |
| 89  | 1     | 4218 | 3KD  | C9-C10-C11 | -3.42 | 103.87      | 111.31   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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   | 2     | 1750/1800 (97%) | -0.08  | 60 (3%) 43 8 | 42, 78, 158, 258      | 0     |
| 1   | 6     | 1795/1800 (99%) | -0.12  | 67 (3%) 39 8 | 29, 63, 172, 265      | 0     |
| 2   | S0    | 206/251 (82%)   | 0.22   | 5 (2%) 56 11 | 83, 99, 114, 155      | 0     |
| 2   | s0    | 206/251 (82%)   | 0.05   | 0 100 100    | 60, 80, 95, 110       | 0     |
| 3   | S1    | 214/254 (84%)   | 0.75   | 23 (10%) 6 2 | 86, 123, 151, 162     | 0     |
| 3   | s1    | 216/254 (85%)   | -0.02  | 1 (0%) 88 36 | 58, 74, 96, 110       | 0     |
| 4   | S2    | 217/253 (85%)   | -0.09  | 0 100 100    | 59, 75, 93, 111       | 0     |
| 4   | s2    | 217/253 (85%)   | -0.17  | 1 (0%) 88 36 | 43, 60, 75, 85        | 0     |
| 5   | S3    | 223/239 (93%)   | 0.15   | 2 (0%) 81 24 | 66, 82, 112, 142      | 0     |
| 5   | s3    | 223/239 (93%)   | 0.11   | 1 (0%) 90 41 | 61, 92, 119, 126      | 0     |
| 6   | S4    | 260/260 (100%)  | 0.13   | 6 (2%) 57 12 | 52, 77, 91, 138       | 0     |
| 6   | s4    | 260/260 (100%)  | -0.11  | 1 (0%) 90 41 | 39, 62, 80, 119       | 0     |
| 7   | S5    | 206/224 (91%)   | 0.22   | 9 (4%) 33 7  | 86, 108, 129, 147     | 0     |
| 7   | s5    | 206/224 (91%)   | 0.06   | 3 (1%) 70 16 | 55, 79, 109, 137      | 0     |
| 8   | S6    | 226/236 (95%)   | 0.14   | 3 (1%) 74 19 | 54, 91, 116, 159      | 0     |
| 8   | s6    | 218/236 (92%)   | -0.04  | 1 (0%) 88 36 | 41, 69, 97, 133       | 0     |
| 9   | S7    | 184/189 (97%)   | 0.27   | 3 (1%) 68 16 | 74, 104, 135, 145     | 0     |
| 9   | s7    | 186/189 (98%)   | 0.20   | 3 (1%) 68 16 | 56, 91, 133, 145      | 0     |
| 10  | S8    | 188/200 (94%)   | 0.07   | 1 (0%) 88 36 | 44, 59, 101, 118      | 0     |
| 10  | s8    | 188/200 (94%)   | 0.06   | 3 (1%) 68 16 | 36, 55, 102, 119      | 0     |
| 11  | S9    | 185/196 (94%)   | 0.33   | 6 (3%) 45 9  | 70, 87, 124, 168      | 0     |
| 11  | s9    | 185/196 (94%)   | 0.14   | 1 (0%) 88 36 | 52, 65, 106, 145      | 0     |
| 12  | C0    | 96/105 (91%)    | 0.29   | 0 100 100    | 73, 94, 132, 148      | 0     |
| 12  | c0    | 96/105 (91%)    | 0.95   | 13 (13%) 4 1 | 86, 120, 150, 176     | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 13  | C1    | 155/155 (100%) | 0.30   | 11 (7%) 16 4 | 49, 60, 129, 138      | 0     |
| 13  | c1    | 146/155 (94%)  | 0.20   | 8 (5%) 24 5  | 37, 53, 92, 122       | 0     |
| 14  | C2    | 124/142 (87%)  | 1.26   | 25 (20%) 2 1 | 120, 135, 163, 180    | 0     |
| 14  | c2    | 124/142 (87%)  | 1.70   | 40 (32%) 1 0 | 168, 188, 215, 223    | 0     |
| 15  | C3    | 150/150 (100%) | 0.17   | 1 (0%) 84 28 | 58, 77, 93, 104       | 0     |
| 15  | c3    | 150/150 (100%) | -0.18  | 0 100 100    | 46, 61, 81, 94        | 0     |
| 16  | C4    | 127/136 (93%)  | 0.47   | 3 (2%) 56 11 | 59, 115, 135, 140     | 0     |
| 16  | c4    | 128/136 (94%)  | 0.03   | 0 100 100    | 40, 72, 82, 92        | 0     |
| 17  | C5    | 124/141 (87%)  | 0.37   | 2 (1%) 68 16 | 69, 87, 128, 156      | 0     |
| 17  | c5    | 135/141 (95%)  | 0.51   | 11 (8%) 12 3 | 65, 91, 119, 128      | 0     |
| 18  | C6    | 141/142 (99%)  | 0.38   | 7 (4%) 28 6  | 71, 99, 107, 111      | 0     |
| 18  | c6    | 142/142 (100%) | 0.12   | 1 (0%) 84 28 | 54, 71, 87, 113       | 0     |
| 19  | C7    | 120/136 (88%)  | 0.06   | 2 (1%) 67 15 | 79, 100, 133, 137     | 0     |
| 19  | c7    | 117/136 (86%)  | 0.09   | 1 (0%) 81 24 | 65, 80, 109, 119      | 0     |
| 20  | C8    | 145/145 (100%) | 0.23   | 3 (2%) 60 12 | 69, 98, 127, 134      | 0     |
| 20  | c8    | 145/145 (100%) | -0.05  | 0 100 100    | 55, 74, 106, 120      | 0     |
| 21  | C9    | 143/143 (100%) | 0.05   | 0 100 100    | 79, 96, 116, 129      | 0     |
| 21  | c9    | 143/143 (100%) | -0.05  | 0 100 100    | 52, 62, 84, 106       | 0     |
| 22  | D0    | 107/120 (89%)  | 0.42   | 2 (1%) 64 13 | 65, 98, 139, 145      | 0     |
| 22  | d0    | 110/120 (91%)  | 0.04   | 1 (0%) 81 24 | 56, 94, 140, 156      | 0     |
| 23  | D1    | 87/87 (100%)   | 0.01   | 0 100 100    | 78, 86, 105, 116      | 0     |
| 23  | d1    | 87/87 (100%)   | -0.16  | 0 100 100    | 58, 66, 90, 101       | 0     |
| 24  | D2    | 129/129 (100%) | -0.13  | 0 100 100    | 58, 70, 77, 87        | 0     |
| 24  | d2    | 129/129 (100%) | -0.29  | 0 100 100    | 41, 52, 59, 68        | 0     |
| 25  | D3    | 144/144 (100%) | 0.03   | 0 100 100    | 48, 53, 66, 81        | 0     |
| 25  | d3    | 144/144 (100%) | -0.18  | 0 100 100    | 34, 38, 50, 70        | 0     |
| 26  | D4    | 134/134 (100%) | 0.27   | 0 100 100    | 63, 91, 114, 125      | 0     |
| 26  | d4    | 134/134 (100%) | -0.07  | 0 100 100    | 47, 69, 87, 115       | 0     |
| 27  | D5    | 70/107 (65%)   | 0.68   | 4 (5%) 23 5  | 102, 124, 133, 140    | 0     |
| 27  | d5    | 69/107 (64%)   | 0.26   | 1 (1%) 72 18 | 71, 97, 114, 120      | 0     |
| 28  | D6    | 97/97 (100%)   | 0.42   | 3 (3%) 47 9  | 62, 77, 140, 145      | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 28  | d6    | 97/97 (100%)    | 0.01   | 1 (1%) 79 22  | 44, 53, 87, 98        | 0     |
| 29  | D7    | 81/81 (100%)    | 0.43   | 6 (7%) 14 3   | 73, 90, 135, 148      | 0     |
| 29  | d7    | 81/81 (100%)    | 0.14   | 1 (1%) 75 20  | 56, 73, 126, 135      | 0     |
| 30  | D8    | 63/66 (95%)     | 0.42   | 1 (1%) 68 16  | 102, 120, 137, 154    | 0     |
| 30  | d8    | 63/66 (95%)     | 0.47   | 2 (3%) 45 9   | 76, 94, 111, 126      | 0     |
| 31  | D9    | 53/55 (96%)     | 0.03   | 1 (1%) 64 13  | 66, 71, 92, 100       | 0     |
| 31  | d9    | 53/55 (96%)     | 0.36   | 2 (3%) 38 7   | 58, 69, 112, 128      | 0     |
| 32  | E0    | 60/60 (100%)    | 0.25   | 3 (5%) 28 6   | 52, 84, 139, 149      | 0     |
| 33  | E1    | 71/76 (93%)     | 0.63   | 6 (8%) 11 3   | 99, 118, 132, 136     | 0     |
| 33  | e1    | 76/76 (100%)    | 1.80   | 24 (31%) 1 0  | 136, 154, 168, 169    | 0     |
| 34  | SR    | 318/318 (100%)  | 0.31   | 7 (2%) 59 12  | 65, 105, 130, 151     | 0     |
| 34  | sR    | 318/318 (100%)  | 0.21   | 4 (1%) 74 19  | 80, 100, 120, 147     | 0     |
| 35  | SM    | 159/273 (58%)   | 0.35   | 9 (5%) 23 5   | 58, 81, 135, 140      | 0     |
| 36  | 1     | 3149/3396 (92%) | -0.28  | 55 (1%) 67 15 | 18, 39, 125, 256      | 0     |
| 36  | 5     | 3150/3396 (92%) | -0.30  | 49 (1%) 68 16 | 18, 38, 110, 247      | 0     |
| 37  | 3     | 121/121 (100%)  | -0.52  | 0 100 100     | 30, 57, 74, 80        | 0     |
| 37  | 7     | 121/121 (100%)  | -0.56  | 0 100 100     | 24, 40, 53, 59        | 0     |
| 38  | 4     | 158/158 (100%)  | -0.41  | 2 (1%) 74 19  | 23, 41, 77, 127       | 0     |
| 38  | 8     | 158/158 (100%)  | -0.41  | 2 (1%) 74 19  | 27, 49, 86, 114       | 0     |
| 39  | L2    | 252/253 (99%)   | -0.24  | 0 100 100     | 23, 38, 55, 65        | 0     |
| 39  | l2    | 252/253 (99%)   | -0.20  | 2 (0%) 83 26  | 24, 42, 61, 73        | 0     |
| 40  | L3    | 386/386 (100%)  | -0.30  | 1 (0%) 91 48  | 22, 44, 58, 97        | 0     |
| 40  | l3    | 386/386 (100%)  | -0.33  | 1 (0%) 91 48  | 17, 29, 43, 75        | 0     |
| 41  | L4    | 361/361 (100%)  | -0.32  | 0 100 100     | 18, 32, 50, 62        | 0     |
| 41  | l4    | 361/361 (100%)  | -0.32  | 0 100 100     | 21, 38, 58, 73        | 0     |
| 42  | L5    | 296/296 (100%)  | -0.09  | 2 (0%) 84 28  | 39, 63, 84, 122       | 0     |
| 42  | l5    | 294/296 (99%)   | -0.20  | 0 100 100     | 29, 44, 72, 118       | 0     |
| 43  | L6    | 156/175 (89%)   | -0.27  | 0 100 100     | 29, 35, 54, 74        | 0     |
| 43  | l6    | 157/175 (89%)   | -0.31  | 0 100 100     | 28, 37, 58, 70        | 0     |
| 44  | L7    | 222/243 (91%)   | -0.27  | 0 100 100     | 21, 30, 64, 117       | 0     |
| 44  | l7    | 223/243 (91%)   | -0.31  | 0 100 100     | 20, 27, 68, 126       | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 45  | L8    | 233/255 (91%)  | 0.05   | 0 100 100    | 46, 60, 102, 131      | 0     |
| 45  | l8    | 231/255 (90%)  | 0.17   | 4 (1%) 67 15 | 57, 71, 103, 109      | 0     |
| 46  | L9    | 191/191 (100%) | -0.17  | 0 100 100    | 40, 51, 64, 86        | 0     |
| 46  | l9    | 191/191 (100%) | -0.31  | 0 100 100    | 25, 34, 55, 82        | 0     |
| 47  | M0    | 211/220 (95%)  | -0.16  | 0 100 100    | 28, 42, 82, 102       | 0     |
| 47  | m0    | 213/220 (96%)  | -0.22  | 2 (0%) 81 24 | 30, 46, 70, 89        | 0     |
| 48  | M1    | 169/173 (97%)  | -0.08  | 0 100 100    | 49, 69, 83, 93        | 0     |
| 48  | m1    | 169/173 (97%)  | -0.18  | 1 (0%) 86 32 | 31, 49, 64, 74        | 0     |
| 49  | M3    | 193/198 (97%)  | -0.16  | 0 100 100    | 22, 42, 87, 117       | 0     |
| 49  | m3    | 194/198 (97%)  | -0.01  | 1 (0%) 88 36 | 28, 52, 97, 132       | 0     |
| 50  | M4    | 136/137 (99%)  | -0.33  | 0 100 100    | 31, 41, 54, 65        | 0     |
| 50  | m4    | 137/137 (100%) | -0.35  | 0 100 100    | 26, 30, 51, 64        | 0     |
| 51  | M5    | 203/203 (100%) | -0.31  | 0 100 100    | 21, 36, 47, 51        | 0     |
| 51  | m5    | 203/203 (100%) | -0.26  | 0 100 100    | 27, 46, 57, 62        | 0     |
| 52  | M6    | 197/198 (99%)  | -0.27  | 0 100 100    | 22, 30, 53, 58        | 0     |
| 52  | m6    | 197/198 (99%)  | -0.34  | 0 100 100    | 18, 21, 47, 52        | 0     |
| 53  | M7    | 183/183 (100%) | -0.05  | 6 (3%) 44 8  | 25, 32, 93, 144       | 0     |
| 53  | m7    | 155/183 (84%)  | -0.27  | 0 100 100    | 20, 29, 43, 89        | 0     |
| 54  | M8    | 185/185 (100%) | -0.33  | 0 100 100    | 23, 33, 48, 66        | 0     |
| 54  | m8    | 185/185 (100%) | -0.27  | 0 100 100    | 26, 38, 45, 52        | 0     |
| 55  | M9    | 188/188 (100%) | 0.14   | 1 (0%) 88 36 | 39, 56, 160, 170      | 0     |
| 55  | m9    | 188/188 (100%) | -0.09  | 0 100 100    | 37, 49, 124, 142      | 0     |
| 56  | N0    | 172/172 (100%) | -0.39  | 1 (0%) 86 32 | 31, 38, 52, 60        | 0     |
| 56  | n0    | 172/172 (100%) | -0.40  | 0 100 100    | 23, 29, 39, 53        | 0     |
| 57  | N1    | 159/159 (100%) | -0.26  | 0 100 100    | 29, 37, 85, 97        | 0     |
| 57  | n1    | 159/159 (100%) | -0.29  | 0 100 100    | 25, 31, 74, 82        | 0     |
| 58  | N2    | 100/120 (83%)  | 0.00   | 3 (3%) 48 9  | 70, 88, 104, 131      | 0     |
| 58  | n2    | 98/120 (81%)   | 0.65   | 6 (6%) 21 5  | 63, 78, 91, 93        | 0     |
| 59  | N3    | 136/136 (100%) | -0.13  | 0 100 100    | 28, 38, 50, 57        | 0     |
| 59  | n3    | 136/136 (100%) | -0.15  | 0 100 100    | 18, 27, 41, 46        | 0     |
| 60  | N4    | 98/155 (63%)   | 1.00   | 24 (24%) 1 1 | 39, 53, 163, 167      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 60  | n4    | 135/155 (87%)  | 0.36   | 8 (5%) 22 5  | 28, 80, 133, 156      | 0     |
| 61  | N5    | 121/141 (85%)  | -0.19  | 2 (1%) 67 15 | 35, 47, 66, 101       | 0     |
| 61  | n5    | 120/141 (85%)  | 0.05   | 1 (0%) 83 26 | 39, 54, 75, 82        | 0     |
| 62  | N6    | 126/126 (100%) | -0.05  | 1 (0%) 83 26 | 30, 42, 53, 62        | 0     |
| 62  | n6    | 126/126 (100%) | 0.08   | 0 100 100    | 35, 48, 63, 70        | 0     |
| 63  | N7    | 135/135 (100%) | 0.06   | 0 100 100    | 57, 73, 88, 98        | 0     |
| 63  | n7    | 135/135 (100%) | 0.45   | 7 (5%) 26 6  | 65, 82, 103, 113      | 0     |
| 64  | N8    | 148/148 (100%) | -0.15  | 0 100 100    | 18, 34, 56, 66        | 0     |
| 64  | n8    | 148/148 (100%) | -0.17  | 0 100 100    | 19, 40, 58, 62        | 0     |
| 65  | N9    | 58/58 (100%)   | -0.08  | 0 100 100    | 24, 41, 97, 116       | 0     |
| 65  | n9    | 58/58 (100%)   | -0.14  | 0 100 100    | 21, 40, 65, 75        | 0     |
| 66  | O0    | 97/104 (93%)   | 0.10   | 1 (1%) 79 22 | 57, 67, 100, 108      | 0     |
| 66  | o0    | 100/104 (96%)  | 0.01   | 0 100 100    | 57, 70, 99, 111       | 0     |
| 67  | O1    | 109/112 (97%)  | 0.12   | 2 (1%) 65 14 | 37, 50, 89, 103       | 0     |
| 67  | o1    | 109/112 (97%)  | -0.11  | 0 100 100    | 29, 40, 84, 110       | 0     |
| 68  | O2    | 127/129 (98%)  | -0.12  | 1 (0%) 83 26 | 17, 29, 38, 51        | 0     |
| 68  | o2    | 127/129 (98%)  | -0.05  | 2 (1%) 68 16 | 17, 35, 48, 73        | 0     |
| 69  | O3    | 106/106 (100%) | -0.35  | 0 100 100    | 22, 27, 45, 54        | 0     |
| 69  | o3    | 106/106 (100%) | -0.32  | 0 100 100    | 21, 26, 51, 62        | 0     |
| 70  | O4    | 112/119 (94%)  | 0.05   | 2 (1%) 65 14 | 35, 54, 96, 113       | 0     |
| 70  | o4    | 112/119 (94%)  | 0.07   | 0 100 100    | 37, 57, 103, 117      | 0     |
| 71  | O5    | 119/119 (100%) | -0.18  | 0 100 100    | 34, 49, 57, 62        | 0     |
| 71  | o5    | 119/119 (100%) | -0.06  | 1 (0%) 83 26 | 44, 56, 69, 77        | 0     |
| 72  | O6    | 99/99 (100%)   | -0.21  | 0 100 100    | 38, 51, 88, 103       | 0     |
| 72  | o6    | 99/99 (100%)   | -0.01  | 0 100 100    | 45, 61, 86, 111       | 0     |
| 73  | O7    | 87/87 (100%)   | -0.32  | 0 100 100    | 23, 29, 54, 74        | 0     |
| 73  | o7    | 87/87 (100%)   | -0.14  | 2 (2%) 57 12 | 28, 34, 64, 102       | 0     |
| 74  | O8    | 77/77 (100%)   | 0.10   | 0 100 100    | 61, 73, 103, 112      | 0     |
| 74  | o8    | 77/77 (100%)   | 0.23   | 0 100 100    | 65, 77, 101, 107      | 0     |
| 75  | O9    | 50/50 (100%)   | -0.13  | 0 100 100    | 34, 36, 42, 45        | 0     |
| 75  | o9    | 50/50 (100%)   | -0.05  | 0 100 100    | 39, 41, 48, 57        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2                                  | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|--|-----------------------|-------|
| 76  | Q0    | 52/52 (100%)      | -0.02  | 0 <span>100</span> <span>100</span>      | 37, 43, 60, 69        | 0     |
| 76  | q0    | 52/52 (100%)      | -0.15  | 0 <span>100</span> <span>100</span>      | 21, 25, 34, 41        | 0     |
| 77  | Q1    | 25/25 (100%)      | 0.56   | 1 (4%) <span>36</span> <span>7</span>    | 43, 45, 49, 50        | 0     |
| 77  | q1    | 25/25 (100%)      | 0.23   | 0 <span>100</span> <span>100</span>      | 33, 35, 43, 51        | 0     |
| 78  | Q2    | 105/105 (100%)    | -0.05  | 1 (0%) <span>79</span> <span>22</span>   | 23, 42, 64, 105       | 0     |
| 78  | q2    | 105/105 (100%)    | -0.03  | 0 <span>100</span> <span>100</span>      | 29, 41, 57, 99        | 0     |
| 79  | Q3    | 91/91 (100%)      | -0.35  | 0 <span>100</span> <span>100</span>      | 31, 41, 58, 74        | 0     |
| 79  | q3    | 91/91 (100%)      | -0.24  | 0 <span>100</span> <span>100</span>      | 30, 43, 56, 67        | 0     |
| 80  | e0    | 62/62 (100%)      | 0.11   | 2 (3%) <span>45</span> <span>9</span>    | 44, 66, 120, 125      | 0     |
| 81  | sM    | 104/273 (38%)     | 0.45   | 7 (6%) <span>17</span> <span>4</span>    | 53, 91, 163, 183      | 0     |
| 82  | m2    | 0/160             | -      | -  | -                     | -     |
| 83  | p0    | 143/311 (45%)     | 0.77   | 10 (6%) <span>16</span> <span>4</span>   | 76, 96, 181, 185      | 0     |
| 84  | p1    | 0/47              | -      | -  | -                     | -     |
| 85  | p2    | 0/46              | -      | -  | -                     | -     |
| All | All   | 33063/35344 (93%) | -0.06  | 620 (1%) <span>64</span> <span>13</span> | 17, 56, 125, 265      | 0     |

The worst 5 of 620 RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 60  | N4    | 76   | VAL  | 11.0 |
| 33  | e1    | 77   | GLY  | 10.4 |
| 36  | 5     | 2506 | U    | 8.2  |
| 1   | 6     | 662  | U    | 8.2  |
| 60  | N4    | 75   | THR  | 7.6  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF    | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|---------|----------------------------|-------|
| 86  | MG   | 2     | 1958 | 1/1   | 0.87 | 1461.00 | 74,74,74,74                | 0     |
| 86  | MG   | 1     | 3537 | 1/1   | 0.55 | 837.00  | 33,33,33,33                | 0     |
| 86  | MG   | 5     | 3478 | 1/1   | 0.36 | 443.00  | 49,49,49,49                | 0     |
| 86  | MG   | 5     | 3521 | 1/1   | 0.35 | 359.00  | 32,32,32,32                | 0     |
| 86  | MG   | 1     | 3409 | 1/1   | 0.38 | 284.14  | 16,16,16,16                | 0     |
| 86  | MG   | 5     | 3690 | 1/1   | 0.61 | 277.67  | 39,39,39,39                | 0     |
| 86  | MG   | 1     | 3592 | 1/1   | 0.33 | 231.48  | 27,27,27,27                | 0     |
| 86  | MG   | 5     | 3863 | 1/1   | 0.35 | 214.00  | 47,47,47,47                | 0     |
| 86  | MG   | 1     | 3682 | 1/1   | 0.47 | 203.67  | 52,52,52,52                | 0     |
| 86  | MG   | 1     | 3787 | 1/1   | 0.31 | 169.00  | 34,34,34,34                | 0     |
| 86  | MG   | 1     | 3705 | 1/1   | 0.40 | 155.67  | 39,39,39,39                | 0     |
| 86  | MG   | 1     | 3468 | 1/1   | 0.58 | 155.07  | 46,46,46,46                | 0     |
| 86  | MG   | 6     | 1925 | 1/1   | 0.69 | 149.86  | 107,107,107,107            | 0     |
| 86  | MG   | 2     | 1982 | 1/1   | 0.98 | 146.51  | 75,75,75,75                | 0     |
| 86  | MG   | 2     | 1996 | 1/1   | 0.48 | 138.41  | 95,95,95,95                | 0     |
| 86  | MG   | 5     | 3881 | 1/1   | 0.41 | 137.00  | 84,84,84,84                | 0     |
| 86  | MG   | 5     | 3453 | 1/1   | 0.65 | 127.94  | 34,34,34,34                | 0     |
| 86  | MG   | 6     | 2041 | 1/1   | 0.47 | 121.40  | 58,58,58,58                | 0     |
| 86  | MG   | 5     | 3883 | 1/1   | 0.55 | 119.67  | 43,43,43,43                | 0     |
| 86  | MG   | 5     | 3886 | 1/1   | 0.45 | 119.40  | 74,74,74,74                | 0     |
| 86  | MG   | 5     | 3853 | 1/1   | 0.81 | 109.67  | 50,50,50,50                | 0     |
| 86  | MG   | 6     | 1903 | 1/1   | 0.63 | 106.02  | 40,40,40,40                | 0     |
| 86  | MG   | 5     | 3645 | 1/1   | 0.67 | 103.49  | 58,58,58,58                | 0     |
| 86  | MG   | 5     | 3490 | 1/1   | 0.41 | 102.60  | 36,36,36,36                | 0     |
| 86  | MG   | 6     | 1929 | 1/1   | 0.90 | 101.56  | 61,61,61,61                | 0     |
| 86  | MG   | 2     | 2000 | 1/1   | 0.37 | 101.40  | 112,112,112,112            | 0     |
| 86  | MG   | 5     | 3482 | 1/1   | 0.19 | 101.00  | 43,43,43,43                | 0     |
| 87  | OHX  | 6     | 2186 | 7/7   | 0.53 | 99.57   | 128,128,128,128            | 0     |
| 86  | MG   | 1     | 3501 | 1/1   | 0.33 | 98.00   | 67,67,67,67                | 0     |
| 86  | MG   | 5     | 3673 | 1/1   | 0.59 | 96.58   | 44,44,44,44                | 0     |
| 86  | MG   | 5     | 3709 | 1/1   | 0.43 | 92.00   | 85,85,85,85                | 0     |
| 86  | MG   | 7     | 216  | 1/1   | 0.35 | 91.00   | 46,46,46,46                | 0     |
| 86  | MG   | 5     | 3430 | 1/1   | 0.31 | 86.50   | 67,67,67,67                | 0     |
| 86  | MG   | 5     | 3567 | 1/1   | 0.49 | 84.60   | 17,17,17,17                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 2     | 1988 | 1/1   | 0.64 | 84.37 | 52,52,52,52                 | 0     |
| 86  | MG   | 1     | 3661 | 1/1   | 0.51 | 79.50 | 34,34,34,34                 | 0     |
| 86  | MG   | 1     | 3789 | 1/1   | 0.46 | 78.87 | 32,32,32,32                 | 0     |
| 86  | MG   | 5     | 3797 | 1/1   | 0.45 | 77.86 | 40,40,40,40                 | 0     |
| 86  | MG   | 4     | 202  | 1/1   | 0.54 | 76.34 | 46,46,46,46                 | 0     |
| 86  | MG   | 2     | 1957 | 1/1   | 0.76 | 74.50 | 60,60,60,60                 | 0     |
| 86  | MG   | 5     | 3858 | 1/1   | 1.11 | 71.46 | 67,67,67,67                 | 0     |
| 86  | MG   | 2     | 1999 | 1/1   | 0.47 | 71.46 | 87,87,87,87                 | 0     |
| 86  | MG   | 1     | 3477 | 1/1   | 0.60 | 70.33 | 46,46,46,46                 | 0     |
| 86  | MG   | 1     | 3862 | 1/1   | 0.87 | 69.96 | 56,56,56,56                 | 0     |
| 86  | MG   | 5     | 3549 | 1/1   | 0.65 | 69.33 | 32,32,32,32                 | 0     |
| 86  | MG   | L3    | 402  | 1/1   | 0.41 | 69.00 | 31,31,31,31                 | 0     |
| 86  | MG   | 1     | 3528 | 1/1   | 0.56 | 66.71 | 22,22,22,22                 | 0     |
| 86  | MG   | 5     | 3591 | 1/1   | 0.51 | 65.24 | 29,29,29,29                 | 0     |
| 86  | MG   | 1     | 3448 | 1/1   | 0.39 | 63.65 | 21,21,21,21                 | 0     |
| 86  | MG   | 5     | 3436 | 1/1   | 0.43 | 63.02 | 37,37,37,37                 | 0     |
| 86  | MG   | 5     | 3850 | 1/1   | 0.41 | 61.29 | 41,41,41,41                 | 0     |
| 87  | OHX  | 1     | 4176 | 7/7   | 0.39 | 60.65 | 115,115,115,115             | 0     |
| 86  | MG   | 1     | 3843 | 1/1   | 0.55 | 59.31 | 43,43,43,43                 | 0     |
| 86  | MG   | 1     | 3431 | 1/1   | 0.46 | 58.98 | 39,39,39,39                 | 0     |
| 87  | OHX  | M9    | 202  | 7/7   | 0.26 | 58.33 | 139,139,139,139             | 0     |
| 86  | MG   | 2     | 1913 | 1/1   | 1.23 | 57.86 | 85,85,85,85                 | 0     |
| 86  | MG   | 1     | 3493 | 1/1   | 0.61 | 57.43 | 52,52,52,52                 | 0     |
| 86  | MG   | 1     | 3485 | 1/1   | 0.38 | 56.29 | 35,35,35,35                 | 0     |
| 86  | MG   | 5     | 3780 | 1/1   | 0.48 | 53.74 | 75,75,75,75                 | 0     |
| 86  | MG   | 2     | 1925 | 1/1   | 0.65 | 53.59 | 59,59,59,59                 | 0     |
| 86  | MG   | 5     | 3553 | 1/1   | 0.65 | 53.44 | 37,37,37,37                 | 0     |
| 86  | MG   | 6     | 1945 | 1/1   | 0.54 | 53.18 | 52,52,52,52                 | 0     |
| 86  | MG   | 1     | 3591 | 1/1   | 0.62 | 53.12 | 38,38,38,38                 | 0     |
| 86  | MG   | 2     | 2008 | 1/1   | 0.56 | 52.85 | 55,55,55,55                 | 0     |
| 87  | OHX  | 5     | 4230 | 7/7   | 0.46 | 52.56 | 99,99,99,99                 | 0     |
| 86  | MG   | 6     | 2013 | 1/1   | 0.30 | 52.08 | 52,52,52,52                 | 0     |
| 86  | MG   | 6     | 1981 | 1/1   | 0.76 | 51.74 | 57,57,57,57                 | 0     |
| 86  | MG   | 5     | 3433 | 1/1   | 0.66 | 49.82 | 75,75,75,75                 | 0     |
| 86  | MG   | 2     | 1981 | 1/1   | 0.79 | 49.02 | 50,50,50,50                 | 0     |
| 86  | MG   | 1     | 3580 | 1/1   | 0.43 | 48.34 | 26,26,26,26                 | 0     |
| 86  | MG   | 2     | 1906 | 1/1   | 0.33 | 47.76 | 43,43,43,43                 | 0     |
| 86  | MG   | 5     | 3845 | 1/1   | 0.27 | 47.68 | 26,26,26,26                 | 0     |
| 86  | MG   | 5     | 3487 | 1/1   | 0.49 | 47.66 | 43,43,43,43                 | 0     |
| 86  | MG   | 1     | 3572 | 1/1   | 0.55 | 46.76 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 3507 | 1/1   | 0.53 | 45.68 | 29,29,29,29                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 5     | 3728 | 1/1   | 0.42 | 44.90 | 87,87,87,87                 | 0     |
| 86  | MG   | 6     | 1986 | 1/1   | 0.55 | 44.71 | 76,76,76,76                 | 0     |
| 86  | MG   | 5     | 3885 | 1/1   | 0.76 | 44.47 | 61,61,61,61                 | 0     |
| 86  | MG   | 1     | 3589 | 1/1   | 0.51 | 44.37 | 19,19,19,19                 | 0     |
| 86  | MG   | 4     | 210  | 1/1   | 0.39 | 44.19 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 3786 | 1/1   | 0.85 | 44.03 | 76,76,76,76                 | 0     |
| 86  | MG   | 1     | 3516 | 1/1   | 0.52 | 43.68 | 19,19,19,19                 | 0     |
| 86  | MG   | 2     | 1915 | 1/1   | 1.06 | 43.55 | 63,63,63,63                 | 0     |
| 86  | MG   | 6     | 1922 | 1/1   | 0.43 | 43.31 | 35,35,35,35                 | 0     |
| 86  | MG   | 1     | 3637 | 1/1   | 0.29 | 43.29 | 61,61,61,61                 | 0     |
| 86  | MG   | 1     | 3854 | 1/1   | 0.61 | 43.14 | 49,49,49,49                 | 0     |
| 86  | MG   | 6     | 1977 | 1/1   | 0.73 | 43.05 | 59,59,59,59                 | 0     |
| 87  | OHX  | 5     | 4171 | 7/7   | 0.36 | 43.02 | 110,110,110,110             | 0     |
| 87  | OHX  | 1     | 4171 | 7/7   | 0.36 | 43.01 | 86,86,86,86                 | 0     |
| 86  | MG   | 5     | 3632 | 1/1   | 0.55 | 42.58 | 77,77,77,77                 | 0     |
| 86  | MG   | 3     | 209  | 1/1   | 0.61 | 42.46 | 52,52,52,52                 | 0     |
| 86  | MG   | 2     | 1975 | 1/1   | 1.04 | 42.17 | 74,74,74,74                 | 0     |
| 86  | MG   | 1     | 3509 | 1/1   | 0.44 | 42.07 | 22,22,22,22                 | 0     |
| 86  | MG   | 2     | 2012 | 1/1   | 0.54 | 41.94 | 55,55,55,55                 | 0     |
| 86  | MG   | 5     | 3578 | 1/1   | 0.80 | 41.39 | 36,36,36,36                 | 0     |
| 86  | MG   | 5     | 3665 | 1/1   | 0.86 | 40.88 | 54,54,54,54                 | 0     |
| 86  | MG   | 5     | 3582 | 1/1   | 0.54 | 40.63 | 34,34,34,34                 | 0     |
| 86  | MG   | 5     | 3896 | 1/1   | 0.57 | 39.70 | 88,88,88,88                 | 0     |
| 86  | MG   | 6     | 1917 | 1/1   | 0.75 | 39.38 | 49,49,49,49                 | 0     |
| 86  | MG   | 5     | 3781 | 1/1   | 0.46 | 39.27 | 72,72,72,72                 | 0     |
| 86  | MG   | 5     | 3575 | 1/1   | 0.41 | 39.20 | 20,20,20,20                 | 0     |
| 86  | MG   | 6     | 1941 | 1/1   | 0.63 | 38.91 | 75,75,75,75                 | 0     |
| 86  | MG   | 1     | 3849 | 1/1   | 0.54 | 38.69 | 57,57,57,57                 | 0     |
| 86  | MG   | 1     | 3419 | 1/1   | 0.44 | 38.39 | 83,83,83,83                 | 0     |
| 86  | MG   | 5     | 3625 | 1/1   | 0.41 | 38.37 | 30,30,30,30                 | 0     |
| 87  | OHX  | 1     | 4151 | 7/7   | 0.34 | 38.34 | 108,108,108,108             | 0     |
| 86  | MG   | 1     | 3544 | 1/1   | 0.48 | 38.27 | 28,28,28,28                 | 0     |
| 86  | MG   | 1     | 3543 | 1/1   | 0.64 | 38.26 | 27,27,27,27                 | 0     |
| 86  | MG   | 4     | 219  | 1/1   | 0.71 | 38.16 | 73,73,73,73                 | 0     |
| 86  | MG   | 5     | 3584 | 1/1   | 0.41 | 37.81 | 21,21,21,21                 | 0     |
| 86  | MG   | 5     | 3458 | 1/1   | 0.39 | 37.44 | 58,58,58,58                 | 0     |
| 86  | MG   | 2     | 1924 | 1/1   | 0.52 | 36.94 | 73,73,73,73                 | 0     |
| 86  | MG   | 5     | 3538 | 1/1   | 0.41 | 36.92 | 29,29,29,29                 | 0     |
| 86  | MG   | 2     | 1935 | 1/1   | 0.54 | 36.61 | 44,44,44,44                 | 0     |
| 86  | MG   | 5     | 3775 | 1/1   | 0.30 | 36.42 | 26,26,26,26                 | 0     |
| 86  | MG   | 5     | 3466 | 1/1   | 0.48 | 36.21 | 81,81,81,81                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 1     | 3599 | 1/1   | 0.49 | 36.13 | 29,29,29,29                 | 0     |
| 86  | MG   | 2     | 1917 | 1/1   | 0.68 | 36.07 | 50,50,50,50                 | 0     |
| 86  | MG   | 1     | 3575 | 1/1   | 0.48 | 35.86 | 29,29,29,29                 | 0     |
| 86  | MG   | 2     | 2020 | 1/1   | 0.88 | 35.72 | 109,109,109,109             | 0     |
| 86  | MG   | 1     | 3530 | 1/1   | 0.63 | 35.70 | 27,27,27,27                 | 0     |
| 86  | MG   | 7     | 204  | 1/1   | 0.57 | 35.63 | 70,70,70,70                 | 0     |
| 86  | MG   | 6     | 2049 | 1/1   | 0.43 | 35.40 | 62,62,62,62                 | 0     |
| 86  | MG   | 7     | 207  | 1/1   | 0.27 | 35.36 | 46,46,46,46                 | 0     |
| 86  | MG   | 1     | 3556 | 1/1   | 0.53 | 35.22 | 19,19,19,19                 | 0     |
| 86  | MG   | 2     | 1962 | 1/1   | 0.56 | 35.17 | 69,69,69,69                 | 0     |
| 86  | MG   | 6     | 2015 | 1/1   | 0.33 | 35.00 | 141,141,141,141             | 0     |
| 86  | MG   | 5     | 3539 | 1/1   | 0.43 | 34.84 | 14,14,14,14                 | 0     |
| 86  | MG   | 1     | 3620 | 1/1   | 0.33 | 34.82 | 47,47,47,47                 | 0     |
| 86  | MG   | 1     | 3465 | 1/1   | 0.37 | 34.65 | 50,50,50,50                 | 0     |
| 86  | MG   | 2     | 1903 | 1/1   | 0.65 | 34.57 | 51,51,51,51                 | 0     |
| 86  | MG   | 5     | 3880 | 1/1   | 0.39 | 34.47 | 48,48,48,48                 | 0     |
| 87  | OHX  | 5     | 4181 | 7/7   | 0.41 | 34.34 | 139,139,139,139             | 0     |
| 86  | MG   | 5     | 3719 | 1/1   | 0.51 | 34.31 | 61,61,61,61                 | 0     |
| 86  | MG   | 7     | 205  | 1/1   | 0.42 | 34.28 | 19,19,19,19                 | 0     |
| 86  | MG   | 1     | 3408 | 1/1   | 0.44 | 34.04 | 25,25,25,25                 | 0     |
| 86  | MG   | 2     | 1973 | 1/1   | 0.43 | 34.01 | 69,69,69,69                 | 0     |
| 86  | MG   | 5     | 3527 | 1/1   | 0.46 | 33.95 | 23,23,23,23                 | 0     |
| 86  | MG   | 2     | 1934 | 1/1   | 0.54 | 33.87 | 44,44,44,44                 | 0     |
| 86  | MG   | 1     | 3841 | 1/1   | 0.45 | 33.64 | 24,24,24,24                 | 0     |
| 86  | MG   | 5     | 3598 | 1/1   | 0.58 | 33.56 | 22,22,22,22                 | 0     |
| 86  | MG   | 5     | 3502 | 1/1   | 0.47 | 33.55 | 38,38,38,38                 | 0     |
| 86  | MG   | 3     | 213  | 1/1   | 0.51 | 33.50 | 50,50,50,50                 | 0     |
| 86  | MG   | 1     | 3413 | 1/1   | 0.61 | 33.46 | 50,50,50,50                 | 0     |
| 86  | MG   | 1     | 3538 | 1/1   | 0.64 | 33.36 | 26,26,26,26                 | 0     |
| 86  | MG   | 5     | 3431 | 1/1   | 0.29 | 33.15 | 26,26,26,26                 | 0     |
| 86  | MG   | 1     | 3865 | 1/1   | 0.37 | 33.08 | 32,32,32,32                 | 0     |
| 86  | MG   | 6     | 1940 | 1/1   | 0.65 | 32.68 | 53,53,53,53                 | 0     |
| 86  | MG   | 5     | 3531 | 1/1   | 0.51 | 32.56 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 3542 | 1/1   | 0.34 | 32.45 | 18,18,18,18                 | 0     |
| 86  | MG   | 1     | 3576 | 1/1   | 0.43 | 32.19 | 15,15,15,15                 | 0     |
| 86  | MG   | 5     | 3604 | 1/1   | 0.50 | 32.03 | 31,31,31,31                 | 0     |
| 86  | MG   | 6     | 1934 | 1/1   | 0.74 | 31.94 | 54,54,54,54                 | 0     |
| 86  | MG   | 17    | 302  | 1/1   | 0.43 | 31.80 | 41,41,41,41                 | 0     |
| 86  | MG   | 6     | 2046 | 1/1   | 0.32 | 31.73 | 38,38,38,38                 | 0     |
| 86  | MG   | 2     | 1943 | 1/1   | 0.62 | 31.73 | 59,59,59,59                 | 0     |
| 86  | MG   | 5     | 3537 | 1/1   | 0.44 | 31.69 | 30,30,30,30                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 5     | 3414 | 1/1   | 0.45 | 31.46 | 21,21,21,21                 | 0     |
| 86  | MG   | 5     | 3874 | 1/1   | 0.39 | 31.40 | 39,39,39,39                 | 0     |
| 86  | MG   | 5     | 3557 | 1/1   | 0.39 | 31.37 | 17,17,17,17                 | 0     |
| 86  | MG   | 1     | 3685 | 1/1   | 0.25 | 31.33 | 44,44,44,44                 | 0     |
| 86  | MG   | 5     | 3480 | 1/1   | 0.74 | 31.25 | 57,57,57,57                 | 0     |
| 86  | MG   | 6     | 2020 | 1/1   | 0.60 | 31.15 | 45,45,45,45                 | 0     |
| 86  | MG   | 1     | 3846 | 1/1   | 0.56 | 31.15 | 44,44,44,44                 | 0     |
| 86  | MG   | 5     | 3762 | 1/1   | 0.40 | 31.12 | 63,63,63,63                 | 0     |
| 86  | MG   | 1     | 3563 | 1/1   | 0.44 | 31.10 | 19,19,19,19                 | 0     |
| 86  | MG   | 5     | 3530 | 1/1   | 0.47 | 31.04 | 17,17,17,17                 | 0     |
| 86  | MG   | 6     | 1905 | 1/1   | 0.66 | 30.99 | 49,49,49,49                 | 0     |
| 86  | MG   | 1     | 3480 | 1/1   | 0.53 | 30.91 | 70,70,70,70                 | 0     |
| 86  | MG   | 1     | 3521 | 1/1   | 0.56 | 30.81 | 34,34,34,34                 | 0     |
| 86  | MG   | 1     | 3460 | 1/1   | 0.41 | 30.79 | 17,17,17,17                 | 0     |
| 86  | MG   | 5     | 3524 | 1/1   | 0.56 | 30.78 | 29,29,29,29                 | 0     |
| 86  | MG   | 5     | 3681 | 1/1   | 0.33 | 30.63 | 36,36,36,36                 | 0     |
| 86  | MG   | 6     | 1927 | 1/1   | 0.60 | 30.54 | 39,39,39,39                 | 0     |
| 86  | MG   | 5     | 3507 | 1/1   | 0.65 | 30.45 | 29,29,29,29                 | 0     |
| 86  | MG   | 5     | 3793 | 1/1   | 0.45 | 30.38 | 87,87,87,87                 | 0     |
| 86  | MG   | 5     | 3564 | 1/1   | 0.54 | 30.35 | 22,22,22,22                 | 0     |
| 86  | MG   | 6     | 2048 | 1/1   | 0.36 | 30.33 | 90,90,90,90                 | 0     |
| 86  | MG   | 5     | 3571 | 1/1   | 0.54 | 30.30 | 20,20,20,20                 | 0     |
| 86  | MG   | 5     | 3563 | 1/1   | 0.68 | 30.17 | 27,27,27,27                 | 0     |
| 86  | MG   | 6     | 1959 | 1/1   | 0.52 | 29.57 | 46,46,46,46                 | 0     |
| 87  | OHX  | 5     | 4236 | 7/7   | 0.50 | 29.46 | 141,141,141,141             | 0     |
| 87  | OHX  | 5     | 4220 | 7/7   | 0.36 | 29.43 | 111,111,111,111             | 0     |
| 86  | MG   | 1     | 3557 | 1/1   | 0.47 | 29.43 | 27,27,27,27                 | 0     |
| 86  | MG   | 1     | 3838 | 1/1   | 0.35 | 29.25 | 19,19,19,19                 | 0     |
| 86  | MG   | 3     | 204  | 1/1   | 0.48 | 28.91 | 46,46,46,46                 | 0     |
| 86  | MG   | 5     | 3621 | 1/1   | 0.32 | 28.82 | 37,37,37,37                 | 0     |
| 87  | OHX  | 5     | 4189 | 7/7   | 0.56 | 28.82 | 88,88,88,88                 | 0     |
| 86  | MG   | 1     | 3590 | 1/1   | 0.40 | 28.75 | 22,22,22,22                 | 0     |
| 86  | MG   | 1     | 3729 | 1/1   | 0.50 | 28.68 | 24,24,24,24                 | 0     |
| 86  | MG   | 5     | 3738 | 1/1   | 0.27 | 28.60 | 35,35,35,35                 | 0     |
| 87  | OHX  | 1     | 4193 | 7/7   | 0.45 | 28.50 | 97,97,97,97                 | 0     |
| 86  | MG   | 1     | 3402 | 1/1   | 0.51 | 28.49 | 42,42,42,42                 | 0     |
| 86  | MG   | 1     | 3856 | 1/1   | 0.76 | 28.40 | 75,75,75,75                 | 0     |
| 86  | MG   | 1     | 3562 | 1/1   | 0.60 | 28.39 | 32,32,32,32                 | 0     |
| 86  | MG   | 5     | 3525 | 1/1   | 0.51 | 28.35 | 21,21,21,21                 | 0     |
| 86  | MG   | 5     | 3656 | 1/1   | 0.27 | 28.33 | 59,59,59,59                 | 0     |
| 86  | MG   | 5     | 3541 | 1/1   | 0.49 | 28.28 | 24,24,24,24                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 6     | 1951 | 1/1   | 0.38 | 28.19 | 36,36,36,36                 | 0     |
| 86  | MG   | 6     | 1952 | 1/1   | 0.65 | 28.15 | 59,59,59,59                 | 0     |
| 86  | MG   | 6     | 1921 | 1/1   | 0.53 | 27.81 | 54,54,54,54                 | 0     |
| 86  | MG   | 5     | 3518 | 1/1   | 0.45 | 27.81 | 18,18,18,18                 | 0     |
| 86  | MG   | 1     | 3860 | 1/1   | 0.31 | 27.67 | 53,53,53,53                 | 0     |
| 86  | MG   | 1     | 3549 | 1/1   | 0.41 | 27.67 | 42,42,42,42                 | 0     |
| 86  | MG   | 1     | 3597 | 1/1   | 0.48 | 27.63 | 16,16,16,16                 | 0     |
| 86  | MG   | 1     | 3532 | 1/1   | 0.41 | 27.47 | 19,19,19,19                 | 0     |
| 86  | MG   | 6     | 1912 | 1/1   | 0.61 | 27.39 | 76,76,76,76                 | 0     |
| 86  | MG   | 6     | 1969 | 1/1   | 0.41 | 27.29 | 71,71,71,71                 | 0     |
| 86  | MG   | 2     | 2016 | 1/1   | 0.50 | 27.21 | 69,69,69,69                 | 0     |
| 86  | MG   | 2     | 2017 | 1/1   | 1.22 | 27.20 | 65,65,65,65                 | 0     |
| 87  | OHX  | 1     | 4167 | 7/7   | 0.33 | 27.17 | 132,132,132,132             | 0     |
| 86  | MG   | 1     | 3773 | 1/1   | 0.23 | 26.87 | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 3556 | 1/1   | 0.42 | 26.72 | 26,26,26,26                 | 0     |
| 86  | MG   | 6     | 1957 | 1/1   | 0.50 | 26.70 | 38,38,38,38                 | 0     |
| 86  | MG   | 6     | 2037 | 1/1   | 0.65 | 26.70 | 58,58,58,58                 | 0     |
| 86  | MG   | 2     | 1994 | 1/1   | 0.30 | 26.67 | 82,82,82,82                 | 0     |
| 86  | MG   | 8     | 205  | 1/1   | 0.48 | 26.66 | 46,46,46,46                 | 0     |
| 86  | MG   | 1     | 3478 | 1/1   | 0.41 | 26.56 | 39,39,39,39                 | 0     |
| 86  | MG   | 7     | 210  | 1/1   | 0.31 | 26.33 | 44,44,44,44                 | 0     |
| 86  | MG   | 5     | 3771 | 1/1   | 0.34 | 26.29 | 58,58,58,58                 | 0     |
| 86  | MG   | 3     | 205  | 1/1   | 0.33 | 26.27 | 29,29,29,29                 | 0     |
| 86  | MG   | 1     | 3458 | 1/1   | 0.68 | 26.23 | 62,62,62,62                 | 0     |
| 86  | MG   | 1     | 3565 | 1/1   | 0.49 | 26.22 | 26,26,26,26                 | 0     |
| 86  | MG   | 5     | 3585 | 1/1   | 0.56 | 26.08 | 22,22,22,22                 | 0     |
| 87  | OHX  | 2     | 2123 | 7/7   | 0.31 | 26.02 | 104,104,104,104             | 0     |
| 86  | MG   | 6     | 2032 | 1/1   | 0.56 | 26.02 | 76,76,76,76                 | 0     |
| 87  | OHX  | 1     | 4144 | 7/7   | 0.44 | 26.01 | 88,88,88,88                 | 0     |
| 86  | MG   | 1     | 3802 | 1/1   | 0.29 | 26.00 | 42,42,42,42                 | 0     |
| 86  | MG   | 1     | 3579 | 1/1   | 0.44 | 25.97 | 18,18,18,18                 | 0     |
| 87  | OHX  | 1     | 4132 | 7/7   | 0.45 | 25.87 | 134,134,134,134             | 0     |
| 86  | MG   | 2     | 1931 | 1/1   | 0.49 | 25.77 | 53,53,53,53                 | 0     |
| 86  | MG   | 6     | 1914 | 1/1   | 0.39 | 25.75 | 31,31,31,31                 | 0     |
| 87  | OHX  | 5     | 4141 | 7/7   | 0.23 | 25.74 | 118,118,118,118             | 0     |
| 87  | OHX  | 1     | 4150 | 7/7   | 0.35 | 25.70 | 124,124,124,124             | 0     |
| 86  | MG   | 4     | 204  | 1/1   | 0.51 | 25.66 | 40,40,40,40                 | 0     |
| 86  | MG   | 5     | 3545 | 1/1   | 0.71 | 25.63 | 45,45,45,45                 | 0     |
| 86  | MG   | 5     | 3570 | 1/1   | 0.46 | 25.52 | 23,23,23,23                 | 0     |
| 86  | MG   | 5     | 3551 | 1/1   | 0.45 | 25.44 | 22,22,22,22                 | 0     |
| 86  | MG   | 1     | 3461 | 1/1   | 0.38 | 25.37 | 18,18,18,18                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 4     | 207  | 1/1   | 0.31 | 25.34 | 29,29,29,29                 | 0     |
| 86  | MG   | 1     | 3457 | 1/1   | 0.33 | 25.30 | 31,31,31,31                 | 0     |
| 86  | MG   | 1     | 4221 | 1/1   | 0.47 | 25.23 | 24,24,24,24                 | 0     |
| 86  | MG   | 1     | 3698 | 1/1   | 0.25 | 25.22 | 39,39,39,39                 | 0     |
| 86  | MG   | 2     | 2009 | 1/1   | 1.00 | 25.12 | 62,62,62,62                 | 0     |
| 87  | OHX  | 1     | 4189 | 7/7   | 0.40 | 25.07 | 103,103,103,103             | 0     |
| 86  | MG   | 8     | 214  | 1/1   | 0.37 | 25.00 | 30,30,30,30                 | 0     |
| 86  | MG   | 6     | 1946 | 1/1   | 0.41 | 24.99 | 37,37,37,37                 | 0     |
| 86  | MG   | 2     | 1912 | 1/1   | 0.47 | 24.93 | 59,59,59,59                 | 0     |
| 86  | MG   | 5     | 3857 | 1/1   | 0.33 | 24.88 | 64,64,64,64                 | 0     |
| 86  | MG   | 5     | 3529 | 1/1   | 0.43 | 24.78 | 22,22,22,22                 | 0     |
| 86  | MG   | 6     | 1904 | 1/1   | 0.49 | 24.77 | 58,58,58,58                 | 0     |
| 86  | MG   | n3    | 201  | 1/1   | 0.50 | 24.72 | 17,17,17,17                 | 0     |
| 86  | MG   | 1     | 3552 | 1/1   | 0.48 | 24.71 | 25,25,25,25                 | 0     |
| 86  | MG   | 5     | 3865 | 1/1   | 0.30 | 24.70 | 46,46,46,46                 | 0     |
| 86  | MG   | 5     | 3467 | 1/1   | 0.23 | 24.67 | 23,23,23,23                 | 0     |
| 86  | MG   | 2     | 1923 | 1/1   | 0.48 | 24.65 | 48,48,48,48                 | 0     |
| 86  | MG   | 1     | 3837 | 1/1   | 0.50 | 24.64 | 44,44,44,44                 | 0     |
| 86  | MG   | 1     | 3595 | 1/1   | 0.47 | 24.52 | 20,20,20,20                 | 0     |
| 86  | MG   | 1     | 3524 | 1/1   | 0.36 | 24.49 | 18,18,18,18                 | 0     |
| 86  | MG   | 6     | 1960 | 1/1   | 0.34 | 24.38 | 46,46,46,46                 | 0     |
| 87  | OHX  | 5     | 4239 | 7/7   | 0.42 | 24.34 | 138,138,138,138             | 0     |
| 86  | MG   | 5     | 3635 | 1/1   | 0.49 | 24.34 | 71,71,71,71                 | 0     |
| 86  | MG   | 1     | 3850 | 1/1   | 0.71 | 24.33 | 48,48,48,48                 | 0     |
| 86  | MG   | 5     | 3498 | 1/1   | 0.32 | 24.26 | 38,38,38,38                 | 0     |
| 86  | MG   | 1     | 3429 | 1/1   | 0.46 | 24.22 | 35,35,35,35                 | 0     |
| 86  | MG   | 5     | 3497 | 1/1   | 0.43 | 24.18 | 25,25,25,25                 | 0     |
| 86  | MG   | 6     | 1923 | 1/1   | 0.65 | 24.07 | 47,47,47,47                 | 0     |
| 86  | MG   | 2     | 2013 | 1/1   | 0.74 | 24.03 | 62,62,62,62                 | 0     |
| 86  | MG   | 2     | 1905 | 1/1   | 0.73 | 23.91 | 52,52,52,52                 | 0     |
| 86  | MG   | 3     | 214  | 1/1   | 0.43 | 23.90 | 48,48,48,48                 | 0     |
| 87  | OHX  | 5     | 4070 | 7/7   | 0.19 | 23.83 | 119,119,119,119             | 0     |
| 87  | OHX  | 5     | 4160 | 7/7   | 0.29 | 23.78 | 84,84,84,84                 | 0     |
| 87  | OHX  | 5     | 4231 | 7/7   | 0.26 | 23.76 | 171,171,171,171             | 0     |
| 86  | MG   | 1     | 3628 | 1/1   | 0.25 | 23.75 | 26,26,26,26                 | 0     |
| 86  | MG   | 5     | 3869 | 1/1   | 0.49 | 23.67 | 24,24,24,24                 | 0     |
| 86  | MG   | 5     | 3577 | 1/1   | 0.40 | 23.61 | 25,25,25,25                 | 0     |
| 86  | MG   | 1     | 3858 | 1/1   | 0.41 | 23.60 | 50,50,50,50                 | 0     |
| 86  | MG   | 1     | 3766 | 1/1   | 0.40 | 23.43 | 31,31,31,31                 | 0     |
| 86  | MG   | 5     | 3595 | 1/1   | 0.53 | 23.42 | 29,29,29,29                 | 0     |
| 86  | MG   | 7     | 201  | 1/1   | 0.47 | 23.41 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 1     | 3668 | 1/1   | 0.38 | 23.40 | 74,74,74,74                 | 0     |
| 86  | MG   | 7     | 206  | 1/1   | 0.26 | 23.38 | 32,32,32,32                 | 0     |
| 86  | MG   | 5     | 3596 | 1/1   | 0.49 | 23.38 | 18,18,18,18                 | 0     |
| 86  | MG   | 6     | 1939 | 1/1   | 0.32 | 23.36 | 34,34,34,34                 | 0     |
| 87  | OHX  | 5     | 4127 | 7/7   | 0.28 | 23.36 | 118,118,118,118             | 0     |
| 86  | MG   | 7     | 215  | 1/1   | 0.53 | 23.19 | 65,65,65,65                 | 0     |
| 86  | MG   | 1     | 3514 | 1/1   | 0.38 | 23.12 | 17,17,17,17                 | 0     |
| 86  | MG   | 1     | 3553 | 1/1   | 0.53 | 23.00 | 31,31,31,31                 | 0     |
| 86  | MG   | 1     | 3560 | 1/1   | 0.40 | 23.00 | 17,17,17,17                 | 0     |
| 86  | MG   | 1     | 3692 | 1/1   | 0.49 | 22.97 | 45,45,45,45                 | 0     |
| 86  | MG   | 1     | 3731 | 1/1   | 0.45 | 22.96 | 22,22,22,22                 | 0     |
| 86  | MG   | 2     | 1945 | 1/1   | 0.40 | 22.79 | 79,79,79,79                 | 0     |
| 86  | MG   | 1     | 3462 | 1/1   | 0.39 | 22.65 | 18,18,18,18                 | 0     |
| 86  | MG   | 1     | 3745 | 1/1   | 0.27 | 22.55 | 50,50,50,50                 | 0     |
| 87  | OHX  | 5     | 4150 | 7/7   | 0.38 | 22.55 | 111,111,111,111             | 0     |
| 86  | MG   | 6     | 2028 | 1/1   | 0.56 | 22.51 | 55,55,55,55                 | 0     |
| 87  | OHX  | 5     | 4161 | 7/7   | 0.42 | 22.45 | 111,111,111,111             | 0     |
| 86  | MG   | 5     | 3894 | 1/1   | 0.61 | 22.43 | 42,42,42,42                 | 0     |
| 86  | MG   | 2     | 1950 | 1/1   | 0.59 | 22.37 | 78,78,78,78                 | 0     |
| 86  | MG   | 5     | 3649 | 1/1   | 0.57 | 22.35 | 44,44,44,44                 | 0     |
| 86  | MG   | 1     | 3608 | 1/1   | 0.55 | 22.18 | 45,45,45,45                 | 0     |
| 87  | OHX  | 1     | 4194 | 7/7   | 0.49 | 22.11 | 122,122,122,122             | 0     |
| 86  | MG   | 1     | 3723 | 1/1   | 0.31 | 22.05 | 42,42,42,42                 | 0     |
| 86  | MG   | 2     | 1979 | 1/1   | 0.48 | 22.02 | 51,51,51,51                 | 0     |
| 86  | MG   | 5     | 3536 | 1/1   | 0.34 | 22.01 | 30,30,30,30                 | 0     |
| 86  | MG   | 4     | 215  | 1/1   | 0.25 | 21.91 | 51,51,51,51                 | 0     |
| 86  | MG   | 13    | 401  | 1/1   | 0.50 | 21.88 | 17,17,17,17                 | 0     |
| 86  | MG   | 1     | 3517 | 1/1   | 0.45 | 21.80 | 31,31,31,31                 | 0     |
| 86  | MG   | 2     | 1919 | 1/1   | 0.61 | 21.78 | 62,62,62,62                 | 0     |
| 86  | MG   | 2     | 1998 | 1/1   | 0.38 | 21.72 | 70,70,70,70                 | 0     |
| 86  | MG   | 6     | 1944 | 1/1   | 0.36 | 21.69 | 29,29,29,29                 | 0     |
| 86  | MG   | 2     | 1956 | 1/1   | 0.41 | 21.68 | 50,50,50,50                 | 0     |
| 86  | MG   | 5     | 3491 | 1/1   | 0.37 | 21.63 | 51,51,51,51                 | 0     |
| 87  | OHX  | 1     | 4201 | 7/7   | 0.39 | 21.56 | 145,145,145,145             | 0     |
| 86  | MG   | o1    | 202  | 1/1   | 0.62 | 21.56 | 61,61,61,61                 | 0     |
| 86  | MG   | 1     | 3711 | 1/1   | 0.34 | 21.52 | 24,24,24,24                 | 0     |
| 86  | MG   | 1     | 3547 | 1/1   | 0.19 | 21.49 | 56,56,56,56                 | 0     |
| 86  | MG   | 5     | 3745 | 1/1   | 0.43 | 21.41 | 34,34,34,34                 | 0     |
| 86  | MG   | 2     | 1978 | 1/1   | 0.34 | 21.41 | 94,94,94,94                 | 0     |
| 87  | OHX  | 5     | 4233 | 7/7   | 0.43 | 21.38 | 92,92,92,92                 | 0     |
| 86  | MG   | 6     | 1943 | 1/1   | 0.30 | 21.24 | 26,26,26,26                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 5     | 3457 | 1/1   | 0.22 | 21.16 | 28,28,28,28                 | 0     |
| 86  | MG   | 5     | 3445 | 1/1   | 0.32 | 21.12 | 33,33,33,33                 | 0     |
| 86  | MG   | 1     | 3515 | 1/1   | 0.39 | 21.09 | 15,15,15,15                 | 0     |
| 87  | OHX  | 6     | 2150 | 7/7   | 0.27 | 21.07 | 89,89,89,89                 | 0     |
| 86  | MG   | 2     | 1911 | 1/1   | 0.64 | 21.06 | 47,47,47,47                 | 0     |
| 86  | MG   | 2     | 1902 | 1/1   | 0.42 | 21.06 | 40,40,40,40                 | 0     |
| 86  | MG   | 5     | 3590 | 1/1   | 0.36 | 21.03 | 25,25,25,25                 | 0     |
| 86  | MG   | 1     | 3600 | 1/1   | 0.44 | 20.97 | 17,17,17,17                 | 0     |
| 86  | MG   | 1     | 3450 | 1/1   | 0.29 | 20.93 | 29,29,29,29                 | 0     |
| 86  | MG   | 1     | 3574 | 1/1   | 0.55 | 20.92 | 26,26,26,26                 | 0     |
| 86  | MG   | 1     | 3567 | 1/1   | 0.43 | 20.79 | 22,22,22,22                 | 0     |
| 86  | MG   | 6     | 2035 | 1/1   | 0.46 | 20.75 | 55,55,55,55                 | 0     |
| 86  | MG   | 2     | 2010 | 1/1   | 0.36 | 20.71 | 45,45,45,45                 | 0     |
| 86  | MG   | 1     | 3825 | 1/1   | 0.33 | 20.68 | 49,49,49,49                 | 0     |
| 86  | MG   | 6     | 2014 | 1/1   | 0.47 | 20.68 | 60,60,60,60                 | 0     |
| 86  | MG   | 5     | 3418 | 1/1   | 0.44 | 20.67 | 18,18,18,18                 | 0     |
| 86  | MG   | 1     | 3768 | 1/1   | 0.53 | 20.66 | 40,40,40,40                 | 0     |
| 87  | OHX  | 5     | 4194 | 7/7   | 0.35 | 20.64 | 99,99,99,99                 | 0     |
| 86  | MG   | 12    | 301  | 1/1   | 0.73 | 20.55 | 38,38,38,38                 | 0     |
| 86  | MG   | 6     | 2040 | 1/1   | 0.41 | 20.55 | 58,58,58,58                 | 0     |
| 86  | MG   | 1     | 3616 | 1/1   | 0.41 | 20.52 | 27,27,27,27                 | 0     |
| 86  | MG   | 1     | 3504 | 1/1   | 0.39 | 20.39 | 19,19,19,19                 | 0     |
| 86  | MG   | 1     | 3845 | 1/1   | 0.64 | 20.39 | 46,46,46,46                 | 0     |
| 86  | MG   | 5     | 3504 | 1/1   | 0.41 | 20.35 | 22,22,22,22                 | 0     |
| 87  | OHX  | 1     | 4175 | 7/7   | 0.41 | 20.34 | 151,151,151,151             | 0     |
| 86  | MG   | 1     | 3435 | 1/1   | 0.42 | 20.34 | 32,32,32,32                 | 0     |
| 86  | MG   | 5     | 3452 | 1/1   | 0.18 | 20.33 | 30,30,30,30                 | 0     |
| 86  | MG   | 1     | 3412 | 1/1   | 0.41 | 20.29 | 33,33,33,33                 | 0     |
| 86  | MG   | 1     | 3498 | 1/1   | 0.34 | 20.28 | 35,35,35,35                 | 0     |
| 87  | OHX  | 5     | 4217 | 7/7   | 0.35 | 20.28 | 121,121,121,121             | 0     |
| 86  | MG   | 1     | 3513 | 1/1   | 0.60 | 20.26 | 31,31,31,31                 | 0     |
| 86  | MG   | 5     | 3523 | 1/1   | 0.35 | 20.13 | 33,33,33,33                 | 0     |
| 86  | MG   | M7    | 204  | 1/1   | 0.46 | 20.08 | 24,24,24,24                 | 0     |
| 86  | MG   | 5     | 3532 | 1/1   | 0.27 | 20.05 | 23,23,23,23                 | 0     |
| 86  | MG   | 1     | 3573 | 1/1   | 0.50 | 20.01 | 24,24,24,24                 | 0     |
| 87  | OHX  | 5     | 4180 | 7/7   | 0.41 | 19.95 | 82,82,82,82                 | 0     |
| 87  | OHX  | 5     | 4215 | 7/7   | 0.31 | 19.92 | 93,93,93,93                 | 0     |
| 86  | MG   | 1     | 3459 | 1/1   | 0.53 | 19.91 | 21,21,21,21                 | 0     |
| 86  | MG   | 1     | 3539 | 1/1   | 0.30 | 19.86 | 28,28,28,28                 | 0     |
| 86  | MG   | 1     | 3609 | 1/1   | 0.82 | 19.82 | 62,62,62,62                 | 0     |
| 86  | MG   | 6     | 1956 | 1/1   | 0.50 | 19.82 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 5     | 3405 | 1/1   | 0.41 | 19.79 | 20,20,20,20                 | 0     |
| 86  | MG   | 5     | 3449 | 1/1   | 0.38 | 19.66 | 53,53,53,53                 | 0     |
| 86  | MG   | 8     | 202  | 1/1   | 0.64 | 19.65 | 61,61,61,61                 | 0     |
| 87  | OHX  | 5     | 4163 | 7/7   | 0.36 | 19.60 | 88,88,88,88                 | 0     |
| 87  | OHX  | 5     | 4237 | 7/7   | 0.48 | 19.59 | 120,120,120,120             | 0     |
| 86  | MG   | 2     | 1940 | 1/1   | 0.43 | 19.58 | 58,58,58,58                 | 0     |
| 86  | MG   | 1     | 3857 | 1/1   | 0.38 | 19.57 | 16,16,16,16                 | 0     |
| 86  | MG   | 1     | 3455 | 1/1   | 0.50 | 19.55 | 47,47,47,47                 | 0     |
| 87  | OHX  | 5     | 3931 | 7/7   | 0.40 | 19.55 | 101,101,101,101             | 0     |
| 87  | OHX  | 1     | 4146 | 7/7   | 0.39 | 19.51 | 111,111,111,111             | 0     |
| 86  | MG   | 1     | 3526 | 1/1   | 0.45 | 19.45 | 21,21,21,21                 | 0     |
| 86  | MG   | 5     | 3552 | 1/1   | 0.49 | 19.38 | 37,37,37,37                 | 0     |
| 86  | MG   | 5     | 3822 | 1/1   | 0.40 | 19.34 | 34,34,34,34                 | 0     |
| 86  | MG   | 5     | 3522 | 1/1   | 0.40 | 19.30 | 23,23,23,23                 | 0     |
| 86  | MG   | 1     | 3615 | 1/1   | 0.36 | 19.19 | 29,29,29,29                 | 0     |
| 86  | MG   | 1     | 3588 | 1/1   | 0.46 | 19.19 | 27,27,27,27                 | 0     |
| 87  | OHX  | 1     | 4181 | 7/7   | 0.42 | 19.14 | 94,94,94,94                 | 0     |
| 86  | MG   | 1     | 3535 | 1/1   | 0.44 | 19.12 | 18,18,18,18                 | 0     |
| 86  | MG   | 5     | 3510 | 1/1   | 0.44 | 19.10 | 22,22,22,22                 | 0     |
| 86  | MG   | 5     | 3715 | 1/1   | 0.27 | 19.10 | 31,31,31,31                 | 0     |
| 86  | MG   | 5     | 3428 | 1/1   | 0.36 | 19.06 | 19,19,19,19                 | 0     |
| 86  | MG   | 5     | 3448 | 1/1   | 0.54 | 19.05 | 45,45,45,45                 | 0     |
| 87  | OHX  | 1     | 4210 | 7/7   | 0.43 | 19.01 | 89,89,89,89                 | 0     |
| 86  | MG   | 5     | 3810 | 1/1   | 0.38 | 19.00 | 27,27,27,27                 | 0     |
| 86  | MG   | 2     | 1938 | 1/1   | 0.55 | 18.97 | 59,59,59,59                 | 0     |
| 87  | OHX  | 1     | 4054 | 7/7   | 0.27 | 18.96 | 94,94,94,94                 | 0     |
| 86  | MG   | 1     | 3715 | 1/1   | 0.29 | 18.92 | 75,75,75,75                 | 0     |
| 87  | OHX  | 5     | 4214 | 7/7   | 0.32 | 18.91 | 128,128,128,128             | 0     |
| 86  | MG   | 6     | 1967 | 1/1   | 0.50 | 18.90 | 54,54,54,54                 | 0     |
| 86  | MG   | 1     | 3740 | 1/1   | 0.39 | 18.89 | 43,43,43,43                 | 0     |
| 86  | MG   | M7    | 202  | 1/1   | 0.56 | 18.88 | 25,25,25,25                 | 0     |
| 86  | MG   | 6     | 2045 | 1/1   | 0.49 | 18.86 | 65,65,65,65                 | 0     |
| 86  | MG   | 5     | 3426 | 1/1   | 0.39 | 18.83 | 30,30,30,30                 | 0     |
| 86  | MG   | 2     | 1966 | 1/1   | 0.49 | 18.79 | 79,79,79,79                 | 0     |
| 86  | MG   | 1     | 3784 | 1/1   | 0.45 | 18.75 | 36,36,36,36                 | 0     |
| 87  | OHX  | 1     | 4152 | 7/7   | 0.34 | 18.75 | 128,128,128,128             | 0     |
| 86  | MG   | 2     | 1914 | 1/1   | 0.61 | 18.63 | 56,56,56,56                 | 0     |
| 86  | MG   | 6     | 1949 | 1/1   | 0.34 | 18.62 | 33,33,33,33                 | 0     |
| 87  | OHX  | 6     | 2184 | 7/7   | 0.42 | 18.61 | 115,115,115,115             | 0     |
| 86  | MG   | 4     | 206  | 1/1   | 0.39 | 18.53 | 18,18,18,18                 | 0     |
| 86  | MG   | 5     | 3593 | 1/1   | 0.41 | 18.49 | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 5     | 3814 | 1/1   | 0.38 | 18.41 | 76,76,76,76                 | 0     |
| 86  | MG   | 1     | 3510 | 1/1   | 0.49 | 18.39 | 15,15,15,15                 | 0     |
| 86  | MG   | 1     | 3417 | 1/1   | 0.49 | 18.38 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 3414 | 1/1   | 0.47 | 18.38 | 24,24,24,24                 | 0     |
| 87  | OHX  | 2     | 2170 | 7/7   | 0.43 | 18.36 | 131,131,131,131             | 0     |
| 86  | MG   | 5     | 3676 | 1/1   | 0.43 | 18.35 | 32,32,32,32                 | 0     |
| 86  | MG   | 1     | 3584 | 1/1   | 0.55 | 18.35 | 27,27,27,27                 | 0     |
| 86  | MG   | 8     | 203  | 1/1   | 0.45 | 18.31 | 32,32,32,32                 | 0     |
| 86  | MG   | 5     | 3753 | 1/1   | 0.44 | 18.30 | 34,34,34,34                 | 0     |
| 86  | MG   | 2     | 1916 | 1/1   | 0.44 | 18.29 | 46,46,46,46                 | 0     |
| 86  | MG   | 1     | 3487 | 1/1   | 0.42 | 18.28 | 20,20,20,20                 | 0     |
| 87  | OHX  | 2     | 2157 | 7/7   | 0.36 | 18.25 | 129,129,129,129             | 0     |
| 86  | MG   | 4     | 218  | 1/1   | 0.27 | 18.24 | 44,44,44,44                 | 0     |
| 86  | MG   | 6     | 1901 | 1/1   | 0.51 | 18.23 | 36,36,36,36                 | 0     |
| 86  | MG   | 2     | 1908 | 1/1   | 0.45 | 18.19 | 66,66,66,66                 | 0     |
| 87  | OHX  | 1     | 4174 | 7/7   | 0.38 | 18.19 | 145,145,145,145             | 0     |
| 87  | OHX  | 5     | 4204 | 7/7   | 0.35 | 18.16 | 115,115,115,115             | 0     |
| 86  | MG   | 5     | 3554 | 1/1   | 0.43 | 18.16 | 26,26,26,26                 | 0     |
| 86  | MG   | 2     | 2007 | 1/1   | 0.49 | 18.14 | 67,67,67,67                 | 0     |
| 86  | MG   | 5     | 3562 | 1/1   | 0.45 | 18.13 | 16,16,16,16                 | 0     |
| 87  | OHX  | 1     | 4172 | 7/7   | 0.31 | 18.13 | 93,93,93,93                 | 0     |
| 86  | MG   | 5     | 3519 | 1/1   | 0.43 | 18.10 | 19,19,19,19                 | 0     |
| 86  | MG   | 2     | 1937 | 1/1   | 0.54 | 18.08 | 52,52,52,52                 | 0     |
| 86  | MG   | 5     | 3696 | 1/1   | 0.50 | 18.08 | 64,64,64,64                 | 0     |
| 86  | MG   | 5     | 3475 | 1/1   | 0.20 | 18.00 | 65,65,65,65                 | 0     |
| 86  | MG   | 1     | 3697 | 1/1   | 0.31 | 18.00 | 39,39,39,39                 | 0     |
| 86  | MG   | 1     | 3442 | 1/1   | 0.34 | 18.00 | 18,18,18,18                 | 0     |
| 87  | OHX  | 1     | 4113 | 7/7   | 0.26 | 17.98 | 98,98,98,98                 | 0     |
| 86  | MG   | 6     | 1947 | 1/1   | 0.47 | 17.97 | 56,56,56,56                 | 0     |
| 86  | MG   | 1     | 3859 | 1/1   | 0.31 | 17.92 | 31,31,31,31                 | 0     |
| 86  | MG   | 6     | 1955 | 1/1   | 0.40 | 17.91 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 3735 | 1/1   | 0.31 | 17.82 | 78,78,78,78                 | 0     |
| 86  | MG   | 2     | 1928 | 1/1   | 0.57 | 17.78 | 75,75,75,75                 | 0     |
| 86  | MG   | 1     | 3625 | 1/1   | 0.28 | 17.77 | 40,40,40,40                 | 0     |
| 87  | OHX  | 2     | 2155 | 7/7   | 0.43 | 17.71 | 95,95,95,95                 | 0     |
| 86  | MG   | 2     | 1936 | 1/1   | 0.54 | 17.70 | 48,48,48,48                 | 0     |
| 86  | MG   | 1     | 3421 | 1/1   | 0.38 | 17.61 | 28,28,28,28                 | 0     |
| 86  | MG   | 6     | 1938 | 1/1   | 0.34 | 17.59 | 35,35,35,35                 | 0     |
| 87  | OHX  | 1     | 4195 | 7/7   | 0.30 | 17.54 | 112,112,112,112             | 0     |
| 86  | MG   | 1     | 3761 | 1/1   | 0.25 | 17.53 | 39,39,39,39                 | 0     |
| 86  | MG   | 5     | 3608 | 1/1   | 0.40 | 17.53 | 21,21,21,21                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 2     | 1932 | 1/1   | 0.44 | 17.47 | 61,61,61,61                 | 0     |
| 87  | OHX  | 1     | 4206 | 7/7   | 0.40 | 17.47 | 110,110,110,110             | 0     |
| 86  | MG   | 1     | 3430 | 1/1   | 0.53 | 17.44 | 41,41,41,41                 | 0     |
| 86  | MG   | 1     | 3797 | 1/1   | 0.58 | 17.42 | 30,30,30,30                 | 0     |
| 86  | MG   | 5     | 3667 | 1/1   | 0.23 | 17.42 | 35,35,35,35                 | 0     |
| 86  | MG   | 5     | 3402 | 1/1   | 0.38 | 17.38 | 18,18,18,18                 | 0     |
| 87  | OHX  | 1     | 4046 | 7/7   | 0.24 | 17.36 | 96,96,96,96                 | 0     |
| 86  | MG   | 6     | 1928 | 1/1   | 0.43 | 17.34 | 39,39,39,39                 | 0     |
| 86  | MG   | 2     | 1921 | 1/1   | 0.45 | 17.25 | 43,43,43,43                 | 0     |
| 86  | MG   | 5     | 3692 | 1/1   | 0.38 | 17.24 | 39,39,39,39                 | 0     |
| 86  | MG   | 1     | 3820 | 1/1   | 0.58 | 17.17 | 101,101,101,101             | 0     |
| 87  | OHX  | 6     | 2182 | 7/7   | 0.22 | 17.13 | 133,133,133,133             | 0     |
| 87  | OHX  | 1     | 4072 | 7/7   | 0.42 | 17.12 | 112,112,112,112             | 0     |
| 86  | MG   | n8    | 204  | 1/1   | 0.40 | 17.11 | 33,33,33,33                 | 0     |
| 86  | MG   | 5     | 3550 | 1/1   | 0.52 | 17.08 | 43,43,43,43                 | 0     |
| 86  | MG   | 2     | 2015 | 1/1   | 0.47 | 17.06 | 71,71,71,71                 | 0     |
| 86  | MG   | 5     | 3626 | 1/1   | 0.30 | 17.03 | 21,21,21,21                 | 0     |
| 86  | MG   | 5     | 3574 | 1/1   | 0.47 | 17.01 | 31,31,31,31                 | 0     |
| 87  | OHX  | 5     | 4143 | 7/7   | 0.36 | 17.00 | 104,104,104,104             | 0     |
| 87  | OHX  | 1     | 4050 | 7/7   | 0.31 | 16.98 | 85,85,85,85                 | 0     |
| 87  | OHX  | 1     | 4147 | 7/7   | 0.32 | 16.98 | 119,119,119,119             | 0     |
| 86  | MG   | 6     | 1918 | 1/1   | 0.50 | 16.97 | 48,48,48,48                 | 0     |
| 86  | MG   | 1     | 3432 | 1/1   | 0.51 | 16.96 | 36,36,36,36                 | 0     |
| 87  | OHX  | 2     | 2141 | 7/7   | 0.46 | 16.95 | 104,104,104,104             | 0     |
| 87  | OHX  | 5     | 4129 | 7/7   | 0.37 | 16.94 | 117,117,117,117             | 0     |
| 87  | OHX  | 5     | 4211 | 7/7   | 0.32 | 16.92 | 123,123,123,123             | 0     |
| 86  | MG   | 1     | 3540 | 1/1   | 0.45 | 16.90 | 18,18,18,18                 | 0     |
| 86  | MG   | n8    | 205  | 1/1   | 0.44 | 16.89 | 31,31,31,31                 | 0     |
| 86  | MG   | 1     | 3720 | 1/1   | 0.51 | 16.89 | 31,31,31,31                 | 0     |
| 86  | MG   | 1     | 3527 | 1/1   | 0.42 | 16.89 | 19,19,19,19                 | 0     |
| 87  | OHX  | 8     | 227  | 7/7   | 0.32 | 16.82 | 106,106,106,106             | 0     |
| 86  | MG   | 2     | 1961 | 1/1   | 0.44 | 16.81 | 49,49,49,49                 | 0     |
| 86  | MG   | 5     | 3804 | 1/1   | 0.34 | 16.73 | 57,57,57,57                 | 0     |
| 86  | MG   | 5     | 3435 | 1/1   | 0.25 | 16.71 | 24,24,24,24                 | 0     |
| 87  | OHX  | 1     | 4168 | 7/7   | 0.36 | 16.66 | 143,143,143,143             | 0     |
| 86  | MG   | 1     | 3732 | 1/1   | 0.44 | 16.65 | 18,18,18,18                 | 0     |
| 86  | MG   | 2     | 2004 | 1/1   | 0.59 | 16.64 | 77,77,77,77                 | 0     |
| 87  | OHX  | 6     | 2164 | 7/7   | 0.29 | 16.61 | 102,102,102,102             | 0     |
| 86  | MG   | 1     | 3847 | 1/1   | 0.49 | 16.59 | 47,47,47,47                 | 0     |
| 87  | OHX  | 1     | 4138 | 7/7   | 0.35 | 16.59 | 114,114,114,114             | 0     |
| 86  | MG   | 1     | 3643 | 1/1   | 0.25 | 16.55 | 27,27,27,27                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 1     | 3561 | 1/1   | 0.44 | 16.54 | 30,30,30,30                 | 0     |
| 86  | MG   | 1     | 3852 | 1/1   | 0.28 | 16.52 | 43,43,43,43                 | 0     |
| 86  | MG   | 5     | 3743 | 1/1   | 0.35 | 16.51 | 27,27,27,27                 | 0     |
| 87  | OHX  | 1     | 4143 | 7/7   | 0.38 | 16.49 | 118,118,118,118             | 0     |
| 86  | MG   | 1     | 3693 | 1/1   | 0.40 | 16.49 | 25,25,25,25                 | 0     |
| 86  | MG   | 1     | 3690 | 1/1   | 0.36 | 16.44 | 38,38,38,38                 | 0     |
| 86  | MG   | 5     | 3561 | 1/1   | 0.49 | 16.42 | 22,22,22,22                 | 0     |
| 86  | MG   | 5     | 3439 | 1/1   | 0.33 | 16.38 | 23,23,23,23                 | 0     |
| 86  | MG   | 5     | 3411 | 1/1   | 0.36 | 16.37 | 30,30,30,30                 | 0     |
| 86  | MG   | 1     | 3440 | 1/1   | 0.36 | 16.33 | 27,27,27,27                 | 0     |
| 87  | OHX  | 5     | 4162 | 7/7   | 0.30 | 16.27 | 97,97,97,97                 | 0     |
| 87  | OHX  | M7    | 207  | 7/7   | 0.44 | 16.26 | 78,78,78,78                 | 0     |
| 86  | MG   | 1     | 3481 | 1/1   | 0.51 | 16.25 | 35,35,35,35                 | 0     |
| 86  | MG   | 6     | 1911 | 1/1   | 0.46 | 16.25 | 40,40,40,40                 | 0     |
| 86  | MG   | 1     | 3648 | 1/1   | 0.21 | 16.14 | 25,25,25,25                 | 0     |
| 86  | MG   | 6     | 1987 | 1/1   | 0.38 | 16.01 | 36,36,36,36                 | 0     |
| 86  | MG   | 2     | 1909 | 1/1   | 0.50 | 15.97 | 65,65,65,65                 | 0     |
| 86  | MG   | 1     | 3650 | 1/1   | 0.46 | 15.95 | 36,36,36,36                 | 0     |
| 87  | OHX  | 5     | 4247 | 7/7   | 0.30 | 15.94 | 126,126,126,126             | 0     |
| 86  | MG   | 1     | 3525 | 1/1   | 0.41 | 15.93 | 32,32,32,32                 | 0     |
| 86  | MG   | 1     | 3401 | 1/1   | 0.56 | 15.86 | 34,34,34,34                 | 0     |
| 86  | MG   | 1     | 3505 | 1/1   | 0.33 | 15.84 | 28,28,28,28                 | 0     |
| 86  | MG   | 1     | 3780 | 1/1   | 0.25 | 15.81 | 24,24,24,24                 | 0     |
| 86  | MG   | 1     | 3659 | 1/1   | 0.38 | 15.80 | 31,31,31,31                 | 0     |
| 86  | MG   | 5     | 3573 | 1/1   | 0.46 | 15.79 | 22,22,22,22                 | 0     |
| 86  | MG   | 5     | 3682 | 1/1   | 0.17 | 15.74 | 33,33,33,33                 | 0     |
| 86  | MG   | 5     | 3795 | 1/1   | 0.38 | 15.72 | 37,37,37,37                 | 0     |
| 86  | MG   | 4     | 205  | 1/1   | 0.40 | 15.72 | 23,23,23,23                 | 0     |
| 86  | MG   | 1     | 3660 | 1/1   | 0.47 | 15.71 | 19,19,19,19                 | 0     |
| 87  | OHX  | 1     | 4117 | 7/7   | 0.39 | 15.67 | 89,89,89,89                 | 0     |
| 86  | MG   | 6     | 1992 | 1/1   | 0.47 | 15.63 | 65,65,65,65                 | 0     |
| 86  | MG   | 1     | 3503 | 1/1   | 0.47 | 15.62 | 39,39,39,39                 | 0     |
| 86  | MG   | 6     | 1930 | 1/1   | 0.44 | 15.60 | 45,45,45,45                 | 0     |
| 86  | MG   | 5     | 3555 | 1/1   | 0.65 | 15.59 | 42,42,42,42                 | 0     |
| 86  | MG   | 5     | 3572 | 1/1   | 0.33 | 15.57 | 32,32,32,32                 | 0     |
| 86  | MG   | 6     | 1974 | 1/1   | 0.29 | 15.55 | 42,42,42,42                 | 0     |
| 87  | OHX  | 6     | 2207 | 7/7   | 0.41 | 15.52 | 124,124,124,124             | 0     |
| 87  | OHX  | 5     | 4155 | 7/7   | 0.44 | 15.49 | 95,95,95,95                 | 0     |
| 87  | OHX  | 6     | 2171 | 7/7   | 0.36 | 15.46 | 95,95,95,95                 | 0     |
| 86  | MG   | 6     | 1909 | 1/1   | 0.39 | 15.43 | 100,100,100,100             | 0     |
| 86  | MG   | 1     | 3520 | 1/1   | 0.46 | 15.38 | 20,20,20,20                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 87  | OHX  | 1     | 4119 | 7/7   | 0.40 | 15.36 | 101,101,101,101             | 0     |
| 86  | MG   | 1     | 3619 | 1/1   | 0.27 | 15.33 | 46,46,46,46                 | 0     |
| 86  | MG   | 3     | 212  | 1/1   | 0.34 | 15.33 | 66,66,66,66                 | 0     |
| 87  | OHX  | 1     | 4173 | 7/7   | 0.34 | 15.30 | 89,89,89,89                 | 0     |
| 87  | OHX  | 7     | 226  | 7/7   | 0.35 | 15.24 | 99,99,99,99                 | 0     |
| 86  | MG   | 1     | 3675 | 1/1   | 0.35 | 15.21 | 52,52,52,52                 | 0     |
| 86  | MG   | 1     | 3652 | 1/1   | 0.37 | 15.20 | 59,59,59,59                 | 0     |
| 86  | MG   | 5     | 3486 | 1/1   | 0.42 | 15.17 | 32,32,32,32                 | 0     |
| 87  | OHX  | 6     | 2129 | 7/7   | 0.42 | 15.14 | 86,86,86,86                 | 0     |
| 86  | MG   | D0    | 201  | 1/1   | 0.76 | 15.08 | 65,65,65,65                 | 0     |
| 86  | MG   | 5     | 3576 | 1/1   | 0.40 | 15.03 | 32,32,32,32                 | 0     |
| 86  | MG   | 5     | 3848 | 1/1   | 0.20 | 15.00 | 41,41,41,41                 | 0     |
| 87  | OHX  | 6     | 2177 | 7/7   | 0.43 | 14.99 | 103,103,103,103             | 0     |
| 86  | MG   | 1     | 3473 | 1/1   | 0.36 | 14.97 | 15,15,15,15                 | 0     |
| 86  | MG   | 5     | 3640 | 1/1   | 0.30 | 14.96 | 37,37,37,37                 | 0     |
| 86  | MG   | 3     | 202  | 1/1   | 0.47 | 14.90 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 3512 | 1/1   | 0.53 | 14.87 | 25,25,25,25                 | 0     |
| 86  | MG   | 5     | 3503 | 1/1   | 0.39 | 14.86 | 35,35,35,35                 | 0     |
| 87  | OHX  | 5     | 4188 | 7/7   | 0.31 | 14.83 | 99,99,99,99                 | 0     |
| 86  | MG   | 6     | 2021 | 1/1   | 0.38 | 14.81 | 41,41,41,41                 | 0     |
| 86  | MG   | 6     | 1996 | 1/1   | 0.31 | 14.79 | 36,36,36,36                 | 0     |
| 87  | OHX  | 5     | 4114 | 7/7   | 0.34 | 14.73 | 82,82,82,82                 | 0     |
| 86  | MG   | 5     | 3534 | 1/1   | 0.40 | 14.72 | 28,28,28,28                 | 0     |
| 87  | OHX  | 1     | 4211 | 7/7   | 0.40 | 14.65 | 111,111,111,111             | 0     |
| 86  | MG   | o3    | 202  | 1/1   | 0.43 | 14.64 | 22,22,22,22                 | 0     |
| 86  | MG   | 5     | 3607 | 1/1   | 0.41 | 14.60 | 39,39,39,39                 | 0     |
| 87  | OHX  | 5     | 4187 | 7/7   | 0.43 | 14.56 | 103,103,103,103             | 0     |
| 86  | MG   | 5     | 3508 | 1/1   | 0.36 | 14.53 | 17,17,17,17                 | 0     |
| 86  | MG   | 1     | 3570 | 1/1   | 0.39 | 14.48 | 17,17,17,17                 | 0     |
| 87  | OHX  | 6     | 2130 | 7/7   | 0.34 | 14.47 | 98,98,98,98                 | 0     |
| 87  | OHX  | 5     | 4207 | 7/7   | 0.50 | 14.46 | 127,127,127,127             | 0     |
| 86  | MG   | 1     | 3673 | 1/1   | 0.23 | 14.45 | 38,38,38,38                 | 0     |
| 86  | MG   | 5     | 3481 | 1/1   | 0.40 | 14.44 | 33,33,33,33                 | 0     |
| 87  | OHX  | 1     | 4200 | 7/7   | 0.40 | 14.44 | 109,109,109,109             | 0     |
| 86  | MG   | 8     | 213  | 1/1   | 0.29 | 14.42 | 48,48,48,48                 | 0     |
| 86  | MG   | 2     | 1965 | 1/1   | 0.38 | 14.41 | 55,55,55,55                 | 0     |
| 87  | OHX  | 1     | 4212 | 7/7   | 0.39 | 14.38 | 96,96,96,96                 | 0     |
| 87  | OHX  | 1     | 4130 | 7/7   | 0.37 | 14.38 | 98,98,98,98                 | 0     |
| 86  | MG   | 5     | 3438 | 1/1   | 0.44 | 14.37 | 52,52,52,52                 | 0     |
| 87  | OHX  | 1     | 4049 | 7/7   | 0.32 | 14.33 | 88,88,88,88                 | 0     |
| 86  | MG   | 1     | 3433 | 1/1   | 0.35 | 14.32 | 23,23,23,23                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 5     | 3675 | 1/1   | 0.23 | 14.30 | 56,56,56,56                 | 0     |
| 87  | OHX  | 5     | 4177 | 7/7   | 0.46 | 14.27 | 119,119,119,119             | 0     |
| 86  | MG   | 2     | 2006 | 1/1   | 0.47 | 14.27 | 48,48,48,48                 | 0     |
| 87  | OHX  | 3     | 225  | 7/7   | 0.33 | 14.24 | 107,107,107,107             | 0     |
| 86  | MG   | N3    | 201  | 1/1   | 0.38 | 14.18 | 25,25,25,25                 | 0     |
| 86  | MG   | 1     | 3418 | 1/1   | 0.27 | 14.16 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 3688 | 1/1   | 0.26 | 14.15 | 28,28,28,28                 | 0     |
| 86  | MG   | 1     | 3641 | 1/1   | 0.29 | 14.12 | 48,48,48,48                 | 0     |
| 86  | MG   | 1     | 3598 | 1/1   | 0.54 | 14.11 | 17,17,17,17                 | 0     |
| 86  | MG   | 6     | 1926 | 1/1   | 0.50 | 14.10 | 31,31,31,31                 | 0     |
| 86  | MG   | 1     | 3423 | 1/1   | 0.39 | 14.07 | 33,33,33,33                 | 0     |
| 86  | MG   | 5     | 3624 | 1/1   | 0.36 | 14.04 | 35,35,35,35                 | 0     |
| 86  | MG   | 6     | 1932 | 1/1   | 0.47 | 14.03 | 47,47,47,47                 | 0     |
| 87  | OHX  | 4     | 233  | 7/7   | 0.39 | 14.01 | 120,120,120,120             | 0     |
| 86  | MG   | 5     | 3877 | 1/1   | 0.50 | 13.99 | 18,18,18,18                 | 0     |
| 86  | MG   | 6     | 1963 | 1/1   | 0.34 | 13.96 | 39,39,39,39                 | 0     |
| 86  | MG   | 1     | 3490 | 1/1   | 0.44 | 13.96 | 24,24,24,24                 | 0     |
| 86  | MG   | 5     | 3587 | 1/1   | 0.29 | 13.95 | 18,18,18,18                 | 0     |
| 86  | MG   | 5     | 3559 | 1/1   | 0.37 | 13.94 | 24,24,24,24                 | 0     |
| 86  | MG   | 1     | 3518 | 1/1   | 0.31 | 13.92 | 32,32,32,32                 | 0     |
| 87  | OHX  | m4    | 201  | 7/7   | 0.33 | 13.84 | 217,217,217,217             | 0     |
| 86  | MG   | 6     | 1970 | 1/1   | 0.43 | 13.84 | 59,59,59,59                 | 0     |
| 86  | MG   | 1     | 3511 | 1/1   | 0.28 | 13.84 | 37,37,37,37                 | 0     |
| 86  | MG   | 1     | 3785 | 1/1   | 0.41 | 13.82 | 28,28,28,28                 | 0     |
| 86  | MG   | 1     | 3644 | 1/1   | 0.34 | 13.80 | 29,29,29,29                 | 0     |
| 86  | MG   | 5     | 3568 | 1/1   | 0.38 | 13.79 | 19,19,19,19                 | 0     |
| 87  | OHX  | 1     | 4180 | 7/7   | 0.38 | 13.77 | 130,130,130,130             | 0     |
| 86  | MG   | 5     | 3501 | 1/1   | 0.32 | 13.71 | 20,20,20,20                 | 0     |
| 86  | MG   | 5     | 3705 | 1/1   | 0.13 | 13.67 | 42,42,42,42                 | 0     |
| 87  | OHX  | 8     | 221  | 7/7   | 0.24 | 13.64 | 93,93,93,93                 | 0     |
| 87  | OHX  | 5     | 4073 | 7/7   | 0.24 | 13.61 | 99,99,99,99                 | 0     |
| 87  | OHX  | 1     | 4100 | 7/7   | 0.27 | 13.58 | 128,128,128,128             | 0     |
| 86  | MG   | 3     | 206  | 1/1   | 0.50 | 13.56 | 26,26,26,26                 | 0     |
| 86  | MG   | 5     | 3500 | 1/1   | 0.46 | 13.53 | 27,27,27,27                 | 0     |
| 86  | MG   | 2     | 1971 | 1/1   | 0.44 | 13.52 | 63,63,63,63                 | 0     |
| 86  | MG   | 1     | 3867 | 1/1   | 0.44 | 13.52 | 52,52,52,52                 | 0     |
| 86  | MG   | 1     | 3649 | 1/1   | 0.28 | 13.51 | 27,27,27,27                 | 0     |
| 86  | MG   | 5     | 3629 | 1/1   | 0.54 | 13.49 | 54,54,54,54                 | 0     |
| 87  | OHX  | 6     | 2187 | 7/7   | 0.34 | 13.42 | 114,114,114,114             | 0     |
| 87  | OHX  | 1     | 4214 | 7/7   | 0.44 | 13.41 | 96,96,96,96                 | 0     |
| 86  | MG   | 5     | 3714 | 1/1   | 0.35 | 13.40 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 1     | 3836 | 1/1   | 0.54 | 13.24 | 18,18,18,18                 | 0     |
| 87  | OHX  | 2     | 2146 | 7/7   | 0.36 | 13.18 | 90,90,90,90                 | 0     |
| 86  | MG   | 2     | 1918 | 1/1   | 0.51 | 13.15 | 43,43,43,43                 | 0     |
| 87  | OHX  | 2     | 2162 | 7/7   | 0.43 | 13.12 | 116,116,116,116             | 0     |
| 86  | MG   | 1     | 3680 | 1/1   | 0.23 | 13.09 | 35,35,35,35                 | 0     |
| 87  | OHX  | 5     | 4219 | 7/7   | 0.34 | 13.06 | 125,125,125,125             | 0     |
| 87  | OHX  | 5     | 4183 | 7/7   | 0.36 | 13.06 | 114,114,114,114             | 0     |
| 87  | OHX  | 5     | 4152 | 7/7   | 0.33 | 13.03 | 95,95,95,95                 | 0     |
| 87  | OHX  | 5     | 4090 | 7/7   | 0.34 | 13.02 | 83,83,83,83                 | 0     |
| 86  | MG   | 7     | 202  | 1/1   | 0.28 | 13.02 | 19,19,19,19                 | 0     |
| 86  | MG   | 6     | 2026 | 1/1   | 0.40 | 13.02 | 42,42,42,42                 | 0     |
| 86  | MG   | 5     | 3609 | 1/1   | 0.26 | 13.00 | 22,22,22,22                 | 0     |
| 86  | MG   | 5     | 3427 | 1/1   | 0.34 | 12.99 | 36,36,36,36                 | 0     |
| 86  | MG   | 5     | 3513 | 1/1   | 0.29 | 12.97 | 52,52,52,52                 | 0     |
| 86  | MG   | 1     | 3496 | 1/1   | 0.27 | 12.93 | 38,38,38,38                 | 0     |
| 87  | OHX  | 6     | 2168 | 7/7   | 0.29 | 12.88 | 125,125,125,125             | 0     |
| 87  | OHX  | O9    | 101  | 7/7   | 0.48 | 12.85 | 85,85,85,85                 | 0     |
| 86  | MG   | 1     | 3834 | 1/1   | 0.35 | 12.85 | 18,18,18,18                 | 0     |
| 86  | MG   | 1     | 3486 | 1/1   | 0.25 | 12.84 | 28,28,28,28                 | 0     |
| 86  | MG   | 5     | 3588 | 1/1   | 0.68 | 12.82 | 42,42,42,42                 | 0     |
| 86  | MG   | 1     | 3500 | 1/1   | 0.41 | 12.82 | 50,50,50,50                 | 0     |
| 87  | OHX  | 5     | 4195 | 7/7   | 0.31 | 12.81 | 92,92,92,92                 | 0     |
| 86  | MG   | 5     | 3465 | 1/1   | 0.30 | 12.79 | 51,51,51,51                 | 0     |
| 86  | MG   | 5     | 3864 | 1/1   | 0.40 | 12.78 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 3742 | 1/1   | 0.32 | 12.76 | 16,16,16,16                 | 0     |
| 87  | OHX  | 5     | 4241 | 7/7   | 0.39 | 12.75 | 125,125,125,125             | 0     |
| 86  | MG   | 5     | 3884 | 1/1   | 0.38 | 12.71 | 62,62,62,62                 | 0     |
| 86  | MG   | 5     | 3639 | 1/1   | 0.40 | 12.71 | 49,49,49,49                 | 0     |
| 87  | OHX  | 5     | 4164 | 7/7   | 0.30 | 12.70 | 94,94,94,94                 | 0     |
| 87  | OHX  | 1     | 4102 | 7/7   | 0.25 | 12.69 | 139,139,139,139             | 0     |
| 86  | MG   | 5     | 3623 | 1/1   | 0.38 | 12.67 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 3586 | 1/1   | 0.50 | 12.66 | 16,16,16,16                 | 0     |
| 86  | MG   | 1     | 3453 | 1/1   | 0.34 | 12.64 | 35,35,35,35                 | 0     |
| 86  | MG   | 6     | 1950 | 1/1   | 0.49 | 12.56 | 42,42,42,42                 | 0     |
| 86  | MG   | 5     | 3661 | 1/1   | 0.25 | 12.54 | 20,20,20,20                 | 0     |
| 86  | MG   | 1     | 3684 | 1/1   | 0.18 | 12.53 | 29,29,29,29                 | 0     |
| 87  | OHX  | 5     | 4212 | 7/7   | 0.34 | 12.48 | 89,89,89,89                 | 0     |
| 86  | MG   | 5     | 3748 | 1/1   | 0.34 | 12.46 | 29,29,29,29                 | 0     |
| 86  | MG   | 5     | 3813 | 1/1   | 0.28 | 12.43 | 31,31,31,31                 | 0     |
| 87  | OHX  | 1     | 4157 | 7/7   | 0.33 | 12.41 | 118,118,118,118             | 0     |
| 86  | MG   | 5     | 3699 | 1/1   | 0.41 | 12.41 | 36,36,36,36                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 5     | 3495 | 1/1   | 0.35 | 12.39 | 19,19,19,19                 | 0     |
| 86  | MG   | 7     | 212  | 1/1   | 0.33 | 12.37 | 58,58,58,58                 | 0     |
| 86  | MG   | 1     | 3410 | 1/1   | 0.43 | 12.35 | 39,39,39,39                 | 0     |
| 86  | MG   | 5     | 3852 | 1/1   | 0.19 | 12.33 | 58,58,58,58                 | 0     |
| 86  | MG   | 1     | 3696 | 1/1   | 0.27 | 12.31 | 28,28,28,28                 | 0     |
| 87  | OHX  | 6     | 2147 | 7/7   | 0.33 | 12.26 | 112,112,112,112             | 0     |
| 87  | OHX  | 1     | 4182 | 7/7   | 0.40 | 12.25 | 130,130,130,130             | 0     |
| 87  | OHX  | 5     | 4071 | 7/7   | 0.33 | 12.25 | 107,107,107,107             | 0     |
| 86  | MG   | 1     | 3559 | 1/1   | 0.44 | 12.25 | 43,43,43,43                 | 0     |
| 87  | OHX  | 2     | 2176 | 7/7   | 0.35 | 12.23 | 163,163,163,163             | 0     |
| 86  | MG   | 5     | 3836 | 1/1   | 0.34 | 12.17 | 28,28,28,28                 | 0     |
| 87  | OHX  | 8     | 229  | 7/7   | 0.32 | 12.16 | 108,108,108,108             | 0     |
| 87  | OHX  | 2     | 2169 | 7/7   | 0.34 | 12.16 | 126,126,126,126             | 0     |
| 87  | OHX  | 5     | 4145 | 7/7   | 0.28 | 12.10 | 88,88,88,88                 | 0     |
| 87  | OHX  | 6     | 2193 | 7/7   | 0.39 | 12.10 | 129,129,129,129             | 0     |
| 87  | OHX  | 4     | 230  | 7/7   | 0.34 | 12.08 | 123,123,123,123             | 0     |
| 86  | MG   | 1     | 3564 | 1/1   | 0.39 | 12.07 | 39,39,39,39                 | 0     |
| 86  | MG   | 5     | 3410 | 1/1   | 0.22 | 12.00 | 51,51,51,51                 | 0     |
| 87  | OHX  | 1     | 4087 | 7/7   | 0.28 | 11.98 | 104,104,104,104             | 0     |
| 86  | MG   | 5     | 3520 | 1/1   | 0.33 | 11.97 | 24,24,24,24                 | 0     |
| 87  | OHX  | 5     | 4205 | 7/7   | 0.46 | 11.97 | 129,129,129,129             | 0     |
| 86  | MG   | 1     | 3596 | 1/1   | 0.48 | 11.94 | 17,17,17,17                 | 0     |
| 86  | MG   | 5     | 3653 | 1/1   | 0.54 | 11.94 | 69,69,69,69                 | 0     |
| 86  | MG   | 1     | 3506 | 1/1   | 0.28 | 11.94 | 25,25,25,25                 | 0     |
| 86  | MG   | 7     | 209  | 1/1   | 0.36 | 11.92 | 32,32,32,32                 | 0     |
| 87  | OHX  | 1     | 4062 | 7/7   | 0.28 | 11.83 | 94,94,94,94                 | 0     |
| 86  | MG   | 1     | 3406 | 1/1   | 0.34 | 11.82 | 30,30,30,30                 | 0     |
| 86  | MG   | 5     | 3630 | 1/1   | 0.33 | 11.80 | 31,31,31,31                 | 0     |
| 87  | OHX  | 5     | 4005 | 7/7   | 0.27 | 11.80 | 97,97,97,97                 | 0     |
| 86  | MG   | 5     | 3492 | 1/1   | 0.41 | 11.77 | 51,51,51,51                 | 0     |
| 87  | OHX  | 1     | 4131 | 7/7   | 0.27 | 11.72 | 121,121,121,121             | 0     |
| 86  | MG   | 6     | 2006 | 1/1   | 0.35 | 11.68 | 94,94,94,94                 | 0     |
| 86  | MG   | 5     | 3506 | 1/1   | 0.43 | 11.52 | 23,23,23,23                 | 0     |
| 86  | MG   | 5     | 3698 | 1/1   | 0.33 | 11.48 | 42,42,42,42                 | 0     |
| 87  | OHX  | 1     | 4162 | 7/7   | 0.28 | 11.48 | 124,124,124,124             | 0     |
| 86  | MG   | 4     | 208  | 1/1   | 0.36 | 11.48 | 35,35,35,35                 | 0     |
| 87  | OHX  | 1     | 4216 | 7/7   | 0.42 | 11.46 | 110,110,110,110             | 0     |
| 87  | OHX  | 5     | 4238 | 7/7   | 0.34 | 11.45 | 115,115,115,115             | 0     |
| 86  | MG   | 2     | 1901 | 1/1   | 0.97 | 11.37 | 66,66,66,66                 | 0     |
| 86  | MG   | 1     | 3678 | 1/1   | 0.35 | 11.32 | 54,54,54,54                 | 0     |
| 86  | MG   | 1     | 3550 | 1/1   | 0.31 | 11.32 | 26,26,26,26                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 5     | 3432 | 1/1   | 0.18 | 11.31 | 33,33,33,33                 | 0     |
| 87  | OHX  | 1     | 4033 | 7/7   | 0.28 | 11.29 | 87,87,87,87                 | 0     |
| 87  | OHX  | 5     | 4222 | 7/7   | 0.35 | 11.29 | 117,117,117,117             | 0     |
| 86  | MG   | 6     | 1961 | 1/1   | 0.45 | 11.29 | 34,34,34,34                 | 0     |
| 86  | MG   | 5     | 3560 | 1/1   | 0.33 | 11.27 | 28,28,28,28                 | 0     |
| 86  | MG   | 4     | 211  | 1/1   | 0.29 | 11.25 | 44,44,44,44                 | 0     |
| 86  | MG   | 2     | 1926 | 1/1   | 0.47 | 11.24 | 84,84,84,84                 | 0     |
| 86  | MG   | 6     | 1966 | 1/1   | 0.25 | 11.21 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 3616 | 1/1   | 0.34 | 11.14 | 28,28,28,28                 | 0     |
| 87  | OHX  | 5     | 4197 | 7/7   | 0.34 | 11.11 | 105,105,105,105             | 0     |
| 86  | MG   | 5     | 3544 | 1/1   | 0.32 | 11.08 | 24,24,24,24                 | 0     |
| 86  | MG   | 2     | 1952 | 1/1   | 0.41 | 11.01 | 89,89,89,89                 | 0     |
| 86  | MG   | 1     | 3548 | 1/1   | 0.41 | 11.01 | 34,34,34,34                 | 0     |
| 87  | OHX  | 1     | 4197 | 7/7   | 0.44 | 11.00 | 123,123,123,123             | 0     |
| 87  | OHX  | 1     | 4164 | 7/7   | 0.42 | 10.97 | 134,134,134,134             | 0     |
| 86  | MG   | 6     | 1920 | 1/1   | 0.37 | 10.97 | 35,35,35,35                 | 0     |
| 86  | MG   | 5     | 3891 | 1/1   | 0.41 | 10.96 | 73,73,73,73                 | 0     |
| 87  | OHX  | 5     | 4052 | 7/7   | 0.23 | 10.94 | 86,86,86,86                 | 0     |
| 86  | MG   | 5     | 3796 | 1/1   | 0.26 | 10.94 | 37,37,37,37                 | 0     |
| 86  | MG   | 1     | 3627 | 1/1   | 0.29 | 10.91 | 27,27,27,27                 | 0     |
| 86  | MG   | 1     | 3866 | 1/1   | 0.28 | 10.87 | 66,66,66,66                 | 0     |
| 86  | MG   | 5     | 3776 | 1/1   | 0.31 | 10.86 | 19,19,19,19                 | 0     |
| 86  | MG   | 5     | 3456 | 1/1   | 0.33 | 10.85 | 18,18,18,18                 | 0     |
| 86  | MG   | 1     | 3689 | 1/1   | 0.22 | 10.85 | 79,79,79,79                 | 0     |
| 86  | MG   | 5     | 3893 | 1/1   | 0.40 | 10.85 | 112,112,112,112             | 0     |
| 86  | MG   | 5     | 3581 | 1/1   | 0.35 | 10.84 | 25,25,25,25                 | 0     |
| 86  | MG   | 6     | 1948 | 1/1   | 0.40 | 10.83 | 43,43,43,43                 | 0     |
| 86  | MG   | 4     | 213  | 1/1   | 0.32 | 10.76 | 50,50,50,50                 | 0     |
| 86  | MG   | 1     | 3748 | 1/1   | 0.41 | 10.75 | 41,41,41,41                 | 0     |
| 86  | MG   | S8    | 301  | 1/1   | 0.39 | 10.72 | 49,49,49,49                 | 0     |
| 87  | OHX  | 1     | 4187 | 7/7   | 0.43 | 10.71 | 117,117,117,117             | 0     |
| 86  | MG   | 5     | 3825 | 1/1   | 0.22 | 10.69 | 37,37,37,37                 | 0     |
| 86  | MG   | 5     | 3499 | 1/1   | 0.28 | 10.68 | 23,23,23,23                 | 0     |
| 86  | MG   | 2     | 1991 | 1/1   | 0.26 | 10.65 | 60,60,60,60                 | 0     |
| 86  | MG   | N0    | 201  | 1/1   | 0.42 | 10.63 | 35,35,35,35                 | 0     |
| 86  | MG   | 5     | 3759 | 1/1   | 0.36 | 10.62 | 44,44,44,44                 | 0     |
| 86  | MG   | 6     | 2033 | 1/1   | 0.41 | 10.61 | 87,87,87,87                 | 0     |
| 86  | MG   | 1     | 3869 | 1/1   | 0.30 | 10.57 | 21,21,21,21                 | 0     |
| 86  | MG   | 5     | 3702 | 1/1   | 0.26 | 10.55 | 26,26,26,26                 | 0     |
| 86  | MG   | 2     | 2005 | 1/1   | 0.56 | 10.54 | 45,45,45,45                 | 0     |
| 87  | OHX  | 2     | 2134 | 7/7   | 0.34 | 10.52 | 112,112,112,112             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 87  | OHX  | 5     | 4101 | 7/7   | 0.28 | 10.51 | 95,95,95,95                 | 0     |
| 86  | MG   | 7     | 203  | 1/1   | 0.31 | 10.51 | 44,44,44,44                 | 0     |
| 86  | MG   | 5     | 3422 | 1/1   | 0.25 | 10.44 | 31,31,31,31                 | 0     |
| 87  | OHX  | 2     | 2106 | 7/7   | 0.32 | 10.44 | 117,117,117,117             | 0     |
| 86  | MG   | 5     | 3861 | 1/1   | 0.16 | 10.43 | 31,31,31,31                 | 0     |
| 86  | MG   | 5     | 3765 | 1/1   | 0.31 | 10.39 | 29,29,29,29                 | 0     |
| 86  | MG   | 5     | 3648 | 1/1   | 0.30 | 10.38 | 28,28,28,28                 | 0     |
| 86  | MG   | 1     | 3790 | 1/1   | 0.32 | 10.37 | 26,26,26,26                 | 0     |
| 86  | MG   | 6     | 1973 | 1/1   | 0.38 | 10.36 | 58,58,58,58                 | 0     |
| 86  | MG   | 5     | 3488 | 1/1   | 0.39 | 10.32 | 15,15,15,15                 | 0     |
| 87  | OHX  | 5     | 4055 | 7/7   | 0.36 | 10.31 | 88,88,88,88                 | 0     |
| 87  | OHX  | 5     | 4083 | 7/7   | 0.34 | 10.31 | 88,88,88,88                 | 0     |
| 86  | MG   | 5     | 3424 | 1/1   | 0.28 | 10.28 | 25,25,25,25                 | 0     |
| 86  | MG   | 5     | 3890 | 1/1   | 0.31 | 10.26 | 16,16,16,16                 | 0     |
| 86  | MG   | 1     | 3741 | 1/1   | 0.25 | 10.25 | 42,42,42,42                 | 0     |
| 86  | MG   | 1     | 3760 | 1/1   | 0.26 | 10.20 | 22,22,22,22                 | 0     |
| 86  | MG   | 1     | 3441 | 1/1   | 0.30 | 10.19 | 32,32,32,32                 | 0     |
| 86  | MG   | 2     | 2003 | 1/1   | 0.31 | 10.19 | 50,50,50,50                 | 0     |
| 86  | MG   | 5     | 3450 | 1/1   | 0.29 | 10.16 | 24,24,24,24                 | 0     |
| 86  | MG   | 8     | 204  | 1/1   | 0.28 | 10.15 | 46,46,46,46                 | 0     |
| 87  | OHX  | 1     | 4121 | 7/7   | 0.27 | 10.11 | 112,112,112,112             | 0     |
| 87  | OHX  | 5     | 4130 | 7/7   | 0.24 | 10.11 | 133,133,133,133             | 0     |
| 87  | OHX  | 1     | 4074 | 7/7   | 0.33 | 10.07 | 92,92,92,92                 | 0     |
| 86  | MG   | 1     | 3407 | 1/1   | 0.27 | 10.06 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 3571 | 1/1   | 0.43 | 10.06 | 18,18,18,18                 | 0     |
| 86  | MG   | 1     | 3488 | 1/1   | 0.26 | 10.06 | 27,27,27,27                 | 0     |
| 86  | MG   | 1     | 3703 | 1/1   | 0.32 | 10.04 | 31,31,31,31                 | 0     |
| 86  | MG   | 5     | 3612 | 1/1   | 0.22 | 10.01 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 3586 | 1/1   | 0.49 | 10.00 | 43,43,43,43                 | 0     |
| 87  | OHX  | 2     | 2167 | 7/7   | 0.34 | 9.97  | 135,135,135,135             | 0     |
| 86  | MG   | 5     | 3589 | 1/1   | 0.35 | 9.92  | 19,19,19,19                 | 0     |
| 86  | MG   | 6     | 1937 | 1/1   | 0.39 | 9.88  | 67,67,67,67                 | 0     |
| 86  | MG   | 1     | 3800 | 1/1   | 0.25 | 9.87  | 19,19,19,19                 | 0     |
| 86  | MG   | 5     | 3815 | 1/1   | 0.21 | 9.86  | 50,50,50,50                 | 0     |
| 87  | OHX  | 5     | 4251 | 7/7   | 0.42 | 9.81  | 137,137,137,137             | 0     |
| 86  | MG   | 5     | 3610 | 1/1   | 0.30 | 9.80  | 22,22,22,22                 | 0     |
| 87  | OHX  | 1     | 4208 | 7/7   | 0.32 | 9.80  | 108,108,108,108             | 0     |
| 86  | MG   | 5     | 3683 | 1/1   | 0.52 | 9.78  | 75,75,75,75                 | 0     |
| 86  | MG   | L4    | 401  | 1/1   | 0.26 | 9.77  | 46,46,46,46                 | 0     |
| 86  | MG   | 6     | 1962 | 1/1   | 0.34 | 9.77  | 69,69,69,69                 | 0     |
| 86  | MG   | 5     | 4257 | 1/1   | 0.36 | 9.75  | 16,16,16,16                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87  | OHX  | 1     | 4116 | 7/7   | 0.38 | 9.74 | 127,127,127,127             | 0     |
| 86  | MG   | 1     | 3777 | 1/1   | 0.21 | 9.74 | 50,50,50,50                 | 0     |
| 86  | MG   | 5     | 3677 | 1/1   | 0.29 | 9.73 | 33,33,33,33                 | 0     |
| 87  | OHX  | 1     | 4104 | 7/7   | 0.30 | 9.72 | 95,95,95,95                 | 0     |
| 86  | MG   | 8     | 210  | 1/1   | 0.34 | 9.72 | 37,37,37,37                 | 0     |
| 86  | MG   | 2     | 1929 | 1/1   | 0.41 | 9.72 | 59,59,59,59                 | 0     |
| 87  | OHX  | 6     | 2139 | 7/7   | 0.33 | 9.71 | 110,110,110,110             | 0     |
| 86  | MG   | 5     | 3548 | 1/1   | 0.34 | 9.69 | 39,39,39,39                 | 0     |
| 87  | OHX  | 2     | 2135 | 7/7   | 0.30 | 9.68 | 151,151,151,151             | 0     |
| 86  | MG   | 5     | 3889 | 1/1   | 0.38 | 9.68 | 31,31,31,31                 | 0     |
| 87  | OHX  | 1     | 4140 | 7/7   | 0.30 | 9.67 | 93,93,93,93                 | 0     |
| 86  | MG   | 1     | 3456 | 1/1   | 0.29 | 9.63 | 17,17,17,17                 | 0     |
| 87  | OHX  | 1     | 4163 | 7/7   | 0.33 | 9.62 | 108,108,108,108             | 0     |
| 86  | MG   | m7    | 201  | 1/1   | 0.39 | 9.62 | 23,23,23,23                 | 0     |
| 86  | MG   | 1     | 3533 | 1/1   | 0.38 | 9.61 | 25,25,25,25                 | 0     |
| 87  | OHX  | 5     | 4248 | 7/7   | 0.30 | 9.61 | 120,120,120,120             | 0     |
| 87  | OHX  | 1     | 4204 | 7/7   | 0.29 | 9.60 | 104,104,104,104             | 0     |
| 86  | MG   | 5     | 3597 | 1/1   | 0.32 | 9.57 | 23,23,23,23                 | 0     |
| 87  | OHX  | 6     | 2180 | 7/7   | 0.31 | 9.56 | 94,94,94,94                 | 0     |
| 87  | OHX  | 5     | 4199 | 7/7   | 0.31 | 9.55 | 96,96,96,96                 | 0     |
| 86  | MG   | 5     | 3569 | 1/1   | 0.35 | 9.51 | 27,27,27,27                 | 0     |
| 86  | MG   | 5     | 3882 | 1/1   | 0.23 | 9.50 | 19,19,19,19                 | 0     |
| 86  | MG   | 5     | 3844 | 1/1   | 0.38 | 9.49 | 37,37,37,37                 | 0     |
| 87  | OHX  | 1     | 4009 | 7/7   | 0.23 | 9.48 | 87,87,87,87                 | 0     |
| 87  | OHX  | 5     | 4128 | 7/7   | 0.26 | 9.45 | 110,110,110,110             | 0     |
| 87  | OHX  | 14    | 403  | 7/7   | 0.48 | 9.45 | 129,129,129,129             | 0     |
| 86  | MG   | 5     | 3641 | 1/1   | 0.20 | 9.43 | 28,28,28,28                 | 0     |
| 87  | OHX  | 5     | 4110 | 7/7   | 0.30 | 9.42 | 100,100,100,100             | 0     |
| 87  | OHX  | 5     | 4249 | 7/7   | 0.29 | 9.42 | 131,131,131,131             | 0     |
| 87  | OHX  | 2     | 2160 | 7/7   | 0.32 | 9.41 | 154,154,154,154             | 0     |
| 86  | MG   | 1     | 3502 | 1/1   | 0.36 | 9.40 | 19,19,19,19                 | 0     |
| 86  | MG   | l3    | 402  | 1/1   | 0.48 | 9.39 | 23,23,23,23                 | 0     |
| 87  | OHX  | 7     | 227  | 7/7   | 0.27 | 9.37 | 131,131,131,131             | 0     |
| 87  | OHX  | 5     | 4093 | 7/7   | 0.27 | 9.36 | 92,92,92,92                 | 0     |
| 87  | OHX  | 5     | 4221 | 7/7   | 0.31 | 9.34 | 164,164,164,164             | 0     |
| 87  | OHX  | 5     | 4112 | 7/7   | 0.36 | 9.33 | 110,110,110,110             | 0     |
| 86  | MG   | 1     | 3554 | 1/1   | 0.28 | 9.33 | 42,42,42,42                 | 0     |
| 87  | OHX  | 5     | 4154 | 7/7   | 0.30 | 9.29 | 87,87,87,87                 | 0     |
| 86  | MG   | 5     | 3546 | 1/1   | 0.35 | 9.27 | 35,35,35,35                 | 0     |
| 86  | MG   | 1     | 3555 | 1/1   | 0.33 | 9.27 | 25,25,25,25                 | 0     |
| 87  | OHX  | 1     | 4158 | 7/7   | 0.26 | 9.27 | 114,114,114,114             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 2     | 1960 | 1/1   | 0.32 | 9.27 | 59,59,59,59                 | 0     |
| 87  | OHX  | 1     | 3900 | 7/7   | 0.29 | 9.25 | 95,95,95,95                 | 0     |
| 86  | MG   | 2     | 1944 | 1/1   | 0.33 | 9.21 | 60,60,60,60                 | 0     |
| 87  | OHX  | 5     | 4099 | 7/7   | 0.22 | 9.19 | 98,98,98,98                 | 0     |
| 86  | MG   | 5     | 3839 | 1/1   | 0.46 | 9.18 | 37,37,37,37                 | 0     |
| 86  | MG   | 1     | 3798 | 1/1   | 0.26 | 9.17 | 19,19,19,19                 | 0     |
| 86  | MG   | 5     | 3516 | 1/1   | 0.34 | 9.14 | 21,21,21,21                 | 0     |
| 86  | MG   | 2     | 1989 | 1/1   | 0.82 | 9.13 | 104,104,104,104             | 0     |
| 87  | OHX  | 5     | 4208 | 7/7   | 0.33 | 9.12 | 120,120,120,120             | 0     |
| 86  | MG   | 1     | 3656 | 1/1   | 0.20 | 9.11 | 20,20,20,20                 | 0     |
| 86  | MG   | 5     | 3646 | 1/1   | 0.38 | 9.10 | 27,27,27,27                 | 0     |
| 87  | OHX  | 5     | 4232 | 7/7   | 0.30 | 9.09 | 137,137,137,137             | 0     |
| 86  | MG   | 2     | 1976 | 1/1   | 0.39 | 9.09 | 51,51,51,51                 | 0     |
| 87  | OHX  | 5     | 4043 | 7/7   | 0.24 | 9.05 | 108,108,108,108             | 0     |
| 87  | OHX  | 4     | 229  | 7/7   | 0.28 | 9.04 | 93,93,93,93                 | 0     |
| 87  | OHX  | 1     | 4178 | 7/7   | 0.30 | 8.99 | 164,164,164,164             | 0     |
| 86  | MG   | 8     | 211  | 1/1   | 0.32 | 8.96 | 61,61,61,61                 | 0     |
| 87  | OHX  | 6     | 2163 | 7/7   | 0.35 | 8.95 | 112,112,112,112             | 0     |
| 87  | OHX  | 5     | 4033 | 7/7   | 0.25 | 8.94 | 87,87,87,87                 | 0     |
| 86  | MG   | 2     | 1967 | 1/1   | 0.65 | 8.93 | 53,53,53,53                 | 0     |
| 87  | OHX  | 5     | 4117 | 7/7   | 0.26 | 8.91 | 126,126,126,126             | 0     |
| 87  | OHX  | 6     | 2194 | 7/7   | 0.31 | 8.87 | 146,146,146,146             | 0     |
| 86  | MG   | 1     | 3635 | 1/1   | 0.28 | 8.86 | 48,48,48,48                 | 0     |
| 86  | MG   | 5     | 3509 | 1/1   | 0.33 | 8.86 | 30,30,30,30                 | 0     |
| 87  | OHX  | 1     | 4096 | 7/7   | 0.27 | 8.86 | 95,95,95,95                 | 0     |
| 86  | MG   | 5     | 3423 | 1/1   | 0.38 | 8.85 | 51,51,51,51                 | 0     |
| 86  | MG   | 5     | 4258 | 1/1   | 0.23 | 8.85 | 24,24,24,24                 | 0     |
| 87  | OHX  | 5     | 4158 | 7/7   | 0.37 | 8.83 | 109,109,109,109             | 0     |
| 87  | OHX  | 5     | 4167 | 7/7   | 0.36 | 8.81 | 111,111,111,111             | 0     |
| 86  | MG   | 1     | 3497 | 1/1   | 0.27 | 8.79 | 22,22,22,22                 | 0     |
| 86  | MG   | 5     | 3421 | 1/1   | 0.37 | 8.79 | 27,27,27,27                 | 0     |
| 87  | OHX  | 6     | 2128 | 7/7   | 0.28 | 8.78 | 113,113,113,113             | 0     |
| 86  | MG   | 1     | 3812 | 1/1   | 0.24 | 8.77 | 30,30,30,30                 | 0     |
| 87  | OHX  | 5     | 4168 | 7/7   | 0.23 | 8.76 | 109,109,109,109             | 0     |
| 86  | MG   | 5     | 3633 | 1/1   | 0.36 | 8.75 | 40,40,40,40                 | 0     |
| 86  | MG   | 5     | 3895 | 1/1   | 0.28 | 8.72 | 46,46,46,46                 | 0     |
| 86  | MG   | 8     | 201  | 1/1   | 0.28 | 8.71 | 31,31,31,31                 | 0     |
| 86  | MG   | 5     | 3763 | 1/1   | 0.33 | 8.70 | 32,32,32,32                 | 0     |
| 87  | OHX  | 1     | 4191 | 7/7   | 0.45 | 8.66 | 179,179,179,179             | 0     |
| 86  | MG   | 6     | 1972 | 1/1   | 0.20 | 8.62 | 57,57,57,57                 | 0     |
| 86  | MG   | 5     | 3526 | 1/1   | 0.20 | 8.61 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 1     | 3474 | 1/1   | 0.26 | 8.60 | 66,66,66,66                 | 0     |
| 86  | MG   | 5     | 3827 | 1/1   | 0.26 | 8.60 | 29,29,29,29                 | 0     |
| 86  | MG   | M5    | 301  | 1/1   | 0.44 | 8.60 | 40,40,40,40                 | 0     |
| 87  | OHX  | 5     | 4074 | 7/7   | 0.23 | 8.56 | 89,89,89,89                 | 0     |
| 86  | MG   | 5     | 3464 | 1/1   | 0.19 | 8.55 | 25,25,25,25                 | 0     |
| 87  | OHX  | 5     | 4201 | 7/7   | 0.29 | 8.54 | 91,91,91,91                 | 0     |
| 86  | MG   | n8    | 201  | 1/1   | 0.32 | 8.53 | 27,27,27,27                 | 0     |
| 86  | MG   | 5     | 3472 | 1/1   | 0.23 | 8.52 | 28,28,28,28                 | 0     |
| 86  | MG   | S2    | 301  | 1/1   | 0.55 | 8.51 | 59,59,59,59                 | 0     |
| 86  | MG   | 5     | 3622 | 1/1   | 0.30 | 8.51 | 26,26,26,26                 | 0     |
| 87  | OHX  | 6     | 2113 | 7/7   | 0.26 | 8.50 | 88,88,88,88                 | 0     |
| 86  | MG   | 1     | 3695 | 1/1   | 0.32 | 8.49 | 36,36,36,36                 | 0     |
| 87  | OHX  | 2     | 2090 | 7/7   | 0.32 | 8.47 | 98,98,98,98                 | 0     |
| 87  | OHX  | 1     | 3959 | 7/7   | 0.19 | 8.46 | 80,80,80,80                 | 0     |
| 87  | OHX  | 5     | 4136 | 7/7   | 0.28 | 8.46 | 97,97,97,97                 | 0     |
| 86  | MG   | 6     | 1982 | 1/1   | 0.28 | 8.44 | 66,66,66,66                 | 0     |
| 87  | OHX  | 5     | 4053 | 7/7   | 0.26 | 8.43 | 79,79,79,79                 | 0     |
| 86  | MG   | 7     | 213  | 1/1   | 0.20 | 8.42 | 65,65,65,65                 | 0     |
| 86  | MG   | 1     | 3833 | 1/1   | 0.26 | 8.41 | 16,16,16,16                 | 0     |
| 86  | MG   | 2     | 1910 | 1/1   | 0.31 | 8.38 | 48,48,48,48                 | 0     |
| 86  | MG   | 6     | 2034 | 1/1   | 0.26 | 8.33 | 59,59,59,59                 | 0     |
| 86  | MG   | 2     | 1907 | 1/1   | 0.50 | 8.32 | 51,51,51,51                 | 0     |
| 86  | MG   | 1     | 3536 | 1/1   | 0.30 | 8.32 | 35,35,35,35                 | 0     |
| 86  | MG   | 3     | 207  | 1/1   | 0.28 | 8.28 | 58,58,58,58                 | 0     |
| 86  | MG   | 3     | 203  | 1/1   | 0.27 | 8.28 | 85,85,85,85                 | 0     |
| 86  | MG   | 1     | 3651 | 1/1   | 0.30 | 8.27 | 38,38,38,38                 | 0     |
| 87  | OHX  | o7    | 503  | 7/7   | 0.34 | 8.26 | 102,102,102,102             | 0     |
| 87  | OHX  | 2     | 2111 | 7/7   | 0.34 | 8.25 | 113,113,113,113             | 0     |
| 86  | MG   | 1     | 3626 | 1/1   | 0.48 | 8.24 | 76,76,76,76                 | 0     |
| 86  | MG   | 5     | 3470 | 1/1   | 0.40 | 8.24 | 28,28,28,28                 | 0     |
| 87  | OHX  | 1     | 4082 | 7/7   | 0.40 | 8.24 | 99,99,99,99                 | 0     |
| 86  | MG   | 1     | 3622 | 1/1   | 0.28 | 8.23 | 33,33,33,33                 | 0     |
| 87  | OHX  | 5     | 4098 | 7/7   | 0.22 | 8.21 | 131,131,131,131             | 0     |
| 86  | MG   | 5     | 3583 | 1/1   | 0.28 | 8.18 | 30,30,30,30                 | 0     |
| 86  | MG   | l2    | 302  | 1/1   | 0.34 | 8.17 | 28,28,28,28                 | 0     |
| 86  | MG   | 5     | 3476 | 1/1   | 0.27 | 8.17 | 29,29,29,29                 | 0     |
| 87  | OHX  | 2     | 2174 | 7/7   | 0.27 | 8.11 | 124,124,124,124             | 0     |
| 87  | OHX  | 1     | 4067 | 7/7   | 0.41 | 8.09 | 110,110,110,110             | 0     |
| 86  | MG   | 5     | 3788 | 1/1   | 0.27 | 8.06 | 42,42,42,42                 | 0     |
| 86  | MG   | 5     | 3594 | 1/1   | 0.30 | 8.04 | 30,30,30,30                 | 0     |
| 87  | OHX  | 2     | 2121 | 7/7   | 0.25 | 8.04 | 117,117,117,117             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 5     | 3792 | 1/1   | 0.23 | 8.04 | 25,25,25,25                 | 0     |
| 86  | MG   | 5     | 3634 | 1/1   | 0.20 | 8.03 | 27,27,27,27                 | 0     |
| 86  | MG   | 5     | 3441 | 1/1   | 0.37 | 8.01 | 23,23,23,23                 | 0     |
| 87  | OHX  | 1     | 4066 | 7/7   | 0.33 | 8.01 | 124,124,124,124             | 0     |
| 86  | MG   | c1    | 201  | 1/1   | 0.45 | 8.00 | 38,38,38,38                 | 0     |
| 87  | OHX  | 5     | 4080 | 7/7   | 0.29 | 7.98 | 111,111,111,111             | 0     |
| 87  | OHX  | 1     | 4112 | 7/7   | 0.27 | 7.97 | 116,116,116,116             | 0     |
| 87  | OHX  | 5     | 4139 | 7/7   | 0.39 | 7.97 | 103,103,103,103             | 0     |
| 86  | MG   | s8    | 301  | 1/1   | 0.34 | 7.95 | 41,41,41,41                 | 0     |
| 86  | MG   | 6     | 1965 | 1/1   | 0.37 | 7.94 | 87,87,87,87                 | 0     |
| 86  | MG   | 6     | 1936 | 1/1   | 0.64 | 7.91 | 46,46,46,46                 | 0     |
| 87  | OHX  | 2     | 2151 | 7/7   | 0.28 | 7.91 | 160,160,160,160             | 0     |
| 87  | OHX  | 5     | 4186 | 7/7   | 0.31 | 7.91 | 97,97,97,97                 | 0     |
| 87  | OHX  | 5     | 4176 | 7/7   | 0.26 | 7.90 | 101,101,101,101             | 0     |
| 86  | MG   | 5     | 3685 | 1/1   | 0.27 | 7.90 | 25,25,25,25                 | 0     |
| 86  | MG   | 1     | 3712 | 1/1   | 0.23 | 7.90 | 29,29,29,29                 | 0     |
| 86  | MG   | 1     | 3844 | 1/1   | 0.34 | 7.89 | 20,20,20,20                 | 0     |
| 86  | MG   | 1     | 3593 | 1/1   | 0.38 | 7.89 | 39,39,39,39                 | 0     |
| 86  | MG   | 2     | 1970 | 1/1   | 0.30 | 7.89 | 63,63,63,63                 | 0     |
| 86  | MG   | 1     | 3585 | 1/1   | 0.29 | 7.88 | 33,33,33,33                 | 0     |
| 86  | MG   | 5     | 3631 | 1/1   | 0.21 | 7.87 | 35,35,35,35                 | 0     |
| 86  | MG   | 1     | 3671 | 1/1   | 0.23 | 7.87 | 73,73,73,73                 | 0     |
| 86  | MG   | 6     | 1906 | 1/1   | 0.34 | 7.86 | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 3663 | 1/1   | 0.32 | 7.86 | 23,23,23,23                 | 0     |
| 86  | MG   | 2     | 1942 | 1/1   | 0.45 | 7.84 | 59,59,59,59                 | 0     |
| 87  | OHX  | 1     | 4118 | 7/7   | 0.23 | 7.83 | 164,164,164,164             | 0     |
| 87  | OHX  | 5     | 4147 | 7/7   | 0.30 | 7.82 | 98,98,98,98                 | 0     |
| 86  | MG   | 5     | 3514 | 1/1   | 0.41 | 7.78 | 20,20,20,20                 | 0     |
| 87  | OHX  | 6     | 2189 | 7/7   | 0.39 | 7.73 | 124,124,124,124             | 0     |
| 87  | OHX  | 6     | 2190 | 7/7   | 0.32 | 7.73 | 150,150,150,150             | 0     |
| 86  | MG   | 5     | 3756 | 1/1   | 0.32 | 7.72 | 50,50,50,50                 | 0     |
| 86  | MG   | 1     | 3577 | 1/1   | 0.40 | 7.70 | 18,18,18,18                 | 0     |
| 86  | MG   | 1     | 3744 | 1/1   | 0.33 | 7.70 | 35,35,35,35                 | 0     |
| 86  | MG   | 2     | 1983 | 1/1   | 0.24 | 7.70 | 70,70,70,70                 | 0     |
| 87  | OHX  | 1     | 4091 | 7/7   | 0.23 | 7.69 | 115,115,115,115             | 0     |
| 86  | MG   | 5     | 3440 | 1/1   | 0.28 | 7.67 | 32,32,32,32                 | 0     |
| 86  | MG   | 1     | 3733 | 1/1   | 0.25 | 7.67 | 32,32,32,32                 | 0     |
| 87  | OHX  | 1     | 3961 | 7/7   | 0.27 | 7.64 | 91,91,91,91                 | 0     |
| 86  | MG   | 1     | 3483 | 1/1   | 0.36 | 7.64 | 42,42,42,42                 | 0     |
| 87  | OHX  | 1     | 3984 | 7/7   | 0.28 | 7.64 | 73,73,73,73                 | 0     |
| 87  | OHX  | 1     | 4114 | 7/7   | 0.26 | 7.60 | 117,117,117,117             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 5     | 3739 | 1/1   | 0.29 | 7.58 | 64,64,64,64                 | 0     |
| 87  | OHX  | 1     | 4124 | 7/7   | 0.29 | 7.56 | 88,88,88,88                 | 0     |
| 86  | MG   | 1     | 3670 | 1/1   | 0.29 | 7.54 | 34,34,34,34                 | 0     |
| 87  | OHX  | 5     | 4174 | 7/7   | 0.43 | 7.54 | 78,78,78,78                 | 0     |
| 86  | MG   | 6     | 1935 | 1/1   | 0.36 | 7.54 | 64,64,64,64                 | 0     |
| 87  | OHX  | 6     | 2179 | 7/7   | 0.35 | 7.53 | 85,85,85,85                 | 0     |
| 87  | OHX  | 6     | 2106 | 7/7   | 0.30 | 7.51 | 97,97,97,97                 | 0     |
| 86  | MG   | 2     | 1951 | 1/1   | 0.57 | 7.50 | 90,90,90,90                 | 0     |
| 87  | OHX  | 5     | 4250 | 7/7   | 0.36 | 7.50 | 103,103,103,103             | 0     |
| 86  | MG   | 1     | 3605 | 1/1   | 0.28 | 7.49 | 28,28,28,28                 | 0     |
| 86  | MG   | 6     | 1954 | 1/1   | 0.46 | 7.48 | 54,54,54,54                 | 0     |
| 86  | MG   | 1     | 3546 | 1/1   | 0.39 | 7.46 | 46,46,46,46                 | 0     |
| 86  | MG   | 1     | 3826 | 1/1   | 0.37 | 7.46 | 32,32,32,32                 | 0     |
| 87  | OHX  | 6     | 2181 | 7/7   | 0.35 | 7.45 | 118,118,118,118             | 0     |
| 86  | MG   | 1     | 3529 | 1/1   | 0.29 | 7.45 | 38,38,38,38                 | 0     |
| 86  | MG   | 5     | 3752 | 1/1   | 0.20 | 7.44 | 40,40,40,40                 | 0     |
| 86  | MG   | 1     | 3475 | 1/1   | 0.25 | 7.43 | 24,24,24,24                 | 0     |
| 86  | MG   | 1     | 3587 | 1/1   | 0.54 | 7.42 | 38,38,38,38                 | 0     |
| 86  | MG   | 6     | 1984 | 1/1   | 0.51 | 7.41 | 42,42,42,42                 | 0     |
| 86  | MG   | 5     | 3542 | 1/1   | 0.31 | 7.37 | 22,22,22,22                 | 0     |
| 87  | OHX  | 5     | 4140 | 7/7   | 0.41 | 7.33 | 101,101,101,101             | 0     |
| 87  | OHX  | 1     | 4061 | 7/7   | 0.26 | 7.33 | 77,77,77,77                 | 0     |
| 86  | MG   | 2     | 1984 | 1/1   | 0.31 | 7.32 | 44,44,44,44                 | 0     |
| 87  | OHX  | 4     | 225  | 7/7   | 0.24 | 7.30 | 84,84,84,84                 | 0     |
| 86  | MG   | 1     | 3499 | 1/1   | 0.28 | 7.28 | 22,22,22,22                 | 0     |
| 86  | MG   | 5     | 3442 | 1/1   | 0.30 | 7.27 | 30,30,30,30                 | 0     |
| 86  | MG   | 5     | 3446 | 1/1   | 0.20 | 7.24 | 31,31,31,31                 | 0     |
| 86  | MG   | 5     | 3704 | 1/1   | 0.33 | 7.24 | 55,55,55,55                 | 0     |
| 86  | MG   | 3     | 201  | 1/1   | 0.26 | 7.22 | 62,62,62,62                 | 0     |
| 86  | MG   | 5     | 3790 | 1/1   | 0.33 | 7.21 | 42,42,42,42                 | 0     |
| 86  | MG   | 2     | 1974 | 1/1   | 0.30 | 7.19 | 58,58,58,58                 | 0     |
| 87  | OHX  | 1     | 4086 | 7/7   | 0.24 | 7.17 | 123,123,123,123             | 0     |
| 86  | MG   | 5     | 3444 | 1/1   | 0.24 | 7.08 | 23,23,23,23                 | 0     |
| 86  | MG   | 5     | 3618 | 1/1   | 0.18 | 7.08 | 35,35,35,35                 | 0     |
| 86  | MG   | 5     | 3416 | 1/1   | 0.30 | 7.04 | 24,24,24,24                 | 0     |
| 86  | MG   | 2     | 1977 | 1/1   | 0.28 | 7.03 | 77,77,77,77                 | 0     |
| 86  | MG   | 5     | 3899 | 1/1   | 0.26 | 7.02 | 22,22,22,22                 | 0     |
| 86  | MG   | 5     | 3859 | 1/1   | 0.20 | 7.00 | 45,45,45,45                 | 0     |
| 87  | OHX  | 5     | 4225 | 7/7   | 0.33 | 6.99 | 99,99,99,99                 | 0     |
| 86  | MG   | 5     | 3710 | 1/1   | 0.28 | 6.98 | 35,35,35,35                 | 0     |
| 86  | MG   | 6     | 2043 | 1/1   | 0.47 | 6.93 | 80,80,80,80                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87  | OHX  | 2     | 2132 | 7/7   | 0.30 | 6.92 | 122,122,122,122             | 0     |
| 87  | OHX  | 6     | 2199 | 7/7   | 0.23 | 6.92 | 157,157,157,157             | 0     |
| 87  | OHX  | 5     | 4246 | 7/7   | 0.40 | 6.92 | 117,117,117,117             | 0     |
| 87  | OHX  | 5     | 4166 | 7/7   | 0.30 | 6.91 | 160,160,160,160             | 0     |
| 86  | MG   | 6     | 1931 | 1/1   | 0.30 | 6.90 | 47,47,47,47                 | 0     |
| 87  | OHX  | 2     | 2177 | 7/7   | 0.43 | 6.90 | 132,132,132,132             | 0     |
| 86  | MG   | 2     | 1948 | 1/1   | 0.48 | 6.87 | 83,83,83,83                 | 0     |
| 87  | OHX  | 6     | 2203 | 7/7   | 0.33 | 6.87 | 140,140,140,140             | 0     |
| 86  | MG   | 5     | 3805 | 1/1   | 0.23 | 6.87 | 36,36,36,36                 | 0     |
| 87  | OHX  | 1     | 4099 | 7/7   | 0.34 | 6.86 | 107,107,107,107             | 0     |
| 87  | OHX  | 5     | 4203 | 7/7   | 0.31 | 6.84 | 97,97,97,97                 | 0     |
| 86  | MG   | 5     | 3871 | 1/1   | 0.32 | 6.83 | 38,38,38,38                 | 0     |
| 86  | MG   | 1     | 3519 | 1/1   | 0.33 | 6.83 | 23,23,23,23                 | 0     |
| 87  | OHX  | 5     | 4102 | 7/7   | 0.33 | 6.76 | 108,108,108,108             | 0     |
| 86  | MG   | m5    | 302  | 1/1   | 0.29 | 6.75 | 45,45,45,45                 | 0     |
| 86  | MG   | 5     | 4255 | 1/1   | 0.29 | 6.75 | 29,29,29,29                 | 0     |
| 86  | MG   | 6     | 2012 | 1/1   | 0.30 | 6.74 | 44,44,44,44                 | 0     |
| 86  | MG   | 5     | 3729 | 1/1   | 0.35 | 6.72 | 19,19,19,19                 | 0     |
| 87  | OHX  | 2     | 2171 | 7/7   | 0.40 | 6.72 | 127,127,127,127             | 0     |
| 87  | OHX  | 5     | 4151 | 7/7   | 0.38 | 6.71 | 123,123,123,123             | 0     |
| 86  | MG   | 5     | 3809 | 1/1   | 0.27 | 6.71 | 33,33,33,33                 | 0     |
| 86  | MG   | 2     | 1947 | 1/1   | 0.69 | 6.69 | 54,54,54,54                 | 0     |
| 86  | MG   | 1     | 3472 | 1/1   | 0.28 | 6.67 | 23,23,23,23                 | 0     |
| 87  | OHX  | 5     | 4224 | 7/7   | 0.40 | 6.66 | 124,124,124,124             | 0     |
| 86  | MG   | 6     | 1913 | 1/1   | 0.66 | 6.66 | 46,46,46,46                 | 0     |
| 86  | MG   | 2     | 1920 | 1/1   | 0.38 | 6.65 | 50,50,50,50                 | 0     |
| 86  | MG   | 5     | 3674 | 1/1   | 0.33 | 6.65 | 20,20,20,20                 | 0     |
| 87  | OHX  | 5     | 4213 | 7/7   | 0.30 | 6.65 | 114,114,114,114             | 0     |
| 86  | MG   | 6     | 2025 | 1/1   | 0.61 | 6.63 | 57,57,57,57                 | 0     |
| 86  | MG   | 5     | 3854 | 1/1   | 0.23 | 6.63 | 69,69,69,69                 | 0     |
| 87  | OHX  | 6     | 2160 | 7/7   | 0.32 | 6.63 | 115,115,115,115             | 0     |
| 86  | MG   | 1     | 3566 | 1/1   | 0.29 | 6.62 | 24,24,24,24                 | 0     |
| 86  | MG   | 1     | 3762 | 1/1   | 0.24 | 6.62 | 23,23,23,23                 | 0     |
| 87  | OHX  | 6     | 2172 | 7/7   | 0.27 | 6.62 | 138,138,138,138             | 0     |
| 86  | MG   | 1     | 3791 | 1/1   | 0.32 | 6.61 | 17,17,17,17                 | 0     |
| 86  | MG   | 1     | 3476 | 1/1   | 0.27 | 6.56 | 34,34,34,34                 | 0     |
| 87  | OHX  | 5     | 4027 | 7/7   | 0.26 | 6.53 | 84,84,84,84                 | 0     |
| 86  | MG   | 2     | 1964 | 1/1   | 0.43 | 6.52 | 86,86,86,86                 | 0     |
| 86  | MG   | 5     | 3511 | 1/1   | 0.40 | 6.52 | 17,17,17,17                 | 0     |
| 86  | MG   | 5     | 3443 | 1/1   | 0.26 | 6.51 | 17,17,17,17                 | 0     |
| 86  | MG   | 5     | 3879 | 1/1   | 0.26 | 6.50 | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 5     | 3664 | 1/1   | 0.19 | 6.50 | 39,39,39,39                 | 0     |
| 86  | MG   | 1     | 3631 | 1/1   | 0.24 | 6.49 | 28,28,28,28                 | 0     |
| 86  | MG   | 1     | 3676 | 1/1   | 0.22 | 6.47 | 18,18,18,18                 | 0     |
| 86  | MG   | 6     | 1953 | 1/1   | 0.42 | 6.47 | 50,50,50,50                 | 0     |
| 86  | MG   | 1     | 3808 | 1/1   | 0.32 | 6.46 | 24,24,24,24                 | 0     |
| 87  | OHX  | 5     | 4094 | 7/7   | 0.23 | 6.45 | 87,87,87,87                 | 0     |
| 86  | MG   | 1     | 3726 | 1/1   | 0.28 | 6.45 | 32,32,32,32                 | 0     |
| 87  | OHX  | 2     | 2101 | 7/7   | 0.25 | 6.44 | 125,125,125,125             | 0     |
| 86  | MG   | 1     | 3818 | 1/1   | 0.18 | 6.43 | 55,55,55,55                 | 0     |
| 87  | OHX  | 5     | 4125 | 7/7   | 0.27 | 6.42 | 132,132,132,132             | 0     |
| 86  | MG   | 1     | 3713 | 1/1   | 0.23 | 6.42 | 49,49,49,49                 | 0     |
| 86  | MG   | 1     | 3403 | 1/1   | 0.32 | 6.42 | 26,26,26,26                 | 0     |
| 86  | MG   | 1     | 3437 | 1/1   | 0.29 | 6.42 | 23,23,23,23                 | 0     |
| 86  | MG   | 5     | 3535 | 1/1   | 0.48 | 6.39 | 30,30,30,30                 | 0     |
| 86  | MG   | 8     | 212  | 1/1   | 0.26 | 6.39 | 48,48,48,48                 | 0     |
| 86  | MG   | 1     | 3795 | 1/1   | 0.28 | 6.38 | 19,19,19,19                 | 0     |
| 87  | OHX  | 5     | 4142 | 7/7   | 0.26 | 6.37 | 106,106,106,106             | 0     |
| 86  | MG   | 1     | 3809 | 1/1   | 0.28 | 6.37 | 25,25,25,25                 | 0     |
| 86  | MG   | 1     | 3700 | 1/1   | 0.46 | 6.37 | 61,61,61,61                 | 0     |
| 86  | MG   | 1     | 3604 | 1/1   | 0.23 | 6.37 | 24,24,24,24                 | 0     |
| 87  | OHX  | 5     | 4159 | 7/7   | 0.27 | 6.37 | 118,118,118,118             | 0     |
| 86  | MG   | 6     | 1908 | 1/1   | 0.20 | 6.36 | 37,37,37,37                 | 0     |
| 86  | MG   | 1     | 3781 | 1/1   | 0.40 | 6.36 | 55,55,55,55                 | 0     |
| 87  | OHX  | 7     | 225  | 7/7   | 0.24 | 6.30 | 140,140,140,140             | 0     |
| 87  | OHX  | 2     | 2172 | 7/7   | 0.39 | 6.28 | 138,138,138,138             | 0     |
| 86  | MG   | 6     | 1933 | 1/1   | 0.32 | 6.28 | 32,32,32,32                 | 0     |
| 87  | OHX  | 1     | 4148 | 7/7   | 0.24 | 6.26 | 83,83,83,83                 | 0     |
| 86  | MG   | 6     | 1999 | 1/1   | 0.27 | 6.26 | 50,50,50,50                 | 0     |
| 86  | MG   | 5     | 3437 | 1/1   | 0.33 | 6.25 | 43,43,43,43                 | 0     |
| 87  | OHX  | 6     | 2118 | 7/7   | 0.27 | 6.25 | 104,104,104,104             | 0     |
| 86  | MG   | 2     | 2011 | 1/1   | 0.27 | 6.23 | 62,62,62,62                 | 0     |
| 87  | OHX  | 1     | 4145 | 7/7   | 0.26 | 6.20 | 105,105,105,105             | 0     |
| 87  | OHX  | 5     | 4121 | 7/7   | 0.32 | 6.19 | 100,100,100,100             | 0     |
| 86  | MG   | 5     | 3462 | 1/1   | 0.34 | 6.17 | 23,23,23,23                 | 0     |
| 86  | MG   | 1     | 3438 | 1/1   | 0.35 | 6.16 | 39,39,39,39                 | 0     |
| 87  | OHX  | 1     | 4011 | 7/7   | 0.25 | 6.15 | 98,98,98,98                 | 0     |
| 86  | MG   | 5     | 3691 | 1/1   | 0.24 | 6.15 | 37,37,37,37                 | 0     |
| 86  | MG   | 5     | 4261 | 1/1   | 0.28 | 6.14 | 27,27,27,27                 | 0     |
| 86  | MG   | 1     | 3454 | 1/1   | 0.34 | 6.11 | 27,27,27,27                 | 0     |
| 86  | MG   | 5     | 3614 | 1/1   | 0.21 | 6.11 | 19,19,19,19                 | 0     |
| 86  | MG   | 2     | 1980 | 1/1   | 0.32 | 6.10 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87  | OHX  | 3     | 224  | 7/7   | 0.22 | 6.08 | 154,154,154,154             | 0     |
| 87  | OHX  | 2     | 2158 | 7/7   | 0.46 | 6.08 | 113,113,113,113             | 0     |
| 87  | OHX  | 1     | 4021 | 7/7   | 0.27 | 6.07 | 91,91,91,91                 | 0     |
| 86  | MG   | 1     | 3654 | 1/1   | 0.27 | 6.05 | 61,61,61,61                 | 0     |
| 87  | OHX  | 5     | 4045 | 7/7   | 0.23 | 6.04 | 76,76,76,76                 | 0     |
| 86  | MG   | 5     | 3866 | 1/1   | 0.31 | 6.03 | 20,20,20,20                 | 0     |
| 86  | MG   | 1     | 3701 | 1/1   | 0.27 | 6.03 | 33,33,33,33                 | 0     |
| 86  | MG   | 5     | 3740 | 1/1   | 0.29 | 6.02 | 25,25,25,25                 | 0     |
| 86  | MG   | 5     | 3716 | 1/1   | 0.39 | 6.01 | 44,44,44,44                 | 0     |
| 86  | MG   | 5     | 3835 | 1/1   | 0.26 | 6.01 | 27,27,27,27                 | 0     |
| 87  | OHX  | 5     | 4118 | 7/7   | 0.33 | 6.00 | 82,82,82,82                 | 0     |
| 87  | OHX  | 1     | 4125 | 7/7   | 0.27 | 6.00 | 109,109,109,109             | 0     |
| 87  | OHX  | 5     | 4175 | 7/7   | 0.30 | 5.99 | 73,73,73,73                 | 0     |
| 87  | OHX  | 1     | 4207 | 7/7   | 0.51 | 5.99 | 116,116,116,116             | 0     |
| 87  | OHX  | 6     | 2192 | 7/7   | 0.32 | 5.98 | 117,117,117,117             | 0     |
| 86  | MG   | 5     | 3727 | 1/1   | 0.23 | 5.97 | 33,33,33,33                 | 0     |
| 86  | MG   | 2     | 1992 | 1/1   | 0.40 | 5.94 | 77,77,77,77                 | 0     |
| 87  | OHX  | 5     | 4134 | 7/7   | 0.29 | 5.90 | 96,96,96,96                 | 0     |
| 87  | OHX  | 1     | 4059 | 7/7   | 0.27 | 5.90 | 85,85,85,85                 | 0     |
| 86  | MG   | 1     | 3581 | 1/1   | 0.26 | 5.89 | 27,27,27,27                 | 0     |
| 86  | MG   | 1     | 3569 | 1/1   | 0.35 | 5.86 | 22,22,22,22                 | 0     |
| 86  | MG   | 5     | 3717 | 1/1   | 0.35 | 5.86 | 55,55,55,55                 | 0     |
| 86  | MG   | 6     | 1907 | 1/1   | 0.31 | 5.85 | 59,59,59,59                 | 0     |
| 86  | MG   | 5     | 3605 | 1/1   | 0.28 | 5.84 | 21,21,21,21                 | 0     |
| 86  | MG   | 5     | 3485 | 1/1   | 0.27 | 5.84 | 38,38,38,38                 | 0     |
| 86  | MG   | 5     | 3694 | 1/1   | 0.25 | 5.84 | 41,41,41,41                 | 0     |
| 87  | OHX  | 1     | 4092 | 7/7   | 0.28 | 5.82 | 99,99,99,99                 | 0     |
| 86  | MG   | 6     | 2008 | 1/1   | 0.30 | 5.80 | 43,43,43,43                 | 0     |
| 87  | OHX  | 2     | 2089 | 7/7   | 0.26 | 5.80 | 121,121,121,121             | 0     |
| 86  | MG   | 1     | 3707 | 1/1   | 0.20 | 5.79 | 48,48,48,48                 | 0     |
| 87  | OHX  | 1     | 4137 | 7/7   | 0.29 | 5.79 | 91,91,91,91                 | 0     |
| 87  | OHX  | 6     | 2143 | 7/7   | 0.25 | 5.78 | 119,119,119,119             | 0     |
| 87  | OHX  | 2     | 2150 | 7/7   | 0.36 | 5.75 | 129,129,129,129             | 0     |
| 86  | MG   | 2     | 2014 | 1/1   | 0.46 | 5.74 | 66,66,66,66                 | 0     |
| 86  | MG   | 6     | 2039 | 1/1   | 0.62 | 5.74 | 68,68,68,68                 | 0     |
| 87  | OHX  | 5     | 4210 | 7/7   | 0.37 | 5.73 | 88,88,88,88                 | 0     |
| 87  | OHX  | 2     | 2173 | 7/7   | 0.35 | 5.73 | 152,152,152,152             | 0     |
| 86  | MG   | m5    | 301  | 1/1   | 0.26 | 5.73 | 32,32,32,32                 | 0     |
| 87  | OHX  | 5     | 4235 | 7/7   | 0.21 | 5.70 | 85,85,85,85                 | 0     |
| 87  | OHX  | 5     | 4185 | 7/7   | 0.31 | 5.68 | 109,109,109,109             | 0     |
| 86  | MG   | 1     | 3523 | 1/1   | 0.28 | 5.67 | 75,75,75,75                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 6     | 1942 | 1/1   | 0.29 | 5.66 | 41,41,41,41                 | 0     |
| 87  | OHX  | 5     | 4048 | 7/7   | 0.26 | 5.62 | 108,108,108,108             | 0     |
| 86  | MG   | 5     | 3828 | 1/1   | 0.31 | 5.62 | 24,24,24,24                 | 0     |
| 87  | OHX  | 1     | 4077 | 7/7   | 0.29 | 5.61 | 77,77,77,77                 | 0     |
| 86  | MG   | 5     | 3403 | 1/1   | 0.35 | 5.60 | 51,51,51,51                 | 0     |
| 87  | OHX  | 1     | 4068 | 7/7   | 0.28 | 5.60 | 105,105,105,105             | 0     |
| 86  | MG   | 2     | 1949 | 1/1   | 0.25 | 5.58 | 50,50,50,50                 | 0     |
| 87  | OHX  | 1     | 4044 | 7/7   | 0.24 | 5.57 | 90,90,90,90                 | 0     |
| 86  | MG   | 1     | 3708 | 1/1   | 0.23 | 5.56 | 28,28,28,28                 | 0     |
| 87  | OHX  | 6     | 2152 | 7/7   | 0.26 | 5.56 | 88,88,88,88                 | 0     |
| 87  | OHX  | 1     | 4134 | 7/7   | 0.38 | 5.55 | 140,140,140,140             | 0     |
| 87  | OHX  | 1     | 4169 | 7/7   | 0.28 | 5.54 | 98,98,98,98                 | 0     |
| 87  | OHX  | 1     | 4123 | 7/7   | 0.35 | 5.51 | 102,102,102,102             | 0     |
| 87  | OHX  | 6     | 2136 | 7/7   | 0.33 | 5.47 | 148,148,148,148             | 0     |
| 86  | MG   | 1     | 3578 | 1/1   | 0.22 | 5.44 | 20,20,20,20                 | 0     |
| 87  | OHX  | 6     | 2183 | 7/7   | 0.35 | 5.44 | 117,117,117,117             | 0     |
| 87  | OHX  | 5     | 4242 | 7/7   | 0.27 | 5.43 | 178,178,178,178             | 0     |
| 86  | MG   | 5     | 3580 | 1/1   | 0.24 | 5.42 | 25,25,25,25                 | 0     |
| 87  | OHX  | 5     | 4190 | 7/7   | 0.31 | 5.41 | 146,146,146,146             | 0     |
| 86  | MG   | 5     | 3712 | 1/1   | 0.24 | 5.40 | 31,31,31,31                 | 0     |
| 87  | OHX  | 5     | 4193 | 7/7   | 0.22 | 5.37 | 100,100,100,100             | 0     |
| 87  | OHX  | 5     | 3985 | 7/7   | 0.27 | 5.34 | 76,76,76,76                 | 0     |
| 86  | MG   | 6     | 1919 | 1/1   | 0.40 | 5.34 | 61,61,61,61                 | 0     |
| 86  | MG   | 1     | 3848 | 1/1   | 0.33 | 5.33 | 28,28,28,28                 | 0     |
| 86  | MG   | 1     | 3469 | 1/1   | 0.26 | 5.30 | 33,33,33,33                 | 0     |
| 87  | OHX  | 1     | 4115 | 7/7   | 0.34 | 5.29 | 84,84,84,84                 | 0     |
| 86  | MG   | 5     | 3870 | 1/1   | 0.28 | 5.28 | 19,19,19,19                 | 0     |
| 86  | MG   | 1     | 3855 | 1/1   | 0.21 | 5.28 | 30,30,30,30                 | 0     |
| 87  | OHX  | 1     | 4179 | 7/7   | 0.32 | 5.28 | 121,121,121,121             | 0     |
| 86  | MG   | 7     | 214  | 1/1   | 0.26 | 5.27 | 31,31,31,31                 | 0     |
| 86  | MG   | 5     | 3603 | 1/1   | 0.24 | 5.27 | 31,31,31,31                 | 0     |
| 86  | MG   | 1     | 3545 | 1/1   | 0.28 | 5.27 | 29,29,29,29                 | 0     |
| 86  | MG   | 1     | 3658 | 1/1   | 0.24 | 5.26 | 26,26,26,26                 | 0     |
| 86  | MG   | 1     | 3629 | 1/1   | 0.32 | 5.25 | 66,66,66,66                 | 0     |
| 86  | MG   | 1     | 3799 | 1/1   | 0.23 | 5.25 | 42,42,42,42                 | 0     |
| 86  | MG   | 6     | 2011 | 1/1   | 0.23 | 5.25 | 37,37,37,37                 | 0     |
| 86  | MG   | 5     | 3654 | 1/1   | 0.26 | 5.24 | 23,23,23,23                 | 0     |
| 87  | OHX  | 6     | 2159 | 7/7   | 0.46 | 5.22 | 154,154,154,154             | 0     |
| 86  | MG   | 6     | 1958 | 1/1   | 0.70 | 5.17 | 42,42,42,42                 | 0     |
| 87  | OHX  | 5     | 4149 | 7/7   | 0.29 | 5.17 | 107,107,107,107             | 0     |
| 86  | MG   | 5     | 3483 | 1/1   | 0.40 | 5.16 | 23,23,23,23                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87  | OHX  | 1     | 4202 | 7/7   | 0.39 | 5.15 | 99,99,99,99                 | 0     |
| 86  | MG   | 5     | 3834 | 1/1   | 0.18 | 5.14 | 31,31,31,31                 | 0     |
| 87  | OHX  | 2     | 2082 | 7/7   | 0.28 | 5.12 | 105,105,105,105             | 0     |
| 87  | OHX  | 5     | 4060 | 7/7   | 0.23 | 5.09 | 100,100,100,100             | 0     |
| 87  | OHX  | 1     | 3991 | 7/7   | 0.25 | 5.09 | 80,80,80,80                 | 0     |
| 86  | MG   | 1     | 3765 | 1/1   | 0.23 | 5.08 | 36,36,36,36                 | 0     |
| 87  | OHX  | 1     | 3979 | 7/7   | 0.22 | 5.07 | 88,88,88,88                 | 0     |
| 86  | MG   | 1     | 3666 | 1/1   | 0.28 | 5.07 | 43,43,43,43                 | 0     |
| 87  | OHX  | 5     | 4086 | 7/7   | 0.20 | 5.07 | 95,95,95,95                 | 0     |
| 86  | MG   | 1     | 3725 | 1/1   | 0.35 | 5.06 | 44,44,44,44                 | 0     |
| 87  | OHX  | 5     | 4046 | 7/7   | 0.22 | 5.05 | 101,101,101,101             | 0     |
| 87  | OHX  | 5     | 4135 | 7/7   | 0.21 | 5.03 | 109,109,109,109             | 0     |
| 87  | OHX  | 1     | 4133 | 7/7   | 0.18 | 5.02 | 102,102,102,102             | 0     |
| 86  | MG   | 1     | 3755 | 1/1   | 0.24 | 5.01 | 17,17,17,17                 | 0     |
| 87  | OHX  | 6     | 2174 | 7/7   | 0.37 | 5.01 | 91,91,91,91                 | 0     |
| 86  | MG   | 1     | 3463 | 1/1   | 0.14 | 5.00 | 29,29,29,29                 | 0     |
| 86  | MG   | 5     | 3829 | 1/1   | 0.22 | 4.97 | 19,19,19,19                 | 0     |
| 87  | OHX  | 1     | 4126 | 7/7   | 0.26 | 4.96 | 126,126,126,126             | 0     |
| 87  | OHX  | 1     | 4155 | 7/7   | 0.22 | 4.95 | 89,89,89,89                 | 0     |
| 86  | MG   | 1     | 3819 | 1/1   | 0.37 | 4.94 | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 3517 | 1/1   | 0.23 | 4.93 | 30,30,30,30                 | 0     |
| 86  | MG   | 5     | 3868 | 1/1   | 0.28 | 4.93 | 18,18,18,18                 | 0     |
| 86  | MG   | 5     | 3747 | 1/1   | 0.22 | 4.93 | 53,53,53,53                 | 0     |
| 86  | MG   | 1     | 3750 | 1/1   | 0.21 | 4.90 | 34,34,34,34                 | 0     |
| 86  | MG   | 1     | 3534 | 1/1   | 0.30 | 4.89 | 23,23,23,23                 | 0     |
| 87  | OHX  | 1     | 4120 | 7/7   | 0.26 | 4.87 | 104,104,104,104             | 0     |
| 86  | MG   | 1     | 3823 | 1/1   | 0.30 | 4.87 | 47,47,47,47                 | 0     |
| 87  | OHX  | 2     | 2124 | 7/7   | 0.20 | 4.87 | 125,125,125,125             | 0     |
| 87  | OHX  | 2     | 2117 | 7/7   | 0.27 | 4.86 | 124,124,124,124             | 0     |
| 86  | MG   | 7     | 211  | 1/1   | 0.28 | 4.86 | 35,35,35,35                 | 0     |
| 86  | MG   | 5     | 3479 | 1/1   | 0.39 | 4.85 | 54,54,54,54                 | 0     |
| 87  | OHX  | 1     | 4209 | 7/7   | 0.30 | 4.83 | 107,107,107,107             | 0     |
| 87  | OHX  | 5     | 4113 | 7/7   | 0.25 | 4.83 | 106,106,106,106             | 0     |
| 86  | MG   | 5     | 3777 | 1/1   | 0.19 | 4.81 | 70,70,70,70                 | 0     |
| 87  | OHX  | 5     | 4165 | 7/7   | 0.26 | 4.81 | 117,117,117,117             | 0     |
| 86  | MG   | 2     | 1990 | 1/1   | 0.23 | 4.80 | 50,50,50,50                 | 0     |
| 86  | MG   | 1     | 3452 | 1/1   | 0.21 | 4.80 | 25,25,25,25                 | 0     |
| 87  | OHX  | 2     | 2103 | 7/7   | 0.30 | 4.79 | 98,98,98,98                 | 0     |
| 86  | MG   | 5     | 3773 | 1/1   | 0.20 | 4.78 | 22,22,22,22                 | 0     |
| 87  | OHX  | 1     | 4142 | 7/7   | 0.26 | 4.78 | 99,99,99,99                 | 0     |
| 87  | OHX  | 2     | 2114 | 7/7   | 0.35 | 4.78 | 127,127,127,127             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 5     | 3540 | 1/1   | 0.44 | 4.76 | 20,20,20,20                 | 0     |
| 86  | MG   | 6     | 2007 | 1/1   | 0.28 | 4.75 | 63,63,63,63                 | 0     |
| 86  | MG   | 6     | 2019 | 1/1   | 0.27 | 4.74 | 33,33,33,33                 | 0     |
| 87  | OHX  | 5     | 4198 | 7/7   | 0.28 | 4.74 | 141,141,141,141             | 0     |
| 86  | MG   | 2     | 1955 | 1/1   | 0.34 | 4.72 | 59,59,59,59                 | 0     |
| 86  | MG   | 2     | 1959 | 1/1   | 0.53 | 4.68 | 87,87,87,87                 | 0     |
| 86  | MG   | 1     | 3681 | 1/1   | 0.18 | 4.68 | 28,28,28,28                 | 0     |
| 86  | MG   | 5     | 3785 | 1/1   | 0.20 | 4.68 | 24,24,24,24                 | 0     |
| 86  | MG   | 6     | 1995 | 1/1   | 0.27 | 4.66 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 3784 | 1/1   | 0.23 | 4.66 | 20,20,20,20                 | 0     |
| 87  | OHX  | 3     | 226  | 7/7   | 0.24 | 4.66 | 117,117,117,117             | 0     |
| 87  | OHX  | 6     | 2127 | 7/7   | 0.26 | 4.66 | 86,86,86,86                 | 0     |
| 86  | MG   | 1     | 3757 | 1/1   | 0.25 | 4.65 | 38,38,38,38                 | 0     |
| 86  | MG   | 5     | 3808 | 1/1   | 0.24 | 4.65 | 86,86,86,86                 | 0     |
| 87  | OHX  | 1     | 4190 | 7/7   | 0.41 | 4.64 | 125,125,125,125             | 0     |
| 87  | OHX  | 1     | 4139 | 7/7   | 0.37 | 4.63 | 90,90,90,90                 | 0     |
| 86  | MG   | 1     | 3484 | 1/1   | 0.26 | 4.61 | 28,28,28,28                 | 0     |
| 86  | MG   | 6     | 1902 | 1/1   | 0.28 | 4.60 | 44,44,44,44                 | 0     |
| 86  | MG   | 1     | 3471 | 1/1   | 0.24 | 4.60 | 29,29,29,29                 | 0     |
| 86  | MG   | 1     | 3647 | 1/1   | 0.25 | 4.60 | 56,56,56,56                 | 0     |
| 86  | MG   | 5     | 3856 | 1/1   | 0.25 | 4.58 | 34,34,34,34                 | 0     |
| 88  | ZN   | d7    | 101  | 1/1   | 0.67 | 4.57 | 181,181,181,181             | 0     |
| 87  | OHX  | 5     | 4157 | 7/7   | 0.40 | 4.57 | 117,117,117,117             | 0     |
| 86  | MG   | n0    | 201  | 1/1   | 0.29 | 4.56 | 31,31,31,31                 | 0     |
| 87  | OHX  | 5     | 4209 | 7/7   | 0.24 | 4.55 | 135,135,135,135             | 0     |
| 86  | MG   | 2     | 1933 | 1/1   | 0.32 | 4.54 | 71,71,71,71                 | 0     |
| 87  | OHX  | 6     | 2200 | 7/7   | 0.32 | 4.51 | 121,121,121,121             | 0     |
| 86  | MG   | 8     | 207  | 1/1   | 0.21 | 4.51 | 61,61,61,61                 | 0     |
| 86  | MG   | 2     | 1968 | 1/1   | 0.55 | 4.51 | 120,120,120,120             | 0     |
| 87  | OHX  | 3     | 223  | 7/7   | 0.27 | 4.51 | 92,92,92,92                 | 0     |
| 86  | MG   | o3    | 201  | 1/1   | 0.32 | 4.50 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 3863 | 1/1   | 0.40 | 4.50 | 58,58,58,58                 | 0     |
| 87  | OHX  | 5     | 4047 | 7/7   | 0.23 | 4.49 | 81,81,81,81                 | 0     |
| 86  | MG   | 5     | 3533 | 1/1   | 0.20 | 4.49 | 40,40,40,40                 | 0     |
| 86  | MG   | 5     | 3802 | 1/1   | 0.24 | 4.48 | 22,22,22,22                 | 0     |
| 87  | OHX  | 1     | 4084 | 7/7   | 0.28 | 4.48 | 99,99,99,99                 | 0     |
| 86  | MG   | 1     | 3551 | 1/1   | 0.31 | 4.46 | 32,32,32,32                 | 0     |
| 87  | OHX  | 1     | 4101 | 7/7   | 0.27 | 4.46 | 127,127,127,127             | 0     |
| 86  | MG   | 5     | 3447 | 1/1   | 0.25 | 4.45 | 27,27,27,27                 | 0     |
| 86  | MG   | 5     | 3820 | 1/1   | 0.22 | 4.44 | 46,46,46,46                 | 0     |
| 87  | OHX  | 2     | 2129 | 7/7   | 0.28 | 4.44 | 110,110,110,110             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87  | OHX  | 5     | 4234 | 7/7   | 0.30 | 4.44 | 174,174,174,174             | 0     |
| 87  | OHX  | O3    | 201  | 7/7   | 0.26 | 4.42 | 89,89,89,89                 | 0     |
| 87  | OHX  | 2     | 2143 | 7/7   | 0.33 | 4.42 | 126,126,126,126             | 0     |
| 87  | OHX  | 5     | 4108 | 7/7   | 0.26 | 4.42 | 88,88,88,88                 | 0     |
| 86  | MG   | 1     | 3801 | 1/1   | 0.24 | 4.41 | 41,41,41,41                 | 0     |
| 86  | MG   | L3    | 401  | 1/1   | 0.37 | 4.40 | 25,25,25,25                 | 0     |
| 87  | OHX  | 5     | 4228 | 7/7   | 0.28 | 4.39 | 110,110,110,110             | 0     |
| 86  | MG   | 6     | 1985 | 1/1   | 0.24 | 4.39 | 71,71,71,71                 | 0     |
| 86  | MG   | 5     | 3468 | 1/1   | 0.22 | 4.38 | 28,28,28,28                 | 0     |
| 86  | MG   | 6     | 1980 | 1/1   | 0.19 | 4.37 | 66,66,66,66                 | 0     |
| 86  | MG   | 1     | 3610 | 1/1   | 0.41 | 4.37 | 57,57,57,57                 | 0     |
| 87  | OHX  | 5     | 4104 | 7/7   | 0.26 | 4.36 | 79,79,79,79                 | 0     |
| 87  | OHX  | 6     | 2206 | 7/7   | 0.41 | 4.36 | 125,125,125,125             | 0     |
| 86  | MG   | 5     | 3830 | 1/1   | 0.21 | 4.35 | 35,35,35,35                 | 0     |
| 86  | MG   | m7    | 204  | 1/1   | 0.23 | 4.34 | 24,24,24,24                 | 0     |
| 86  | MG   | M3    | 203  | 1/1   | 0.31 | 4.34 | 22,22,22,22                 | 0     |
| 87  | OHX  | 2     | 2133 | 7/7   | 0.35 | 4.33 | 112,112,112,112             | 0     |
| 87  | OHX  | 2     | 2072 | 7/7   | 0.24 | 4.32 | 98,98,98,98                 | 0     |
| 86  | MG   | 6     | 1910 | 1/1   | 0.27 | 4.31 | 60,60,60,60                 | 0     |
| 86  | MG   | 6     | 2023 | 1/1   | 0.24 | 4.31 | 73,73,73,73                 | 0     |
| 87  | OHX  | 1     | 3997 | 7/7   | 0.22 | 4.31 | 85,85,85,85                 | 0     |
| 86  | MG   | 1     | 3694 | 1/1   | 0.19 | 4.29 | 28,28,28,28                 | 0     |
| 86  | MG   | M0    | 301  | 1/1   | 0.24 | 4.29 | 33,33,33,33                 | 0     |
| 86  | MG   | 6     | 1988 | 1/1   | 0.27 | 4.29 | 58,58,58,58                 | 0     |
| 87  | OHX  | 6     | 2111 | 7/7   | 0.26 | 4.28 | 93,93,93,93                 | 0     |
| 86  | MG   | 5     | 4259 | 1/1   | 0.36 | 4.28 | 20,20,20,20                 | 0     |
| 87  | OHX  | 8     | 230  | 7/7   | 0.30 | 4.28 | 118,118,118,118             | 0     |
| 86  | MG   | 5     | 3417 | 1/1   | 0.23 | 4.27 | 19,19,19,19                 | 0     |
| 87  | OHX  | 1     | 4188 | 7/7   | 0.26 | 4.24 | 129,129,129,129             | 0     |
| 86  | MG   | 6     | 1979 | 1/1   | 0.29 | 4.24 | 39,39,39,39                 | 0     |
| 87  | OHX  | 2     | 2152 | 7/7   | 0.26 | 4.22 | 137,137,137,137             | 0     |
| 86  | MG   | 2     | 1972 | 1/1   | 0.36 | 4.21 | 75,75,75,75                 | 0     |
| 86  | MG   | 5     | 3650 | 1/1   | 0.21 | 4.20 | 33,33,33,33                 | 0     |
| 86  | MG   | 1     | 3467 | 1/1   | 0.21 | 4.20 | 34,34,34,34                 | 0     |
| 87  | OHX  | 4     | 231  | 7/7   | 0.24 | 4.20 | 118,118,118,118             | 0     |
| 87  | OHX  | 1     | 4213 | 7/7   | 0.40 | 4.19 | 98,98,98,98                 | 0     |
| 86  | MG   | 5     | 3746 | 1/1   | 0.23 | 4.19 | 53,53,53,53                 | 0     |
| 87  | OHX  | 1     | 4079 | 7/7   | 0.20 | 4.18 | 99,99,99,99                 | 0     |
| 87  | OHX  | 6     | 2154 | 7/7   | 0.28 | 4.17 | 91,91,91,91                 | 0     |
| 87  | OHX  | D9    | 102  | 7/7   | 0.31 | 4.16 | 127,127,127,127             | 0     |
| 86  | MG   | 1     | 3679 | 1/1   | 0.23 | 4.15 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 5     | 3887 | 1/1   | 0.32 | 4.15 | 49,49,49,49                 | 0     |
| 87  | OHX  | 6     | 2151 | 7/7   | 0.27 | 4.12 | 108,108,108,108             | 0     |
| 87  | OHX  | 6     | 2124 | 7/7   | 0.28 | 4.11 | 89,89,89,89                 | 0     |
| 87  | OHX  | 1     | 4135 | 7/7   | 0.31 | 4.11 | 124,124,124,124             | 0     |
| 86  | MG   | 5     | 3566 | 1/1   | 0.44 | 4.09 | 37,37,37,37                 | 0     |
| 87  | OHX  | 5     | 4115 | 7/7   | 0.24 | 4.09 | 90,90,90,90                 | 0     |
| 87  | OHX  | 1     | 4019 | 7/7   | 0.24 | 4.09 | 102,102,102,102             | 0     |
| 86  | MG   | 5     | 3878 | 1/1   | 0.27 | 4.09 | 21,21,21,21                 | 0     |
| 86  | MG   | 2     | 1922 | 1/1   | 0.31 | 4.08 | 56,56,56,56                 | 0     |
| 87  | OHX  | 6     | 2120 | 7/7   | 0.28 | 4.05 | 115,115,115,115             | 0     |
| 87  | OHX  | 2     | 2060 | 7/7   | 0.23 | 4.04 | 112,112,112,112             | 0     |
| 86  | MG   | 1     | 3489 | 1/1   | 0.34 | 4.03 | 43,43,43,43                 | 0     |
| 86  | MG   | 1     | 3739 | 1/1   | 0.20 | 4.03 | 55,55,55,55                 | 0     |
| 86  | MG   | 5     | 3406 | 1/1   | 0.23 | 4.02 | 31,31,31,31                 | 0     |
| 87  | OHX  | 5     | 4245 | 7/7   | 0.22 | 4.01 | 145,145,145,145             | 0     |
| 87  | OHX  | 1     | 3996 | 7/7   | 0.21 | 4.00 | 91,91,91,91                 | 0     |
| 87  | OHX  | 5     | 4089 | 7/7   | 0.23 | 3.98 | 90,90,90,90                 | 0     |
| 86  | MG   | 4     | 203  | 1/1   | 0.48 | 3.98 | 67,67,67,67                 | 0     |
| 87  | OHX  | 1     | 4159 | 7/7   | 0.32 | 3.97 | 107,107,107,107             | 0     |
| 87  | OHX  | 5     | 4040 | 7/7   | 0.25 | 3.95 | 72,72,72,72                 | 0     |
| 86  | MG   | 5     | 3489 | 1/1   | 0.23 | 3.94 | 22,22,22,22                 | 0     |
| 86  | MG   | 1     | 3492 | 1/1   | 0.26 | 3.93 | 20,20,20,20                 | 0     |
| 87  | OHX  | 1     | 4042 | 7/7   | 0.24 | 3.93 | 91,91,91,91                 | 0     |
| 87  | OHX  | 2     | 2145 | 7/7   | 0.31 | 3.93 | 165,165,165,165             | 0     |
| 86  | MG   | 5     | 3867 | 1/1   | 0.27 | 3.93 | 16,16,16,16                 | 0     |
| 87  | OHX  | 5     | 4107 | 7/7   | 0.24 | 3.92 | 82,82,82,82                 | 0     |
| 86  | MG   | 1     | 3427 | 1/1   | 0.24 | 3.92 | 31,31,31,31                 | 0     |
| 86  | MG   | 5     | 3579 | 1/1   | 0.33 | 3.92 | 24,24,24,24                 | 0     |
| 87  | OHX  | 1     | 4073 | 7/7   | 0.23 | 3.90 | 106,106,106,106             | 0     |
| 87  | OHX  | 5     | 4173 | 7/7   | 0.23 | 3.89 | 159,159,159,159             | 0     |
| 86  | MG   | 5     | 3459 | 1/1   | 0.22 | 3.88 | 22,22,22,22                 | 0     |
| 87  | OHX  | 2     | 2126 | 7/7   | 0.23 | 3.87 | 137,137,137,137             | 0     |
| 86  | MG   | 1     | 3674 | 1/1   | 0.51 | 3.87 | 57,57,57,57                 | 0     |
| 86  | MG   | 2     | 1927 | 1/1   | 0.44 | 3.87 | 50,50,50,50                 | 0     |
| 87  | OHX  | 5     | 4034 | 7/7   | 0.20 | 3.86 | 84,84,84,84                 | 0     |
| 87  | OHX  | 1     | 4184 | 7/7   | 0.41 | 3.86 | 111,111,111,111             | 0     |
| 86  | MG   | 5     | 3644 | 1/1   | 0.18 | 3.84 | 31,31,31,31                 | 0     |
| 87  | OHX  | 5     | 4178 | 7/7   | 0.28 | 3.84 | 117,117,117,117             | 0     |
| 87  | OHX  | 5     | 4124 | 7/7   | 0.21 | 3.82 | 116,116,116,116             | 0     |
| 86  | MG   | 1     | 3702 | 1/1   | 0.26 | 3.82 | 29,29,29,29                 | 0     |
| 87  | OHX  | 5     | 4223 | 7/7   | 0.34 | 3.82 | 148,148,148,148             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87  | OHX  | 6     | 2173 | 7/7   | 0.32 | 3.82 | 134,134,134,134             | 0     |
| 87  | OHX  | 1     | 4103 | 7/7   | 0.37 | 3.81 | 89,89,89,89                 | 0     |
| 86  | MG   | 5     | 3636 | 1/1   | 0.21 | 3.81 | 39,39,39,39                 | 0     |
| 86  | MG   | 5     | 3647 | 1/1   | 0.27 | 3.79 | 37,37,37,37                 | 0     |
| 87  | OHX  | 5     | 4120 | 7/7   | 0.25 | 3.79 | 94,94,94,94                 | 0     |
| 86  | MG   | 1     | 3699 | 1/1   | 0.21 | 3.79 | 50,50,50,50                 | 0     |
| 87  | OHX  | 6     | 2198 | 7/7   | 0.25 | 3.76 | 147,147,147,147             | 0     |
| 87  | OHX  | 6     | 2141 | 7/7   | 0.22 | 3.76 | 99,99,99,99                 | 0     |
| 86  | MG   | 5     | 3657 | 1/1   | 0.20 | 3.74 | 50,50,50,50                 | 0     |
| 86  | MG   | 5     | 3627 | 1/1   | 0.32 | 3.74 | 51,51,51,51                 | 0     |
| 86  | MG   | 5     | 3505 | 1/1   | 0.26 | 3.73 | 41,41,41,41                 | 0     |
| 86  | MG   | 1     | 3470 | 1/1   | 0.18 | 3.73 | 33,33,33,33                 | 0     |
| 86  | MG   | 1     | 3657 | 1/1   | 0.28 | 3.71 | 37,37,37,37                 | 0     |
| 87  | OHX  | 4     | 232  | 7/7   | 0.26 | 3.70 | 110,110,110,110             | 0     |
| 86  | MG   | 2     | 1930 | 1/1   | 0.27 | 3.66 | 58,58,58,58                 | 0     |
| 87  | OHX  | 6     | 2202 | 7/7   | 0.29 | 3.65 | 118,118,118,118             | 0     |
| 86  | MG   | 6     | 2010 | 1/1   | 0.21 | 3.62 | 40,40,40,40                 | 0     |
| 86  | MG   | 2     | 1939 | 1/1   | 0.30 | 3.61 | 60,60,60,60                 | 0     |
| 87  | OHX  | 1     | 4165 | 7/7   | 0.27 | 3.61 | 139,139,139,139             | 0     |
| 86  | MG   | 5     | 3670 | 1/1   | 0.25 | 3.60 | 28,28,28,28                 | 0     |
| 87  | OHX  | 5     | 4087 | 7/7   | 0.19 | 3.60 | 96,96,96,96                 | 0     |
| 87  | OHX  | 1     | 4186 | 7/7   | 0.27 | 3.59 | 82,82,82,82                 | 0     |
| 86  | MG   | 1     | 3655 | 1/1   | 0.21 | 3.59 | 35,35,35,35                 | 0     |
| 87  | OHX  | 6     | 2156 | 7/7   | 0.20 | 3.59 | 125,125,125,125             | 0     |
| 86  | MG   | 5     | 3749 | 1/1   | 0.24 | 3.58 | 40,40,40,40                 | 0     |
| 87  | OHX  | s9    | 201  | 7/7   | 0.44 | 3.58 | 104,104,104,104             | 0     |
| 87  | OHX  | 3     | 222  | 7/7   | 0.19 | 3.56 | 124,124,124,124             | 0     |
| 87  | OHX  | 1     | 4071 | 7/7   | 0.29 | 3.56 | 82,82,82,82                 | 0     |
| 86  | MG   | 5     | 3425 | 1/1   | 0.24 | 3.53 | 34,34,34,34                 | 0     |
| 86  | MG   | 5     | 3789 | 1/1   | 0.26 | 3.51 | 17,17,17,17                 | 0     |
| 86  | MG   | 1     | 3411 | 1/1   | 0.25 | 3.50 | 19,19,19,19                 | 0     |
| 86  | MG   | 5     | 3718 | 1/1   | 0.26 | 3.50 | 39,39,39,39                 | 0     |
| 87  | OHX  | 1     | 4020 | 7/7   | 0.22 | 3.49 | 104,104,104,104             | 0     |
| 86  | MG   | 1     | 3451 | 1/1   | 0.29 | 3.47 | 34,34,34,34                 | 0     |
| 87  | OHX  | 2     | 2118 | 7/7   | 0.24 | 3.46 | 115,115,115,115             | 0     |
| 86  | MG   | 1     | 3614 | 1/1   | 0.15 | 3.44 | 50,50,50,50                 | 0     |
| 87  | OHX  | 6     | 2169 | 7/7   | 0.21 | 3.44 | 125,125,125,125             | 0     |
| 87  | OHX  | L3    | 403  | 7/7   | 0.27 | 3.42 | 101,101,101,101             | 0     |
| 87  | OHX  | 5     | 3997 | 7/7   | 0.24 | 3.41 | 81,81,81,81                 | 0     |
| 87  | OHX  | 1     | 4047 | 7/7   | 0.23 | 3.40 | 81,81,81,81                 | 0     |
| 86  | MG   | 4     | 214  | 1/1   | 0.16 | 3.40 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 6     | 2003 | 1/1   | 0.23 | 3.39 | 49,49,49,49                 | 0     |
| 87  | OHX  | 1     | 4080 | 7/7   | 0.25 | 3.38 | 99,99,99,99                 | 0     |
| 86  | MG   | 5     | 3768 | 1/1   | 0.24 | 3.37 | 32,32,32,32                 | 0     |
| 87  | OHX  | 5     | 4148 | 7/7   | 0.29 | 3.36 | 89,89,89,89                 | 0     |
| 87  | OHX  | 4     | 226  | 7/7   | 0.17 | 3.35 | 101,101,101,101             | 0     |
| 87  | OHX  | 5     | 3994 | 7/7   | 0.21 | 3.33 | 74,74,74,74                 | 0     |
| 87  | OHX  | 6     | 2197 | 7/7   | 0.29 | 3.33 | 167,167,167,167             | 0     |
| 87  | OHX  | 1     | 4038 | 7/7   | 0.22 | 3.32 | 87,87,87,87                 | 0     |
| 87  | OHX  | 1     | 4013 | 7/7   | 0.20 | 3.32 | 90,90,90,90                 | 0     |
| 87  | OHX  | 5     | 4062 | 7/7   | 0.25 | 3.31 | 85,85,85,85                 | 0     |
| 86  | MG   | 5     | 3794 | 1/1   | 0.26 | 3.31 | 32,32,32,32                 | 0     |
| 87  | OHX  | 6     | 2178 | 7/7   | 0.34 | 3.31 | 135,135,135,135             | 0     |
| 87  | OHX  | 1     | 4026 | 7/7   | 0.25 | 3.30 | 100,100,100,100             | 0     |
| 86  | MG   | O4    | 201  | 1/1   | 0.35 | 3.28 | 45,45,45,45                 | 0     |
| 86  | MG   | 5     | 3840 | 1/1   | 0.20 | 3.27 | 53,53,53,53                 | 0     |
| 87  | OHX  | 8     | 228  | 7/7   | 0.18 | 3.27 | 121,121,121,121             | 0     |
| 86  | MG   | 5     | 3799 | 1/1   | 0.30 | 3.26 | 35,35,35,35                 | 0     |
| 86  | MG   | 5     | 3547 | 1/1   | 0.27 | 3.25 | 41,41,41,41                 | 0     |
| 87  | OHX  | 2     | 2077 | 7/7   | 0.25 | 3.25 | 103,103,103,103             | 0     |
| 86  | MG   | 1     | 3422 | 1/1   | 0.23 | 3.24 | 24,24,24,24                 | 0     |
| 86  | MG   | 5     | 3558 | 1/1   | 0.23 | 3.24 | 41,41,41,41                 | 0     |
| 86  | MG   | 1     | 3665 | 1/1   | 0.21 | 3.23 | 42,42,42,42                 | 0     |
| 87  | OHX  | 1     | 4081 | 7/7   | 0.17 | 3.23 | 113,113,113,113             | 0     |
| 86  | MG   | 5     | 3463 | 1/1   | 0.25 | 3.22 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 3706 | 1/1   | 0.27 | 3.21 | 44,44,44,44                 | 0     |
| 86  | MG   | n8    | 202  | 1/1   | 0.20 | 3.20 | 20,20,20,20                 | 0     |
| 87  | OHX  | 5     | 4192 | 7/7   | 0.32 | 3.20 | 118,118,118,118             | 0     |
| 87  | OHX  | 6     | 2191 | 7/7   | 0.37 | 3.20 | 130,130,130,130             | 0     |
| 86  | MG   | 5     | 3838 | 1/1   | 0.22 | 3.19 | 25,25,25,25                 | 0     |
| 86  | MG   | 2     | 1987 | 1/1   | 0.17 | 3.19 | 78,78,78,78                 | 0     |
| 86  | MG   | 1     | 3851 | 1/1   | 0.23 | 3.19 | 35,35,35,35                 | 0     |
| 86  | MG   | 3     | 210  | 1/1   | 0.26 | 3.13 | 55,55,55,55                 | 0     |
| 87  | OHX  | 1     | 4004 | 7/7   | 0.20 | 3.13 | 86,86,86,86                 | 0     |
| 87  | OHX  | 6     | 2153 | 7/7   | 0.24 | 3.11 | 120,120,120,120             | 0     |
| 87  | OHX  | 2     | 2084 | 7/7   | 0.23 | 3.11 | 91,91,91,91                 | 0     |
| 87  | OHX  | 5     | 4092 | 7/7   | 0.30 | 3.10 | 86,86,86,86                 | 0     |
| 87  | OHX  | 6     | 2144 | 7/7   | 0.23 | 3.10 | 152,152,152,152             | 0     |
| 86  | MG   | 5     | 3669 | 1/1   | 0.24 | 3.10 | 18,18,18,18                 | 0     |
| 86  | MG   | 5     | 3791 | 1/1   | 0.22 | 3.09 | 44,44,44,44                 | 0     |
| 86  | MG   | 1     | 3444 | 1/1   | 0.16 | 3.08 | 58,58,58,58                 | 0     |
| 87  | OHX  | 1     | 4185 | 7/7   | 0.36 | 3.08 | 109,109,109,109             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87  | OHX  | 2     | 2131 | 7/7   | 0.17 | 3.08 | 143,143,143,143            | 0     |
| 86  | MG   | 1     | 3602 | 1/1   | 0.22 | 3.08 | 19,19,19,19                | 0     |
| 86  | MG   | 1     | 3601 | 1/1   | 0.21 | 3.05 | 28,28,28,28                | 0     |
| 87  | OHX  | 5     | 4226 | 7/7   | 0.35 | 3.05 | 123,123,123,123            | 0     |
| 87  | OHX  | 1     | 4040 | 7/7   | 0.27 | 3.04 | 104,104,104,104            | 0     |
| 86  | MG   | 5     | 3512 | 1/1   | 0.18 | 3.04 | 22,22,22,22                | 0     |
| 87  | OHX  | 1     | 4014 | 7/7   | 0.20 | 3.04 | 104,104,104,104            | 0     |
| 87  | OHX  | 2     | 2161 | 7/7   | 0.27 | 3.03 | 152,152,152,152            | 0     |
| 86  | MG   | 1     | 3479 | 1/1   | 0.26 | 3.02 | 64,64,64,64                | 0     |
| 87  | OHX  | 6     | 2131 | 7/7   | 0.33 | 3.00 | 134,134,134,134            | 0     |
| 86  | MG   | 5     | 3659 | 1/1   | 0.21 | 3.00 | 39,39,39,39                | 0     |
| 86  | MG   | 1     | 3868 | 1/1   | 0.24 | 3.00 | 23,23,23,23                | 0     |
| 87  | OHX  | 1     | 4051 | 7/7   | 0.23 | 2.99 | 88,88,88,88                | 0     |
| 86  | MG   | 1     | 3807 | 1/1   | 0.24 | 2.98 | 47,47,47,47                | 0     |
| 86  | MG   | 1     | 3805 | 1/1   | 0.18 | 2.97 | 49,49,49,49                | 0     |
| 86  | MG   | 5     | 3461 | 1/1   | 0.24 | 2.97 | 32,32,32,32                | 0     |
| 86  | MG   | 1     | 3568 | 1/1   | 0.34 | 2.97 | 20,20,20,20                | 0     |
| 86  | MG   | 1     | 3783 | 1/1   | 0.21 | 2.96 | 39,39,39,39                | 0     |
| 86  | MG   | 1     | 3758 | 1/1   | 0.25 | 2.96 | 20,20,20,20                | 0     |
| 87  | OHX  | 1     | 4075 | 7/7   | 0.31 | 2.96 | 112,112,112,112            | 0     |
| 87  | OHX  | 2     | 2138 | 7/7   | 0.24 | 2.96 | 139,139,139,139            | 0     |
| 87  | OHX  | 1     | 4006 | 7/7   | 0.21 | 2.95 | 90,90,90,90                | 0     |
| 86  | MG   | 5     | 3409 | 1/1   | 0.24 | 2.94 | 35,35,35,35                | 0     |
| 87  | OHX  | 1     | 4177 | 7/7   | 0.20 | 2.92 | 84,84,84,84                | 0     |
| 87  | OHX  | 5     | 4138 | 7/7   | 0.42 | 2.92 | 107,107,107,107            | 0     |
| 87  | OHX  | 5     | 4132 | 7/7   | 0.15 | 2.91 | 91,91,91,91                | 0     |
| 86  | MG   | 5     | 3720 | 1/1   | 0.24 | 2.90 | 39,39,39,39                | 0     |
| 86  | MG   | 1     | 3835 | 1/1   | 0.26 | 2.90 | 24,24,24,24                | 0     |
| 87  | OHX  | 1     | 4199 | 7/7   | 0.44 | 2.89 | 112,112,112,112            | 0     |
| 86  | MG   | 1     | 3405 | 1/1   | 0.40 | 2.88 | 90,90,90,90                | 0     |
| 87  | OHX  | 8     | 226  | 7/7   | 0.22 | 2.87 | 113,113,113,113            | 0     |
| 87  | OHX  | m7    | 206  | 7/7   | 0.40 | 2.84 | 98,98,98,98                | 0     |
| 86  | MG   | 1     | 3653 | 1/1   | 0.40 | 2.83 | 101,101,101,101            | 0     |
| 87  | OHX  | 1     | 4153 | 7/7   | 0.30 | 2.83 | 124,124,124,124            | 0     |
| 86  | MG   | o4    | 201  | 1/1   | 0.41 | 2.82 | 45,45,45,45                | 0     |
| 87  | OHX  | 2     | 2147 | 7/7   | 0.25 | 2.81 | 155,155,155,155            | 0     |
| 86  | MG   | 5     | 3888 | 1/1   | 0.22 | 2.80 | 29,29,29,29                | 0     |
| 87  | OHX  | 1     | 4109 | 7/7   | 0.29 | 2.80 | 101,101,101,101            | 0     |
| 87  | OHX  | 6     | 2135 | 7/7   | 0.28 | 2.79 | 106,106,106,106            | 0     |
| 87  | OHX  | 1     | 4161 | 7/7   | 0.28 | 2.79 | 89,89,89,89                | 0     |
| 86  | MG   | 5     | 3767 | 1/1   | 0.17 | 2.78 | 26,26,26,26                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87  | OHX  | 6     | 2166 | 7/7   | 0.28 | 2.77 | 114,114,114,114             | 0     |
| 86  | MG   | 1     | 3687 | 1/1   | 0.33 | 2.76 | 41,41,41,41                 | 0     |
| 87  | OHX  | 5     | 4063 | 7/7   | 0.22 | 2.75 | 100,100,100,100             | 0     |
| 86  | MG   | 5     | 3744 | 1/1   | 0.22 | 2.75 | 25,25,25,25                 | 0     |
| 86  | MG   | N8    | 201  | 1/1   | 0.24 | 2.74 | 20,20,20,20                 | 0     |
| 86  | MG   | 5     | 3671 | 1/1   | 0.21 | 2.73 | 26,26,26,26                 | 0     |
| 87  | OHX  | 5     | 4077 | 7/7   | 0.30 | 2.73 | 102,102,102,102             | 0     |
| 86  | MG   | 5     | 3707 | 1/1   | 0.26 | 2.72 | 31,31,31,31                 | 0     |
| 87  | OHX  | 1     | 4217 | 7/7   | 0.26 | 2.70 | 119,119,119,119             | 0     |
| 86  | MG   | 4     | 217  | 1/1   | 0.18 | 2.70 | 30,30,30,30                 | 0     |
| 86  | MG   | 6     | 1990 | 1/1   | 0.22 | 2.69 | 76,76,76,76                 | 0     |
| 86  | MG   | 5     | 3496 | 1/1   | 0.22 | 2.69 | 24,24,24,24                 | 0     |
| 86  | MG   | 1     | 3727 | 1/1   | 0.20 | 2.68 | 33,33,33,33                 | 0     |
| 86  | MG   | 5     | 3843 | 1/1   | 0.24 | 2.67 | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 4256 | 1/1   | 0.38 | 2.67 | 28,28,28,28                 | 0     |
| 86  | MG   | n6    | 201  | 1/1   | 0.30 | 2.66 | 47,47,47,47                 | 0     |
| 87  | OHX  | 5     | 4066 | 7/7   | 0.18 | 2.65 | 94,94,94,94                 | 0     |
| 86  | MG   | 1     | 3721 | 1/1   | 0.23 | 2.65 | 25,25,25,25                 | 0     |
| 87  | OHX  | 5     | 4088 | 7/7   | 0.20 | 2.65 | 105,105,105,105             | 0     |
| 86  | MG   | 7     | 208  | 1/1   | 0.23 | 2.63 | 39,39,39,39                 | 0     |
| 86  | MG   | 1     | 3621 | 1/1   | 0.15 | 2.63 | 59,59,59,59                 | 0     |
| 87  | OHX  | 8     | 223  | 7/7   | 0.27 | 2.62 | 97,97,97,97                 | 0     |
| 86  | MG   | m6    | 201  | 1/1   | 0.23 | 2.61 | 23,23,23,23                 | 0     |
| 86  | MG   | 1     | 3782 | 1/1   | 0.28 | 2.61 | 32,32,32,32                 | 0     |
| 87  | OHX  | 1     | 3978 | 7/7   | 0.22 | 2.61 | 78,78,78,78                 | 0     |
| 87  | OHX  | 2     | 2107 | 7/7   | 0.26 | 2.59 | 137,137,137,137             | 0     |
| 86  | MG   | 1     | 3688 | 1/1   | 0.25 | 2.59 | 29,29,29,29                 | 0     |
| 86  | MG   | m7    | 205  | 1/1   | 0.32 | 2.58 | 28,28,28,28                 | 0     |
| 86  | MG   | 1     | 3439 | 1/1   | 0.31 | 2.58 | 35,35,35,35                 | 0     |
| 86  | MG   | 2     | 1941 | 1/1   | 0.27 | 2.57 | 68,68,68,68                 | 0     |
| 87  | OHX  | 5     | 4206 | 7/7   | 0.38 | 2.56 | 113,113,113,113             | 0     |
| 86  | MG   | 1     | 3603 | 1/1   | 0.24 | 2.56 | 23,23,23,23                 | 0     |
| 86  | MG   | 5     | 3816 | 1/1   | 0.17 | 2.56 | 47,47,47,47                 | 0     |
| 86  | MG   | 1     | 3445 | 1/1   | 0.38 | 2.54 | 31,31,31,31                 | 0     |
| 86  | MG   | 1     | 3764 | 1/1   | 0.25 | 2.53 | 41,41,41,41                 | 0     |
| 86  | MG   | d3    | 201  | 1/1   | 0.28 | 2.52 | 41,41,41,41                 | 0     |
| 86  | MG   | 1     | 3691 | 1/1   | 0.22 | 2.50 | 25,25,25,25                 | 0     |
| 87  | OHX  | 5     | 4028 | 7/7   | 0.19 | 2.50 | 84,84,84,84                 | 0     |
| 86  | MG   | 5     | 3898 | 1/1   | 0.21 | 2.49 | 21,21,21,21                 | 0     |
| 86  | MG   | 5     | 3619 | 1/1   | 0.32 | 2.47 | 33,33,33,33                 | 0     |
| 87  | OHX  | s1    | 303  | 7/7   | 0.42 | 2.47 | 140,140,140,140             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87  | OHX  | 2     | 2100 | 7/7   | 0.20 | 2.46 | 129,129,129,129             | 0     |
| 87  | OHX  | 6     | 2196 | 7/7   | 0.31 | 2.46 | 154,154,154,154             | 0     |
| 87  | OHX  | 5     | 4156 | 7/7   | 0.19 | 2.45 | 96,96,96,96                 | 0     |
| 87  | OHX  | 6     | 2201 | 7/7   | 0.28 | 2.44 | 123,123,123,123             | 0     |
| 87  | OHX  | 1     | 4007 | 7/7   | 0.27 | 2.43 | 79,79,79,79                 | 0     |
| 86  | MG   | 1     | 3831 | 1/1   | 0.17 | 2.43 | 20,20,20,20                 | 0     |
| 87  | OHX  | 1     | 4023 | 7/7   | 0.20 | 2.43 | 102,102,102,102             | 0     |
| 86  | MG   | 5     | 3736 | 1/1   | 0.18 | 2.41 | 30,30,30,30                 | 0     |
| 87  | OHX  | 1     | 4127 | 7/7   | 0.32 | 2.40 | 81,81,81,81                 | 0     |
| 87  | OHX  | 6     | 2188 | 7/7   | 0.24 | 2.40 | 165,165,165,165             | 0     |
| 87  | OHX  | 5     | 4072 | 7/7   | 0.20 | 2.38 | 103,103,103,103             | 0     |
| 86  | MG   | m7    | 203  | 1/1   | 0.23 | 2.37 | 38,38,38,38                 | 0     |
| 86  | MG   | 5     | 3846 | 1/1   | 0.19 | 2.37 | 21,21,21,21                 | 0     |
| 87  | OHX  | 2     | 2164 | 7/7   | 0.24 | 2.37 | 144,144,144,144             | 0     |
| 86  | MG   | 1     | 3763 | 1/1   | 0.19 | 2.35 | 34,34,34,34                 | 0     |
| 86  | MG   | 6     | 1976 | 1/1   | 0.26 | 2.35 | 53,53,53,53                 | 0     |
| 86  | MG   | 5     | 3842 | 1/1   | 0.20 | 2.34 | 22,22,22,22                 | 0     |
| 86  | MG   | 6     | 1964 | 1/1   | 0.28 | 2.32 | 67,67,67,67                 | 0     |
| 86  | MG   | L7    | 302  | 1/1   | 0.23 | 2.32 | 34,34,34,34                 | 0     |
| 87  | OHX  | 1     | 4196 | 7/7   | 0.23 | 2.31 | 125,125,125,125             | 0     |
| 86  | MG   | O7    | 102  | 1/1   | 0.26 | 2.31 | 27,27,27,27                 | 0     |
| 86  | MG   | M7    | 206  | 1/1   | 0.21 | 2.30 | 33,33,33,33                 | 0     |
| 87  | OHX  | 2     | 2056 | 7/7   | 0.20 | 2.30 | 90,90,90,90                 | 0     |
| 87  | OHX  | 6     | 2176 | 7/7   | 0.30 | 2.29 | 128,128,128,128             | 0     |
| 86  | MG   | 1     | 3815 | 1/1   | 0.17 | 2.29 | 31,31,31,31                 | 0     |
| 87  | OHX  | 2     | 2073 | 7/7   | 0.22 | 2.28 | 129,129,129,129             | 0     |
| 86  | MG   | 8     | 206  | 1/1   | 0.23 | 2.27 | 40,40,40,40                 | 0     |
| 86  | MG   | 5     | 3722 | 1/1   | 0.21 | 2.25 | 27,27,27,27                 | 0     |
| 89  | 3KD  | 5     | 4254 | 21/21 | 0.21 | 2.25 | 17,17,17,17                 | 0     |
| 86  | MG   | 1     | 3495 | 1/1   | 0.17 | 2.25 | 33,33,33,33                 | 0     |
| 87  | OHX  | 5     | 4191 | 7/7   | 0.28 | 2.25 | 103,103,103,103             | 0     |
| 86  | MG   | L4    | 402  | 1/1   | 0.20 | 2.24 | 20,20,20,20                 | 0     |
| 86  | MG   | M3    | 202  | 1/1   | 0.41 | 2.23 | 87,87,87,87                 | 0     |
| 86  | MG   | SM    | 301  | 1/1   | 0.21 | 2.21 | 48,48,48,48                 | 0     |
| 87  | OHX  | 2     | 2099 | 7/7   | 0.17 | 2.21 | 124,124,124,124             | 0     |
| 86  | MG   | 5     | 3735 | 1/1   | 0.20 | 2.21 | 61,61,61,61                 | 0     |
| 86  | MG   | 5     | 3493 | 1/1   | 0.23 | 2.21 | 31,31,31,31                 | 0     |
| 87  | OHX  | 1     | 4154 | 7/7   | 0.29 | 2.19 | 128,128,128,128             | 0     |
| 87  | OHX  | 1     | 4192 | 7/7   | 0.33 | 2.18 | 116,116,116,116             | 0     |
| 86  | MG   | 2     | 1954 | 1/1   | 0.20 | 2.16 | 96,96,96,96                 | 0     |
| 86  | MG   | 5     | 3689 | 1/1   | 0.15 | 2.16 | 30,30,30,30                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87  | OHX  | 5     | 4229 | 7/7   | 0.30 | 2.16 | 141,141,141,141             | 0     |
| 87  | OHX  | 5     | 4069 | 7/7   | 0.22 | 2.15 | 85,85,85,85                 | 0     |
| 87  | OHX  | 5     | 4252 | 7/7   | 0.34 | 2.14 | 118,118,118,118             | 0     |
| 87  | OHX  | 5     | 4146 | 7/7   | 0.23 | 2.12 | 111,111,111,111             | 0     |
| 87  | OHX  | 5     | 4076 | 7/7   | 0.34 | 2.12 | 100,100,100,100             | 0     |
| 86  | MG   | 6     | 2005 | 1/1   | 0.28 | 2.11 | 66,66,66,66                 | 0     |
| 86  | MG   | 1     | 3613 | 1/1   | 0.15 | 2.11 | 36,36,36,36                 | 0     |
| 87  | OHX  | 5     | 4096 | 7/7   | 0.22 | 2.10 | 111,111,111,111             | 0     |
| 86  | MG   | 1     | 3717 | 1/1   | 0.17 | 2.10 | 31,31,31,31                 | 0     |
| 87  | OHX  | M7    | 208  | 7/7   | 0.41 | 2.09 | 116,116,116,116             | 0     |
| 87  | OHX  | 1     | 4085 | 7/7   | 0.31 | 2.07 | 93,93,93,93                 | 0     |
| 86  | MG   | 5     | 3592 | 1/1   | 0.23 | 2.07 | 18,18,18,18                 | 0     |
| 86  | MG   | 1     | 3775 | 1/1   | 0.22 | 2.06 | 39,39,39,39                 | 0     |
| 86  | MG   | s8    | 302  | 1/1   | 0.22 | 2.05 | 39,39,39,39                 | 0     |
| 87  | OHX  | 1     | 4052 | 7/7   | 0.19 | 2.05 | 103,103,103,103             | 0     |
| 87  | OHX  | 2     | 2166 | 7/7   | 0.22 | 2.04 | 104,104,104,104             | 0     |
| 86  | MG   | 5     | 3872 | 1/1   | 0.21 | 2.04 | 31,31,31,31                 | 0     |
| 86  | MG   | 5     | 3515 | 1/1   | 0.24 | 2.04 | 30,30,30,30                 | 0     |
| 86  | MG   | 1     | 3704 | 1/1   | 0.20 | 2.04 | 37,37,37,37                 | 0     |
| 87  | OHX  | 1     | 4069 | 7/7   | 0.30 | 2.01 | 82,82,82,82                 | 0     |
| 87  | OHX  | 1     | 4043 | 7/7   | 0.25 | 2.01 | 98,98,98,98                 | 0     |
| 87  | OHX  | 5     | 4137 | 7/7   | 0.21 | 2.00 | 114,114,114,114             | 0     |
| 87  | OHX  | 1     | 3960 | 7/7   | 0.20 | 2.00 | 80,80,80,80                 | 0     |
| 86  | MG   | M3    | 201  | 1/1   | 0.19 | 2.00 | 36,36,36,36                 | 0     |
| 86  | MG   | 5     | 3695 | 1/1   | 0.16 | 2.00 | 39,39,39,39                 | 0     |
| 87  | OHX  | 5     | 4123 | 7/7   | 0.18 | 1.99 | 114,114,114,114             | 0     |
| 87  | OHX  | 1     | 4078 | 7/7   | 0.17 | 1.98 | 101,101,101,101             | 0     |
| 86  | MG   | 5     | 3413 | 1/1   | 0.33 | 1.98 | 31,31,31,31                 | 0     |
| 87  | OHX  | 1     | 4076 | 7/7   | 0.26 | 1.97 | 117,117,117,117             | 0     |
| 87  | OHX  | s4    | 302  | 7/7   | 0.21 | 1.96 | 131,131,131,131             | 0     |
| 86  | MG   | 5     | 3651 | 1/1   | 0.17 | 1.95 | 31,31,31,31                 | 0     |
| 87  | OHX  | 1     | 4034 | 7/7   | 0.17 | 1.95 | 109,109,109,109             | 0     |
| 87  | OHX  | 2     | 2163 | 7/7   | 0.17 | 1.94 | 168,168,168,168             | 0     |
| 86  | MG   | 5     | 3672 | 1/1   | 0.22 | 1.94 | 21,21,21,21                 | 0     |
| 86  | MG   | 5     | 3528 | 1/1   | 0.18 | 1.94 | 17,17,17,17                 | 0     |
| 86  | MG   | l5    | 301  | 1/1   | 0.26 | 1.94 | 50,50,50,50                 | 0     |
| 87  | OHX  | 5     | 4020 | 7/7   | 0.24 | 1.93 | 91,91,91,91                 | 0     |
| 86  | MG   | 1     | 3583 | 1/1   | 0.34 | 1.92 | 29,29,29,29                 | 0     |
| 86  | MG   | 5     | 3408 | 1/1   | 0.24 | 1.91 | 19,19,19,19                 | 0     |
| 86  | MG   | 6     | 2038 | 1/1   | 0.29 | 1.90 | 66,66,66,66                 | 0     |
| 86  | MG   | 5     | 3655 | 1/1   | 0.18 | 1.89 | 26,26,26,26                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 1     | 3667 | 1/1   | 0.23 | 1.88 | 29,29,29,29                 | 0     |
| 87  | OHX  | 5     | 4179 | 7/7   | 0.21 | 1.88 | 110,110,110,110             | 0     |
| 87  | OHX  | 5     | 4030 | 7/7   | 0.24 | 1.86 | 75,75,75,75                 | 0     |
| 87  | OHX  | 2     | 2168 | 7/7   | 0.22 | 1.84 | 123,123,123,123             | 0     |
| 87  | OHX  | 1     | 4094 | 7/7   | 0.22 | 1.84 | 113,113,113,113             | 0     |
| 87  | OHX  | 2     | 2115 | 7/7   | 0.28 | 1.84 | 125,125,125,125             | 0     |
| 86  | MG   | 1     | 3824 | 1/1   | 0.22 | 1.83 | 38,38,38,38                 | 0     |
| 86  | MG   | 5     | 3807 | 1/1   | 0.16 | 1.82 | 31,31,31,31                 | 0     |
| 86  | MG   | 5     | 3847 | 1/1   | 0.55 | 1.82 | 49,49,49,49                 | 0     |
| 87  | OHX  | 5     | 3911 | 7/7   | 0.17 | 1.82 | 55,55,55,55                 | 0     |
| 86  | MG   | m7    | 202  | 1/1   | 0.25 | 1.82 | 23,23,23,23                 | 0     |
| 86  | MG   | 1     | 3606 | 1/1   | 0.17 | 1.81 | 30,30,30,30                 | 0     |
| 86  | MG   | 6     | 2017 | 1/1   | 0.16 | 1.81 | 58,58,58,58                 | 0     |
| 87  | OHX  | 1     | 4128 | 7/7   | 0.24 | 1.81 | 121,121,121,121             | 0     |
| 87  | OHX  | 1     | 4031 | 7/7   | 0.18 | 1.81 | 104,104,104,104             | 0     |
| 86  | MG   | 4     | 209  | 1/1   | 0.18 | 1.80 | 38,38,38,38                 | 0     |
| 86  | MG   | 1     | 3861 | 1/1   | 0.16 | 1.80 | 46,46,46,46                 | 0     |
| 87  | OHX  | L4    | 403  | 7/7   | 0.34 | 1.79 | 110,110,110,110             | 0     |
| 87  | OHX  | 5     | 4003 | 7/7   | 0.24 | 1.78 | 57,57,57,57                 | 0     |
| 87  | OHX  | 5     | 4109 | 7/7   | 0.27 | 1.77 | 101,101,101,101             | 0     |
| 86  | MG   | 5     | 3599 | 1/1   | 0.18 | 1.77 | 32,32,32,32                 | 0     |
| 86  | MG   | c7    | 201  | 1/1   | 0.31 | 1.75 | 69,69,69,69                 | 0     |
| 87  | OHX  | 19    | 202  | 7/7   | 0.24 | 1.75 | 99,99,99,99                 | 0     |
| 86  | MG   | 5     | 3849 | 1/1   | 0.19 | 1.73 | 46,46,46,46                 | 0     |
| 86  | MG   | 1     | 3746 | 1/1   | 0.18 | 1.72 | 18,18,18,18                 | 0     |
| 87  | OHX  | 5     | 4253 | 7/7   | 0.35 | 1.72 | 149,149,149,149             | 0     |
| 87  | OHX  | 5     | 4184 | 7/7   | 0.25 | 1.71 | 126,126,126,126             | 0     |
| 86  | MG   | 1     | 3672 | 1/1   | 0.23 | 1.71 | 45,45,45,45                 | 0     |
| 87  | OHX  | 2     | 2130 | 7/7   | 0.17 | 1.71 | 138,138,138,138             | 0     |
| 86  | MG   | 19    | 201  | 1/1   | 0.22 | 1.71 | 37,37,37,37                 | 0     |
| 87  | OHX  | 1     | 4105 | 7/7   | 0.34 | 1.71 | 140,140,140,140             | 0     |
| 87  | OHX  | 14    | 402  | 7/7   | 0.26 | 1.71 | 134,134,134,134             | 0     |
| 87  | OHX  | 5     | 4119 | 7/7   | 0.22 | 1.70 | 105,105,105,105             | 0     |
| 86  | MG   | 5     | 3725 | 1/1   | 0.20 | 1.69 | 30,30,30,30                 | 0     |
| 86  | MG   | 1     | 3482 | 1/1   | 0.22 | 1.69 | 23,23,23,23                 | 0     |
| 87  | OHX  | 1     | 4205 | 7/7   | 0.20 | 1.68 | 139,139,139,139             | 0     |
| 87  | OHX  | 2     | 2094 | 7/7   | 0.25 | 1.68 | 114,114,114,114             | 0     |
| 87  | OHX  | 1     | 3995 | 7/7   | 0.16 | 1.67 | 83,83,83,83                 | 0     |
| 86  | MG   | 1     | 3794 | 1/1   | 0.13 | 1.67 | 42,42,42,42                 | 0     |
| 87  | OHX  | 2     | 2125 | 7/7   | 0.31 | 1.66 | 113,113,113,113             | 0     |
| 87  | OHX  | 5     | 4218 | 7/7   | 0.22 | 1.66 | 82,82,82,82                 | 0     |
| 86  | MG   | 5     | 3477 | 1/1   | 0.19 | 1.66 | 17,17,17,17                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 1     | 3810 | 1/1   | 0.37 | 1.65 | 181,181,181,181             | 0     |
| 86  | MG   | 5     | 3455 | 1/1   | 0.27 | 1.65 | 72,72,72,72                 | 0     |
| 87  | OHX  | M8    | 202  | 7/7   | 0.26 | 1.65 | 113,113,113,113             | 0     |
| 87  | OHX  | 6     | 2175 | 7/7   | 0.24 | 1.65 | 122,122,122,122             | 0     |
| 86  | MG   | 6     | 2024 | 1/1   | 0.34 | 1.65 | 60,60,60,60                 | 0     |
| 86  | MG   | 5     | 3642 | 1/1   | 0.19 | 1.64 | 41,41,41,41                 | 0     |
| 87  | OHX  | 2     | 2110 | 7/7   | 0.25 | 1.64 | 141,141,141,141             | 0     |
| 86  | MG   | 6     | 2027 | 1/1   | 0.27 | 1.63 | 38,38,38,38                 | 0     |
| 86  | MG   | 1     | 3714 | 1/1   | 0.19 | 1.63 | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 3778 | 1/1   | 0.38 | 1.61 | 45,45,45,45                 | 0     |
| 87  | OHX  | 5     | 4202 | 7/7   | 0.26 | 1.61 | 98,98,98,98                 | 0     |
| 87  | OHX  | 5     | 4015 | 7/7   | 0.18 | 1.60 | 85,85,85,85                 | 0     |
| 86  | MG   | 5     | 3757 | 1/1   | 0.14 | 1.60 | 35,35,35,35                 | 0     |
| 87  | OHX  | 2     | 2067 | 7/7   | 0.29 | 1.58 | 96,96,96,96                 | 0     |
| 86  | MG   | O8    | 101  | 1/1   | 0.25 | 1.57 | 56,56,56,56                 | 0     |
| 86  | MG   | 5     | 3658 | 1/1   | 0.14 | 1.57 | 29,29,29,29                 | 0     |
| 87  | OHX  | 5     | 4116 | 7/7   | 0.20 | 1.55 | 100,100,100,100             | 0     |
| 86  | MG   | 1     | 3612 | 1/1   | 0.22 | 1.54 | 33,33,33,33                 | 0     |
| 87  | OHX  | 5     | 4170 | 7/7   | 0.31 | 1.53 | 113,113,113,113             | 0     |
| 86  | MG   | 1     | 3817 | 1/1   | 0.15 | 1.53 | 42,42,42,42                 | 0     |
| 86  | MG   | M7    | 203  | 1/1   | 0.28 | 1.52 | 23,23,23,23                 | 0     |
| 86  | MG   | 5     | 3770 | 1/1   | 0.26 | 1.52 | 95,95,95,95                 | 0     |
| 87  | OHX  | 2     | 2074 | 7/7   | 0.24 | 1.52 | 112,112,112,112             | 0     |
| 86  | MG   | 6     | 1994 | 1/1   | 0.20 | 1.51 | 43,43,43,43                 | 0     |
| 87  | OHX  | 1     | 4032 | 7/7   | 0.16 | 1.50 | 107,107,107,107             | 0     |
| 87  | OHX  | 6     | 2137 | 7/7   | 0.22 | 1.50 | 107,107,107,107             | 0     |
| 89  | 3KD  | 1     | 4218 | 21/21 | 0.19 | 1.49 | 20,20,20,20                 | 0     |
| 86  | MG   | 1     | 3753 | 1/1   | 0.22 | 1.49 | 48,48,48,48                 | 0     |
| 86  | MG   | 6     | 1978 | 1/1   | 0.22 | 1.46 | 35,35,35,35                 | 0     |
| 86  | MG   | 5     | 3412 | 1/1   | 0.18 | 1.46 | 22,22,22,22                 | 0     |
| 86  | MG   | 14    | 401  | 1/1   | 0.19 | 1.46 | 25,25,25,25                 | 0     |
| 87  | OHX  | 6     | 2158 | 7/7   | 0.23 | 1.45 | 92,92,92,92                 | 0     |
| 86  | MG   | 1     | 3749 | 1/1   | 0.24 | 1.44 | 39,39,39,39                 | 0     |
| 86  | MG   | 1     | 3640 | 1/1   | 0.29 | 1.44 | 43,43,43,43                 | 0     |
| 87  | OHX  | 1     | 4097 | 7/7   | 0.26 | 1.43 | 132,132,132,132             | 0     |
| 86  | MG   | 5     | 3711 | 1/1   | 0.21 | 1.43 | 80,80,80,80                 | 0     |
| 87  | OHX  | 5     | 4075 | 7/7   | 0.22 | 1.43 | 96,96,96,96                 | 0     |
| 86  | MG   | 6     | 1991 | 1/1   | 0.26 | 1.43 | 62,62,62,62                 | 0     |
| 87  | OHX  | 6     | 2170 | 7/7   | 0.21 | 1.40 | 165,165,165,165             | 0     |
| 87  | OHX  | 15    | 305  | 7/7   | 0.51 | 1.40 | 128,128,128,128             | 0     |
| 87  | OHX  | 2     | 2127 | 7/7   | 0.24 | 1.39 | 185,185,185,185             | 0     |
| 86  | MG   | 1     | 3645 | 1/1   | 0.16 | 1.37 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87  | OHX  | 2     | 2165 | 7/7   | 0.17 | 1.36 | 142,142,142,142             | 0     |
| 86  | MG   | 1     | 3623 | 1/1   | 0.22 | 1.35 | 30,30,30,30                 | 0     |
| 86  | MG   | 6     | 2018 | 1/1   | 0.36 | 1.35 | 41,41,41,41                 | 0     |
| 87  | OHX  | 6     | 2142 | 7/7   | 0.16 | 1.35 | 117,117,117,117             | 0     |
| 86  | MG   | 5     | 3454 | 1/1   | 0.14 | 1.34 | 29,29,29,29                 | 0     |
| 86  | MG   | 5     | 3474 | 1/1   | 0.37 | 1.33 | 41,41,41,41                 | 0     |
| 87  | OHX  | 5     | 4050 | 7/7   | 0.19 | 1.32 | 86,86,86,86                 | 0     |
| 86  | MG   | 5     | 3730 | 1/1   | 0.32 | 1.31 | 67,67,67,67                 | 0     |
| 87  | OHX  | 1     | 3994 | 7/7   | 0.18 | 1.30 | 102,102,102,102             | 0     |
| 87  | OHX  | 6     | 2161 | 7/7   | 0.20 | 1.30 | 118,118,118,118             | 0     |
| 87  | OHX  | 5     | 4012 | 7/7   | 0.18 | 1.30 | 90,90,90,90                 | 0     |
| 86  | MG   | 1     | 3774 | 1/1   | 0.22 | 1.30 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 3668 | 1/1   | 0.18 | 1.29 | 22,22,22,22                 | 0     |
| 86  | MG   | L5    | 301  | 1/1   | 0.22 | 1.29 | 52,52,52,52                 | 0     |
| 86  | MG   | 1     | 3508 | 1/1   | 0.24 | 1.28 | 26,26,26,26                 | 0     |
| 86  | MG   | 5     | 3875 | 1/1   | 0.16 | 1.28 | 31,31,31,31                 | 0     |
| 86  | MG   | 1     | 3447 | 1/1   | 0.27 | 1.27 | 29,29,29,29                 | 0     |
| 86  | MG   | 1     | 3771 | 1/1   | 0.19 | 1.26 | 19,19,19,19                 | 0     |
| 86  | MG   | 1     | 3806 | 1/1   | 0.39 | 1.26 | 49,49,49,49                 | 0     |
| 86  | MG   | 1     | 3710 | 1/1   | 0.20 | 1.24 | 41,41,41,41                 | 0     |
| 86  | MG   | o1    | 201  | 1/1   | 0.28 | 1.24 | 39,39,39,39                 | 0     |
| 87  | OHX  | 5     | 4144 | 7/7   | 0.20 | 1.23 | 109,109,109,109             | 0     |
| 87  | OHX  | 6     | 2145 | 7/7   | 0.22 | 1.23 | 108,108,108,108             | 0     |
| 86  | MG   | d4    | 201  | 1/1   | 0.21 | 1.23 | 49,49,49,49                 | 0     |
| 87  | OHX  | 5     | 4091 | 7/7   | 0.27 | 1.22 | 81,81,81,81                 | 0     |
| 87  | OHX  | 6     | 2051 | 7/7   | 0.19 | 1.21 | 61,61,61,61                 | 0     |
| 86  | MG   | 1     | 3827 | 1/1   | 0.14 | 1.21 | 48,48,48,48                 | 0     |
| 87  | OHX  | 5     | 4169 | 7/7   | 0.23 | 1.20 | 133,133,133,133             | 0     |
| 87  | OHX  | 5     | 4200 | 7/7   | 0.19 | 1.19 | 70,70,70,70                 | 0     |
| 86  | MG   | L2    | 301  | 1/1   | 0.21 | 1.18 | 25,25,25,25                 | 0     |
| 87  | OHX  | 5     | 4122 | 7/7   | 0.24 | 1.17 | 125,125,125,125             | 0     |
| 87  | OHX  | 1     | 3876 | 7/7   | 0.14 | 1.17 | 46,46,46,46                 | 0     |
| 86  | MG   | 1     | 3840 | 1/1   | 0.49 | 1.15 | 38,38,38,38                 | 0     |
| 87  | OHX  | 2     | 2098 | 7/7   | 0.27 | 1.15 | 130,130,130,130             | 0     |
| 87  | OHX  | 6     | 2056 | 7/7   | 0.16 | 1.12 | 66,66,66,66                 | 0     |
| 87  | OHX  | 1     | 4098 | 7/7   | 0.15 | 1.12 | 123,123,123,123             | 0     |
| 86  | MG   | 5     | 3611 | 1/1   | 0.22 | 1.12 | 29,29,29,29                 | 0     |
| 87  | OHX  | 2     | 2137 | 7/7   | 0.29 | 1.12 | 143,143,143,143             | 0     |
| 86  | MG   | 2     | 2001 | 1/1   | 0.20 | 1.12 | 73,73,73,73                 | 0     |
| 87  | OHX  | 1     | 4005 | 7/7   | 0.17 | 1.12 | 74,74,74,74                 | 0     |
| 86  | MG   | 1     | 3864 | 1/1   | 0.20 | 1.11 | 93,93,93,93                 | 0     |
| 87  | OHX  | 2     | 2144 | 7/7   | 0.19 | 1.11 | 114,114,114,114             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 87  | OHX  | 5     | 4058 | 7/7   | 0.17 | 1.10 | 112,112,112,112            | 0     |
| 87  | OHX  | 2     | 2136 | 7/7   | 0.20 | 1.09 | 122,122,122,122            | 0     |
| 86  | MG   | 1     | 3719 | 1/1   | 0.20 | 1.09 | 70,70,70,70                | 0     |
| 86  | MG   | 1     | 4220 | 1/1   | 0.22 | 1.08 | 57,57,57,57                | 0     |
| 87  | OHX  | 1     | 4111 | 7/7   | 0.23 | 1.07 | 94,94,94,94                | 0     |
| 87  | OHX  | 1     | 4166 | 7/7   | 0.25 | 1.06 | 117,117,117,117            | 0     |
| 86  | MG   | 5     | 3543 | 1/1   | 0.27 | 1.05 | 58,58,58,58                | 0     |
| 87  | OHX  | 1     | 3963 | 7/7   | 0.21 | 1.05 | 78,78,78,78                | 0     |
| 86  | MG   | 1     | 3531 | 1/1   | 0.25 | 1.03 | 55,55,55,55                | 0     |
| 86  | MG   | 1     | 3769 | 1/1   | 0.23 | 1.03 | 53,53,53,53                | 0     |
| 87  | OHX  | 1     | 3895 | 7/7   | 0.15 | 1.02 | 67,67,67,67                | 0     |
| 87  | OHX  | 6     | 2165 | 7/7   | 0.30 | 1.02 | 96,96,96,96                | 0     |
| 87  | OHX  | 5     | 4095 | 7/7   | 0.22 | 1.02 | 96,96,96,96                | 0     |
| 87  | OHX  | 5     | 4038 | 7/7   | 0.19 | 1.00 | 99,99,99,99                | 0     |
| 87  | OHX  | m8    | 201  | 7/7   | 0.23 | 1.00 | 108,108,108,108            | 0     |
| 86  | MG   | 1     | 3829 | 1/1   | 0.15 | 0.98 | 33,33,33,33                | 0     |
| 86  | MG   | 1     | 3832 | 1/1   | 0.21 | 0.97 | 38,38,38,38                | 0     |
| 87  | OHX  | 1     | 4089 | 7/7   | 0.21 | 0.97 | 106,106,106,106            | 0     |
| 87  | OHX  | 5     | 4049 | 7/7   | 0.19 | 0.97 | 96,96,96,96                | 0     |
| 86  | MG   | 5     | 3724 | 1/1   | 0.20 | 0.97 | 35,35,35,35                | 0     |
| 86  | MG   | 4     | 212  | 1/1   | 0.18 | 0.97 | 28,28,28,28                | 0     |
| 87  | OHX  | 5     | 4011 | 7/7   | 0.17 | 0.96 | 84,84,84,84                | 0     |
| 86  | MG   | 2     | 2002 | 1/1   | 0.31 | 0.95 | 58,58,58,58                | 0     |
| 86  | MG   | 5     | 3897 | 1/1   | 0.19 | 0.95 | 34,34,34,34                | 0     |
| 87  | OHX  | 2     | 2063 | 7/7   | 0.21 | 0.94 | 94,94,94,94                | 0     |
| 86  | MG   | 5     | 3469 | 1/1   | 0.16 | 0.94 | 101,101,101,101            | 0     |
| 87  | OHX  | 1     | 4055 | 7/7   | 0.23 | 0.94 | 90,90,90,90                | 0     |
| 87  | OHX  | 1     | 4122 | 7/7   | 0.21 | 0.93 | 102,102,102,102            | 0     |
| 86  | MG   | 8     | 208  | 1/1   | 0.19 | 0.93 | 40,40,40,40                | 0     |
| 87  | OHX  | d4    | 202  | 7/7   | 0.28 | 0.90 | 141,141,141,141            | 0     |
| 87  | OHX  | 1     | 4083 | 7/7   | 0.20 | 0.90 | 100,100,100,100            | 0     |
| 87  | OHX  | 2     | 2023 | 7/7   | 0.17 | 0.89 | 76,76,76,76                | 0     |
| 86  | MG   | 5     | 3662 | 1/1   | 0.17 | 0.89 | 29,29,29,29                | 0     |
| 86  | MG   | 5     | 3700 | 1/1   | 0.19 | 0.88 | 23,23,23,23                | 0     |
| 87  | OHX  | 6     | 2116 | 7/7   | 0.18 | 0.88 | 83,83,83,83                | 0     |
| 87  | OHX  | 1     | 4024 | 7/7   | 0.22 | 0.88 | 116,116,116,116            | 0     |
| 87  | OHX  | 1     | 3916 | 7/7   | 0.19 | 0.87 | 71,71,71,71                | 0     |
| 87  | OHX  | 2     | 2097 | 7/7   | 0.16 | 0.86 | 98,98,98,98                | 0     |
| 87  | OHX  | 6     | 2185 | 7/7   | 0.33 | 0.86 | 111,111,111,111            | 0     |
| 86  | MG   | 6     | 1993 | 1/1   | 0.17 | 0.85 | 42,42,42,42                | 0     |
| 86  | MG   | 1     | 3816 | 1/1   | 0.12 | 0.84 | 42,42,42,42                | 0     |
| 87  | OHX  | 1     | 4106 | 7/7   | 0.27 | 0.84 | 120,120,120,120            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 1     | 3611 | 1/1   | 0.13 | 0.84 | 34,34,34,34                 | 0     |
| 86  | MG   | 1     | 3686 | 1/1   | 0.17 | 0.84 | 42,42,42,42                 | 0     |
| 87  | OHX  | 6     | 2119 | 7/7   | 0.17 | 0.83 | 115,115,115,115             | 0     |
| 86  | MG   | 1     | 3582 | 1/1   | 0.27 | 0.83 | 33,33,33,33                 | 0     |
| 87  | OHX  | 3     | 216  | 7/7   | 0.18 | 0.82 | 89,89,89,89                 | 0     |
| 87  | OHX  | 1     | 4035 | 7/7   | 0.22 | 0.81 | 86,86,86,86                 | 0     |
| 87  | OHX  | 1     | 3990 | 7/7   | 0.16 | 0.81 | 76,76,76,76                 | 0     |
| 87  | OHX  | 2     | 2178 | 7/7   | 0.29 | 0.80 | 148,148,148,148             | 0     |
| 87  | OHX  | 8     | 222  | 7/7   | 0.13 | 0.79 | 105,105,105,105             | 0     |
| 87  | OHX  | d9    | 102  | 7/7   | 0.30 | 0.79 | 152,152,152,152             | 0     |
| 86  | MG   | 6     | 2044 | 1/1   | 0.16 | 0.77 | 51,51,51,51                 | 0     |
| 87  | OHX  | 6     | 2109 | 7/7   | 0.19 | 0.77 | 92,92,92,92                 | 0     |
| 87  | OHX  | 5     | 3939 | 7/7   | 0.15 | 0.77 | 70,70,70,70                 | 0     |
| 87  | OHX  | 1     | 3973 | 7/7   | 0.20 | 0.76 | 75,75,75,75                 | 0     |
| 86  | MG   | 1     | 3617 | 1/1   | 0.18 | 0.76 | 23,23,23,23                 | 0     |
| 87  | OHX  | 5     | 4019 | 7/7   | 0.18 | 0.76 | 85,85,85,85                 | 0     |
| 86  | MG   | 1     | 3449 | 1/1   | 0.15 | 0.75 | 27,27,27,27                 | 0     |
| 86  | MG   | 1     | 3728 | 1/1   | 0.16 | 0.75 | 55,55,55,55                 | 0     |
| 87  | OHX  | 2     | 2149 | 7/7   | 0.19 | 0.74 | 166,166,166,166             | 0     |
| 86  | MG   | 1     | 3639 | 1/1   | 0.20 | 0.74 | 37,37,37,37                 | 0     |
| 87  | OHX  | 6     | 2133 | 7/7   | 0.20 | 0.74 | 102,102,102,102             | 0     |
| 87  | OHX  | 1     | 4108 | 7/7   | 0.24 | 0.73 | 99,99,99,99                 | 0     |
| 87  | OHX  | 6     | 2121 | 7/7   | 0.19 | 0.73 | 88,88,88,88                 | 0     |
| 87  | OHX  | 2     | 2159 | 7/7   | 0.38 | 0.71 | 134,134,134,134             | 0     |
| 86  | MG   | 5     | 3620 | 1/1   | 0.12 | 0.71 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 3814 | 1/1   | 0.16 | 0.70 | 38,38,38,38                 | 0     |
| 86  | MG   | 2     | 1946 | 1/1   | 0.23 | 0.70 | 54,54,54,54                 | 0     |
| 87  | OHX  | 6     | 2204 | 7/7   | 0.29 | 0.70 | 121,121,121,121             | 0     |
| 86  | MG   | m1    | 201  | 1/1   | 0.16 | 0.68 | 49,49,49,49                 | 0     |
| 87  | OHX  | O2    | 201  | 7/7   | 0.23 | 0.68 | 76,76,76,76                 | 0     |
| 87  | OHX  | 8     | 218  | 7/7   | 0.19 | 0.68 | 88,88,88,88                 | 0     |
| 86  | MG   | 5     | 3434 | 1/1   | 0.19 | 0.68 | 22,22,22,22                 | 0     |
| 87  | OHX  | 6     | 2058 | 7/7   | 0.15 | 0.67 | 70,70,70,70                 | 0     |
| 87  | OHX  | 1     | 3874 | 7/7   | 0.17 | 0.67 | 46,46,46,46                 | 0     |
| 87  | OHX  | 1     | 4001 | 7/7   | 0.20 | 0.66 | 83,83,83,83                 | 0     |
| 87  | OHX  | 5     | 4054 | 7/7   | 0.19 | 0.65 | 83,83,83,83                 | 0     |
| 86  | MG   | 5     | 3782 | 1/1   | 0.20 | 0.65 | 74,74,74,74                 | 0     |
| 86  | MG   | 1     | 3618 | 1/1   | 0.18 | 0.64 | 52,52,52,52                 | 0     |
| 87  | OHX  | 5     | 4227 | 7/7   | 0.29 | 0.64 | 123,123,123,123             | 0     |
| 87  | OHX  | 6     | 2122 | 7/7   | 0.17 | 0.64 | 123,123,123,123             | 0     |
| 86  | MG   | d3    | 202  | 1/1   | 0.23 | 0.64 | 36,36,36,36                 | 0     |
| 87  | OHX  | 6     | 2075 | 7/7   | 0.16 | 0.64 | 76,76,76,76                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87  | OHX  | c1    | 202  | 7/7   | 0.31 | 0.64 | 115,115,115,115             | 0     |
| 87  | OHX  | 1     | 4015 | 7/7   | 0.16 | 0.63 | 110,110,110,110             | 0     |
| 86  | MG   | 5     | 3754 | 1/1   | 0.21 | 0.62 | 37,37,37,37                 | 0     |
| 86  | MG   | 5     | 3602 | 1/1   | 0.15 | 0.62 | 48,48,48,48                 | 0     |
| 86  | MG   | 1     | 3779 | 1/1   | 0.17 | 0.60 | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 3832 | 1/1   | 0.20 | 0.60 | 46,46,46,46                 | 0     |
| 87  | OHX  | 1     | 4136 | 7/7   | 0.25 | 0.59 | 134,134,134,134             | 0     |
| 86  | MG   | N3    | 202  | 1/1   | 0.12 | 0.59 | 56,56,56,56                 | 0     |
| 87  | OHX  | 2     | 2140 | 7/7   | 0.20 | 0.57 | 124,124,124,124             | 0     |
| 86  | MG   | 8     | 209  | 1/1   | 0.12 | 0.57 | 55,55,55,55                 | 0     |
| 86  | MG   | 5     | 3687 | 1/1   | 0.19 | 0.57 | 67,67,67,67                 | 0     |
| 87  | OHX  | 6     | 2162 | 7/7   | 0.21 | 0.55 | 89,89,89,89                 | 0     |
| 87  | OHX  | 1     | 3949 | 7/7   | 0.17 | 0.55 | 74,74,74,74                 | 0     |
| 86  | MG   | M8    | 201  | 1/1   | 0.23 | 0.55 | 46,46,46,46                 | 0     |
| 87  | OHX  | 2     | 2128 | 7/7   | 0.20 | 0.54 | 97,97,97,97                 | 0     |
| 86  | MG   | 5     | 3741 | 1/1   | 0.15 | 0.54 | 43,43,43,43                 | 0     |
| 86  | MG   | 1     | 3662 | 1/1   | 0.15 | 0.54 | 26,26,26,26                 | 0     |
| 86  | MG   | 5     | 3693 | 1/1   | 0.17 | 0.54 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 3633 | 1/1   | 0.20 | 0.54 | 21,21,21,21                 | 0     |
| 86  | MG   | 4     | 220  | 1/1   | 0.18 | 0.54 | 36,36,36,36                 | 0     |
| 87  | OHX  | 2     | 2153 | 7/7   | 0.25 | 0.53 | 125,125,125,125             | 0     |
| 87  | OHX  | 2     | 2148 | 7/7   | 0.28 | 0.52 | 146,146,146,146             | 0     |
| 86  | MG   | 2     | 2180 | 1/1   | 0.22 | 0.51 | 78,78,78,78                 | 0     |
| 87  | OHX  | 6     | 2110 | 7/7   | 0.25 | 0.51 | 108,108,108,108             | 0     |
| 87  | OHX  | 2     | 2175 | 7/7   | 0.24 | 0.48 | 160,160,160,160             | 0     |
| 86  | MG   | 17    | 301  | 1/1   | 0.21 | 0.48 | 29,29,29,29                 | 0     |
| 86  | MG   | 5     | 3800 | 1/1   | 0.18 | 0.48 | 65,65,65,65                 | 0     |
| 87  | OHX  | 1     | 4215 | 7/7   | 0.31 | 0.47 | 136,136,136,136             | 0     |
| 87  | OHX  | 5     | 4081 | 7/7   | 0.17 | 0.47 | 97,97,97,97                 | 0     |
| 87  | OHX  | 2     | 2122 | 7/7   | 0.20 | 0.46 | 130,130,130,130             | 0     |
| 87  | OHX  | L3    | 404  | 7/7   | 0.19 | 0.46 | 90,90,90,90                 | 0     |
| 87  | OHX  | 2     | 2086 | 7/7   | 0.18 | 0.44 | 112,112,112,112             | 0     |
| 87  | OHX  | 1     | 4016 | 7/7   | 0.17 | 0.44 | 105,105,105,105             | 0     |
| 87  | OHX  | 5     | 4065 | 7/7   | 0.16 | 0.44 | 134,134,134,134             | 0     |
| 86  | MG   | 1     | 3624 | 1/1   | 0.16 | 0.44 | 35,35,35,35                 | 0     |
| 87  | OHX  | 6     | 2140 | 7/7   | 0.30 | 0.43 | 102,102,102,102             | 0     |
| 86  | MG   | 2     | 1997 | 1/1   | 0.42 | 0.43 | 64,64,64,64                 | 0     |
| 87  | OHX  | 1     | 4012 | 7/7   | 0.20 | 0.42 | 86,86,86,86                 | 0     |
| 86  | MG   | 1     | 3428 | 1/1   | 0.28 | 0.41 | 39,39,39,39                 | 0     |
| 87  | OHX  | 6     | 2157 | 7/7   | 0.13 | 0.41 | 115,115,115,115             | 0     |
| 86  | MG   | 1     | 3420 | 1/1   | 0.31 | 0.41 | 54,54,54,54                 | 0     |
| 86  | MG   | 5     | 3723 | 1/1   | 0.20 | 0.41 | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 1     | 3669 | 1/1   | 0.16 | 0.41 | 45,45,45,45                 | 0     |
| 86  | MG   | 1     | 3638 | 1/1   | 0.24 | 0.41 | 54,54,54,54                 | 0     |
| 87  | OHX  | 1     | 4041 | 7/7   | 0.15 | 0.40 | 127,127,127,127             | 0     |
| 87  | OHX  | 15    | 304  | 7/7   | 0.29 | 0.40 | 122,122,122,122             | 0     |
| 86  | MG   | 2     | 1986 | 1/1   | 0.20 | 0.40 | 96,96,96,96                 | 0     |
| 87  | OHX  | 6     | 2195 | 7/7   | 0.23 | 0.39 | 141,141,141,141             | 0     |
| 86  | MG   | 5     | 3761 | 1/1   | 0.16 | 0.39 | 39,39,39,39                 | 0     |
| 86  | MG   | M7    | 205  | 1/1   | 0.19 | 0.39 | 26,26,26,26                 | 0     |
| 87  | OHX  | 6     | 2155 | 7/7   | 0.18 | 0.39 | 142,142,142,142             | 0     |
| 87  | OHX  | 5     | 4067 | 7/7   | 0.15 | 0.39 | 98,98,98,98                 | 0     |
| 87  | OHX  | 6     | 2132 | 7/7   | 0.17 | 0.38 | 118,118,118,118             | 0     |
| 86  | MG   | N8    | 202  | 1/1   | 0.27 | 0.38 | 40,40,40,40                 | 0     |
| 86  | MG   | 1     | 3793 | 1/1   | 0.17 | 0.38 | 68,68,68,68                 | 0     |
| 86  | MG   | 5     | 3471 | 1/1   | 0.15 | 0.37 | 36,36,36,36                 | 0     |
| 86  | MG   | 5     | 3660 | 1/1   | 0.18 | 0.36 | 40,40,40,40                 | 0     |
| 87  | OHX  | 5     | 4153 | 7/7   | 0.21 | 0.35 | 136,136,136,136             | 0     |
| 87  | OHX  | 2     | 2049 | 7/7   | 0.16 | 0.34 | 87,87,87,87                 | 0     |
| 87  | OHX  | 2     | 2070 | 7/7   | 0.17 | 0.33 | 105,105,105,105             | 0     |
| 87  | OHX  | 5     | 4100 | 7/7   | 0.17 | 0.33 | 115,115,115,115             | 0     |
| 87  | OHX  | 2     | 2113 | 7/7   | 0.19 | 0.33 | 105,105,105,105             | 0     |
| 87  | OHX  | 1     | 3956 | 7/7   | 0.12 | 0.33 | 102,102,102,102             | 0     |
| 86  | MG   | 1     | 3722 | 1/1   | 0.23 | 0.33 | 39,39,39,39                 | 0     |
| 86  | MG   | s1    | 301  | 1/1   | 0.17 | 0.32 | 65,65,65,65                 | 0     |
| 86  | MG   | 5     | 3404 | 1/1   | 0.17 | 0.31 | 39,39,39,39                 | 0     |
| 88  | ZN   | D7    | 101  | 1/1   | 0.39 | 0.31 | 172,172,172,172             | 0     |
| 86  | MG   | 5     | 3803 | 1/1   | 0.12 | 0.31 | 33,33,33,33                 | 0     |
| 87  | OHX  | 1     | 3992 | 7/7   | 0.20 | 0.30 | 102,102,102,102             | 0     |
| 87  | OHX  | 3     | 221  | 7/7   | 0.17 | 0.30 | 109,109,109,109             | 0     |
| 87  | OHX  | 2     | 2119 | 7/7   | 0.23 | 0.30 | 129,129,129,129             | 0     |
| 86  | MG   | n3    | 202  | 1/1   | 0.22 | 0.29 | 32,32,32,32                 | 0     |
| 86  | MG   | s4    | 301  | 1/1   | 0.22 | 0.29 | 45,45,45,45                 | 0     |
| 87  | OHX  | 5     | 4216 | 7/7   | 0.19 | 0.29 | 184,184,184,184             | 0     |
| 87  | OHX  | 1     | 4058 | 7/7   | 0.18 | 0.26 | 110,110,110,110             | 0     |
| 86  | MG   | 6     | 1968 | 1/1   | 0.20 | 0.26 | 74,74,74,74                 | 0     |
| 87  | OHX  | 1     | 4028 | 7/7   | 0.17 | 0.26 | 128,128,128,128             | 0     |
| 87  | OHX  | 6     | 2094 | 7/7   | 0.19 | 0.25 | 95,95,95,95                 | 0     |
| 87  | OHX  | 1     | 4088 | 7/7   | 0.23 | 0.25 | 120,120,120,120             | 0     |
| 87  | OHX  | 2     | 2083 | 7/7   | 0.17 | 0.25 | 124,124,124,124             | 0     |
| 87  | OHX  | 1     | 3975 | 7/7   | 0.15 | 0.25 | 85,85,85,85                 | 0     |
| 87  | OHX  | 5     | 3916 | 7/7   | 0.16 | 0.24 | 49,49,49,49                 | 0     |
| 87  | OHX  | 1     | 4010 | 7/7   | 0.17 | 0.24 | 97,97,97,97                 | 0     |
| 87  | OHX  | 7     | 219  | 7/7   | 0.16 | 0.23 | 84,84,84,84                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87  | OHX  | 5     | 4064 | 7/7   | 0.17 | 0.23 | 107,107,107,107             | 0     |
| 87  | OHX  | m5    | 304  | 7/7   | 0.22 | 0.22 | 107,107,107,107             | 0     |
| 86  | MG   | 1     | 3778 | 1/1   | 0.21 | 0.22 | 62,62,62,62                 | 0     |
| 87  | OHX  | 1     | 3977 | 7/7   | 0.23 | 0.22 | 89,89,89,89                 | 0     |
| 87  | OHX  | 2     | 2061 | 7/7   | 0.16 | 0.21 | 115,115,115,115             | 0     |
| 87  | OHX  | 5     | 4036 | 7/7   | 0.19 | 0.20 | 107,107,107,107             | 0     |
| 86  | MG   | 6     | 1924 | 1/1   | 0.17 | 0.20 | 58,58,58,58                 | 0     |
| 86  | MG   | 5     | 3812 | 1/1   | 0.31 | 0.19 | 58,58,58,58                 | 0     |
| 86  | MG   | M7    | 201  | 1/1   | 0.33 | 0.19 | 57,57,57,57                 | 0     |
| 86  | MG   | 6     | 1916 | 1/1   | 0.16 | 0.18 | 47,47,47,47                 | 0     |
| 86  | MG   | 2     | 1995 | 1/1   | 0.17 | 0.17 | 72,72,72,72                 | 0     |
| 86  | MG   | L7    | 301  | 1/1   | 0.18 | 0.17 | 27,27,27,27                 | 0     |
| 86  | MG   | 1     | 3466 | 1/1   | 0.15 | 0.17 | 39,39,39,39                 | 0     |
| 86  | MG   | 1     | 3737 | 1/1   | 0.16 | 0.16 | 31,31,31,31                 | 0     |
| 87  | OHX  | 1     | 4203 | 7/7   | 0.31 | 0.15 | 112,112,112,112             | 0     |
| 86  | MG   | 6     | 1971 | 1/1   | 0.18 | 0.14 | 52,52,52,52                 | 0     |
| 87  | OHX  | 5     | 4026 | 7/7   | 0.15 | 0.14 | 90,90,90,90                 | 0     |
| 87  | OHX  | 1     | 4048 | 7/7   | 0.21 | 0.13 | 90,90,90,90                 | 0     |
| 86  | MG   | 5     | 3826 | 1/1   | 0.15 | 0.13 | 27,27,27,27                 | 0     |
| 86  | MG   | 1     | 3811 | 1/1   | 0.18 | 0.13 | 40,40,40,40                 | 0     |
| 87  | OHX  | M5    | 302  | 7/7   | 0.22 | 0.13 | 93,93,93,93                 | 0     |
| 86  | MG   | 1     | 3718 | 1/1   | 0.20 | 0.12 | 36,36,36,36                 | 0     |
| 86  | MG   | 6     | 2030 | 1/1   | 0.18 | 0.10 | 76,76,76,76                 | 0     |
| 87  | OHX  | 5     | 4085 | 7/7   | 0.13 | 0.10 | 117,117,117,117             | 0     |
| 86  | MG   | 1     | 3767 | 1/1   | 0.16 | 0.10 | 48,48,48,48                 | 0     |
| 88  | ZN   | q2    | 501  | 1/1   | 0.24 | 0.10 | 67,67,67,67                 | 0     |
| 86  | MG   | 5     | 3798 | 1/1   | 0.17 | 0.10 | 22,22,22,22                 | 0     |
| 86  | MG   | 1     | 3821 | 1/1   | 0.14 | 0.09 | 27,27,27,27                 | 0     |
| 87  | OHX  | 1     | 4029 | 7/7   | 0.19 | 0.09 | 122,122,122,122             | 0     |
| 87  | OHX  | 6     | 2054 | 7/7   | 0.17 | 0.07 | 62,62,62,62                 | 0     |
| 87  | OHX  | 2     | 2091 | 7/7   | 0.18 | 0.06 | 138,138,138,138             | 0     |
| 86  | MG   | 5     | 3460 | 1/1   | 0.18 | 0.06 | 20,20,20,20                 | 0     |
| 87  | OHX  | 5     | 4002 | 7/7   | 0.22 | 0.06 | 79,79,79,79                 | 0     |
| 87  | OHX  | 6     | 2093 | 7/7   | 0.15 | 0.06 | 93,93,93,93                 | 0     |
| 87  | OHX  | 5     | 4097 | 7/7   | 0.16 | 0.05 | 108,108,108,108             | 0     |
| 87  | OHX  | L3    | 405  | 7/7   | 0.42 | 0.05 | 148,148,148,148             | 0     |
| 86  | MG   | m5    | 303  | 1/1   | 0.23 | 0.05 | 84,84,84,84                 | 0     |
| 86  | MG   | 1     | 3434 | 1/1   | 0.15 | 0.04 | 37,37,37,37                 | 0     |
| 87  | OHX  | 4     | 228  | 7/7   | 0.15 | 0.03 | 112,112,112,112             | 0     |
| 86  | MG   | 5     | 3637 | 1/1   | 0.23 | 0.03 | 40,40,40,40                 | 0     |
| 87  | OHX  | 5     | 4016 | 7/7   | 0.16 | 0.03 | 89,89,89,89                 | 0     |
| 87  | OHX  | 5     | 3925 | 7/7   | 0.16 | 0.02 | 59,59,59,59                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|----------------------------|-------|
| 86  | MG   | 1     | 3634 | 1/1   | 0.24 | 0.02  | 67,67,67,67                | 0     |
| 87  | OHX  | 5     | 4024 | 7/7   | 0.17 | 0.02  | 87,87,87,87                | 0     |
| 86  | MG   | 1     | 3522 | 1/1   | 0.16 | 0.01  | 22,22,22,22                | 0     |
| 87  | OHX  | s8    | 303  | 7/7   | 0.38 | 0.01  | 143,143,143,143            | 0     |
| 87  | OHX  | 2     | 2078 | 7/7   | 0.15 | 0.00  | 157,157,157,157            | 0     |
| 87  | OHX  | 4     | 224  | 7/7   | 0.18 | 0.00  | 105,105,105,105            | 0     |
| 87  | OHX  | 5     | 4126 | 7/7   | 0.19 | -0.01 | 134,134,134,134            | 0     |
| 87  | OHX  | 1     | 4053 | 7/7   | 0.18 | -0.01 | 120,120,120,120            | 0     |
| 86  | MG   | M1    | 201  | 1/1   | 0.18 | -0.01 | 67,67,67,67                | 0     |
| 87  | OHX  | m1    | 202  | 7/7   | 0.28 | -0.01 | 136,136,136,136            | 0     |
| 86  | MG   | 5     | 3703 | 1/1   | 0.17 | -0.03 | 49,49,49,49                | 0     |
| 87  | OHX  | 2     | 2109 | 7/7   | 0.19 | -0.03 | 98,98,98,98                | 0     |
| 87  | OHX  | 5     | 4068 | 7/7   | 0.12 | -0.05 | 106,106,106,106            | 0     |
| 87  | OHX  | 2     | 2088 | 7/7   | 0.19 | -0.05 | 105,105,105,105            | 0     |
| 87  | OHX  | 5     | 4244 | 7/7   | 0.30 | -0.05 | 80,80,80,80                | 0     |
| 86  | MG   | 2     | 2179 | 1/1   | 0.23 | -0.05 | 56,56,56,56                | 0     |
| 87  | OHX  | 5     | 4172 | 7/7   | 0.17 | -0.06 | 179,179,179,179            | 0     |
| 87  | OHX  | 2     | 2062 | 7/7   | 0.18 | -0.07 | 95,95,95,95                | 0     |
| 87  | OHX  | 2     | 2105 | 7/7   | 0.17 | -0.07 | 94,94,94,94                | 0     |
| 86  | MG   | 1     | 3716 | 1/1   | 0.18 | -0.09 | 27,27,27,27                | 0     |
| 86  | MG   | 5     | 3779 | 1/1   | 0.16 | -0.10 | 32,32,32,32                | 0     |
| 87  | OHX  | 1     | 4095 | 7/7   | 0.19 | -0.10 | 133,133,133,133            | 0     |
| 86  | MG   | L8    | 301  | 1/1   | 0.27 | -0.11 | 45,45,45,45                | 0     |
| 86  | MG   | 1     | 3822 | 1/1   | 0.15 | -0.11 | 44,44,44,44                | 0     |
| 86  | MG   | 1     | 4223 | 1/1   | 0.18 | -0.11 | 32,32,32,32                | 0     |
| 86  | MG   | q3    | 502  | 1/1   | 0.24 | -0.12 | 61,61,61,61                | 0     |
| 86  | MG   | 1     | 3436 | 1/1   | 0.17 | -0.13 | 32,32,32,32                | 0     |
| 87  | OHX  | 1     | 4149 | 7/7   | 0.20 | -0.13 | 131,131,131,131            | 0     |
| 87  | OHX  | l3    | 404  | 7/7   | 0.30 | -0.15 | 116,116,116,116            | 0     |
| 86  | MG   | 5     | 3638 | 1/1   | 0.17 | -0.15 | 43,43,43,43                | 0     |
| 87  | OHX  | 1     | 3989 | 7/7   | 0.18 | -0.15 | 85,85,85,85                | 0     |
| 87  | OHX  | 2     | 2087 | 7/7   | 0.17 | -0.15 | 90,90,90,90                | 0     |
| 87  | OHX  | 2     | 2104 | 7/7   | 0.20 | -0.16 | 113,113,113,113            | 0     |
| 87  | OHX  | l5    | 303  | 7/7   | 0.14 | -0.16 | 117,117,117,117            | 0     |
| 87  | OHX  | 1     | 3885 | 7/7   | 0.15 | -0.17 | 52,52,52,52                | 0     |
| 87  | OHX  | sR    | 401  | 7/7   | 0.21 | -0.17 | 147,147,147,147            | 0     |
| 87  | OHX  | 2     | 2120 | 7/7   | 0.18 | -0.18 | 129,129,129,129            | 0     |
| 86  | MG   | 6     | 2001 | 1/1   | 0.18 | -0.18 | 42,42,42,42                | 0     |
| 86  | MG   | 5     | 3758 | 1/1   | 0.16 | -0.20 | 49,49,49,49                | 0     |
| 87  | OHX  | 6     | 2126 | 7/7   | 0.15 | -0.20 | 122,122,122,122            | 0     |
| 86  | MG   | 5     | 3606 | 1/1   | 0.14 | -0.21 | 28,28,28,28                | 0     |
| 87  | OHX  | 3     | 219  | 7/7   | 0.14 | -0.21 | 101,101,101,101            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 1     | 3424 | 1/1   | 0.15 | -0.21 | 38,38,38,38                 | 0     |
| 86  | MG   | 1     | 3788 | 1/1   | 0.16 | -0.21 | 40,40,40,40                 | 0     |
| 87  | OHX  | 6     | 2101 | 7/7   | 0.15 | -0.23 | 106,106,106,106             | 0     |
| 87  | OHX  | c3    | 201  | 7/7   | 0.28 | -0.23 | 139,139,139,139             | 0     |
| 87  | OHX  | 5     | 3909 | 7/7   | 0.14 | -0.23 | 44,44,44,44                 | 0     |
| 87  | OHX  | o2    | 201  | 7/7   | 0.19 | -0.23 | 77,77,77,77                 | 0     |
| 87  | OHX  | 5     | 4057 | 7/7   | 0.18 | -0.23 | 88,88,88,88                 | 0     |
| 87  | OHX  | q2    | 502  | 7/7   | 0.17 | -0.24 | 67,67,67,67                 | 0     |
| 86  | MG   | 1     | 3636 | 1/1   | 0.20 | -0.24 | 32,32,32,32                 | 0     |
| 87  | OHX  | n6    | 202  | 7/7   | 0.17 | -0.24 | 115,115,115,115             | 0     |
| 87  | OHX  | 5     | 4240 | 7/7   | 0.14 | -0.24 | 127,127,127,127             | 0     |
| 87  | OHX  | m0    | 302  | 7/7   | 0.22 | -0.25 | 100,100,100,100             | 0     |
| 87  | OHX  | 1     | 4107 | 7/7   | 0.16 | -0.26 | 119,119,119,119             | 0     |
| 87  | OHX  | 5     | 3974 | 7/7   | 0.16 | -0.27 | 73,73,73,73                 | 0     |
| 87  | OHX  | 2     | 2116 | 7/7   | 0.16 | -0.27 | 146,146,146,146             | 0     |
| 87  | OHX  | 2     | 2052 | 7/7   | 0.15 | -0.27 | 116,116,116,116             | 0     |
| 87  | OHX  | S8    | 302  | 7/7   | 0.33 | -0.29 | 147,147,147,147             | 0     |
| 87  | OHX  | 1     | 4170 | 7/7   | 0.30 | -0.30 | 198,198,198,198             | 0     |
| 87  | OHX  | 4     | 227  | 7/7   | 0.12 | -0.30 | 125,125,125,125             | 0     |
| 87  | OHX  | 1     | 3972 | 7/7   | 0.15 | -0.31 | 98,98,98,98                 | 0     |
| 87  | OHX  | 1     | 3981 | 7/7   | 0.13 | -0.32 | 88,88,88,88                 | 0     |
| 86  | MG   | 5     | 3419 | 1/1   | 0.17 | -0.32 | 26,26,26,26                 | 0     |
| 86  | MG   | 1     | 4225 | 1/1   | 0.17 | -0.32 | 19,19,19,19                 | 0     |
| 87  | OHX  | 2     | 2093 | 7/7   | 0.17 | -0.32 | 138,138,138,138             | 0     |
| 87  | OHX  | Q2    | 503  | 7/7   | 0.16 | -0.32 | 65,65,65,65                 | 0     |
| 87  | OHX  | 6     | 2067 | 7/7   | 0.13 | -0.33 | 77,77,77,77                 | 0     |
| 87  | OHX  | 2     | 2031 | 7/7   | 0.13 | -0.34 | 102,102,102,102             | 0     |
| 87  | OHX  | 8     | 219  | 7/7   | 0.13 | -0.34 | 112,112,112,112             | 0     |
| 86  | MG   | 1     | 3839 | 1/1   | 0.16 | -0.36 | 30,30,30,30                 | 0     |
| 86  | MG   | 2     | 2019 | 1/1   | 0.15 | -0.37 | 71,71,71,71                 | 0     |
| 86  | MG   | 5     | 3429 | 1/1   | 0.17 | -0.37 | 22,22,22,22                 | 0     |
| 86  | MG   | M0    | 302  | 1/1   | 0.25 | -0.37 | 40,40,40,40                 | 0     |
| 86  | MG   | 6     | 2036 | 1/1   | 0.17 | -0.37 | 41,41,41,41                 | 0     |
| 87  | OHX  | N9    | 101  | 7/7   | 0.15 | -0.38 | 52,52,52,52                 | 0     |
| 87  | OHX  | 6     | 2149 | 7/7   | 0.17 | -0.39 | 115,115,115,115             | 0     |
| 87  | OHX  | 1     | 3926 | 7/7   | 0.13 | -0.42 | 100,100,100,100             | 0     |
| 87  | OHX  | 2     | 2142 | 7/7   | 0.31 | -0.42 | 152,152,152,152             | 0     |
| 87  | OHX  | 5     | 3987 | 7/7   | 0.14 | -0.42 | 75,75,75,75                 | 0     |
| 86  | MG   | 1     | 3541 | 1/1   | 0.15 | -0.42 | 48,48,48,48                 | 0     |
| 87  | OHX  | 4     | 222  | 7/7   | 0.15 | -0.42 | 79,79,79,79                 | 0     |
| 87  | OHX  | 1     | 4063 | 7/7   | 0.22 | -0.43 | 160,160,160,160             | 0     |
| 87  | OHX  | 1     | 4057 | 7/7   | 0.13 | -0.43 | 124,124,124,124             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 1     | 3813 | 1/1   | 0.15 | -0.43 | 25,25,25,25                 | 0     |
| 87  | OHX  | 6     | 2089 | 7/7   | 0.16 | -0.45 | 94,94,94,94                 | 0     |
| 87  | OHX  | 5     | 4037 | 7/7   | 0.14 | -0.45 | 114,114,114,114             | 0     |
| 87  | OHX  | 6     | 2146 | 7/7   | 0.16 | -0.45 | 119,119,119,119             | 0     |
| 87  | OHX  | m9    | 201  | 7/7   | 0.16 | -0.45 | 86,86,86,86                 | 0     |
| 87  | OHX  | 1     | 4060 | 7/7   | 0.16 | -0.46 | 131,131,131,131             | 0     |
| 87  | OHX  | 8     | 225  | 7/7   | 0.21 | -0.46 | 102,102,102,102             | 0     |
| 86  | MG   | 5     | 3643 | 1/1   | 0.17 | -0.47 | 54,54,54,54                 | 0     |
| 86  | MG   | 6     | 1997 | 1/1   | 0.17 | -0.47 | 62,62,62,62                 | 0     |
| 87  | OHX  | 5     | 3900 | 7/7   | 0.15 | -0.47 | 38,38,38,38                 | 0     |
| 87  | OHX  | 1     | 3870 | 7/7   | 0.16 | -0.47 | 34,34,34,34                 | 0     |
| 86  | MG   | 1     | 4222 | 1/1   | 0.14 | -0.48 | 34,34,34,34                 | 0     |
| 86  | MG   | 1     | 4224 | 1/1   | 0.13 | -0.48 | 52,52,52,52                 | 0     |
| 87  | OHX  | 7     | 224  | 7/7   | 0.12 | -0.48 | 113,113,113,113             | 0     |
| 86  | MG   | 1     | 3416 | 1/1   | 0.17 | -0.49 | 23,23,23,23                 | 0     |
| 87  | OHX  | 5     | 4014 | 7/7   | 0.16 | -0.49 | 75,75,75,75                 | 0     |
| 87  | OHX  | 5     | 3928 | 7/7   | 0.15 | -0.50 | 58,58,58,58                 | 0     |
| 87  | OHX  | c5    | 201  | 7/7   | 0.18 | -0.50 | 146,146,146,146             | 0     |
| 86  | MG   | 5     | 3697 | 1/1   | 0.11 | -0.51 | 29,29,29,29                 | 0     |
| 86  | MG   | 5     | 3601 | 1/1   | 0.14 | -0.51 | 29,29,29,29                 | 0     |
| 86  | MG   | 5     | 3451 | 1/1   | 0.16 | -0.53 | 26,26,26,26                 | 0     |
| 87  | OHX  | 5     | 4106 | 7/7   | 0.16 | -0.53 | 108,108,108,108             | 0     |
| 87  | OHX  | 5     | 4061 | 7/7   | 0.16 | -0.53 | 127,127,127,127             | 0     |
| 86  | MG   | 1     | 3415 | 1/1   | 0.13 | -0.54 | 39,39,39,39                 | 0     |
| 86  | MG   | 1     | 4226 | 1/1   | 0.16 | -0.55 | 54,54,54,54                 | 0     |
| 87  | OHX  | D3    | 202  | 7/7   | 0.18 | -0.55 | 121,121,121,121             | 0     |
| 86  | MG   | 5     | 3755 | 1/1   | 0.15 | -0.56 | 37,37,37,37                 | 0     |
| 87  | OHX  | 6     | 2053 | 7/7   | 0.13 | -0.56 | 58,58,58,58                 | 0     |
| 87  | OHX  | 5     | 3901 | 7/7   | 0.16 | -0.57 | 35,35,35,35                 | 0     |
| 87  | OHX  | 1     | 4156 | 7/7   | 0.17 | -0.57 | 112,112,112,112             | 0     |
| 86  | MG   | n8    | 203  | 1/1   | 0.17 | -0.57 | 36,36,36,36                 | 0     |
| 87  | OHX  | 5     | 4000 | 7/7   | 0.13 | -0.58 | 90,90,90,90                 | 0     |
| 86  | MG   | 1     | 3425 | 1/1   | 0.16 | -0.60 | 20,20,20,20                 | 0     |
| 87  | OHX  | 5     | 3966 | 7/7   | 0.13 | -0.60 | 84,84,84,84                 | 0     |
| 87  | OHX  | 1     | 4045 | 7/7   | 0.13 | -0.61 | 109,109,109,109             | 0     |
| 86  | MG   | 5     | 3615 | 1/1   | 0.14 | -0.62 | 39,39,39,39                 | 0     |
| 87  | OHX  | 5     | 4196 | 7/7   | 0.25 | -0.63 | 159,159,159,159             | 0     |
| 87  | OHX  | 5     | 4079 | 7/7   | 0.15 | -0.63 | 81,81,81,81                 | 0     |
| 87  | OHX  | 6     | 2108 | 7/7   | 0.16 | -0.66 | 100,100,100,100             | 0     |
| 87  | OHX  | 5     | 3941 | 7/7   | 0.12 | -0.66 | 67,67,67,67                 | 0     |
| 86  | MG   | D4    | 201  | 1/1   | 0.17 | -0.67 | 69,69,69,69                 | 0     |
| 87  | OHX  | 1     | 3880 | 7/7   | 0.15 | -0.67 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 87  | OHX  | 5     | 3904 | 7/7   | 0.16 | -0.67 | 42,42,42,42                 | 0     |
| 87  | OHX  | 5     | 3975 | 7/7   | 0.09 | -0.69 | 86,86,86,86                 | 0     |
| 87  | OHX  | 5     | 4059 | 7/7   | 0.15 | -0.69 | 120,120,120,120             | 0     |
| 87  | OHX  | 6     | 2134 | 7/7   | 0.15 | -0.71 | 128,128,128,128             | 0     |
| 87  | OHX  | 13    | 403  | 7/7   | 0.15 | -0.71 | 81,81,81,81                 | 0     |
| 87  | OHX  | 1     | 3873 | 7/7   | 0.13 | -0.71 | 43,43,43,43                 | 0     |
| 87  | OHX  | 1     | 3902 | 7/7   | 0.13 | -0.72 | 66,66,66,66                 | 0     |
| 87  | OHX  | 1     | 4064 | 7/7   | 0.14 | -0.72 | 108,108,108,108             | 0     |
| 87  | OHX  | 2     | 2055 | 7/7   | 0.16 | -0.73 | 122,122,122,122             | 0     |
| 87  | OHX  | 2     | 2065 | 7/7   | 0.12 | -0.75 | 121,121,121,121             | 0     |
| 87  | OHX  | 1     | 3945 | 7/7   | 0.11 | -0.75 | 93,93,93,93                 | 0     |
| 87  | OHX  | 1     | 3953 | 7/7   | 0.14 | -0.75 | 75,75,75,75                 | 0     |
| 87  | OHX  | 1     | 4037 | 7/7   | 0.15 | -0.75 | 78,78,78,78                 | 0     |
| 87  | OHX  | 2     | 2050 | 7/7   | 0.15 | -0.75 | 100,100,100,100             | 0     |
| 87  | OHX  | 6     | 2071 | 7/7   | 0.13 | -0.76 | 81,81,81,81                 | 0     |
| 87  | OHX  | 5     | 3952 | 7/7   | 0.13 | -0.76 | 94,94,94,94                 | 0     |
| 87  | OHX  | 1     | 3901 | 7/7   | 0.16 | -0.77 | 63,63,63,63                 | 0     |
| 87  | OHX  | 1     | 3878 | 7/7   | 0.14 | -0.78 | 48,48,48,48                 | 0     |
| 87  | OHX  | 7     | 223  | 7/7   | 0.12 | -0.78 | 87,87,87,87                 | 0     |
| 87  | OHX  | 1     | 3964 | 7/7   | 0.17 | -0.79 | 58,58,58,58                 | 0     |
| 87  | OHX  | 5     | 4182 | 7/7   | 0.19 | -0.79 | 140,140,140,140             | 0     |
| 87  | OHX  | 5     | 4031 | 7/7   | 0.14 | -0.81 | 92,92,92,92                 | 0     |
| 87  | OHX  | 1     | 4030 | 7/7   | 0.17 | -0.82 | 93,93,93,93                 | 0     |
| 87  | OHX  | 1     | 4065 | 7/7   | 0.14 | -0.82 | 136,136,136,136             | 0     |
| 86  | MG   | 5     | 3823 | 1/1   | 0.14 | -0.83 | 86,86,86,86                 | 0     |
| 87  | OHX  | 5     | 3905 | 7/7   | 0.15 | -0.83 | 46,46,46,46                 | 0     |
| 87  | OHX  | 6     | 2123 | 7/7   | 0.14 | -0.83 | 97,97,97,97                 | 0     |
| 87  | OHX  | 1     | 3971 | 7/7   | 0.14 | -0.84 | 84,84,84,84                 | 0     |
| 86  | MG   | 1     | 3736 | 1/1   | 0.16 | -0.84 | 53,53,53,53                 | 0     |
| 87  | OHX  | 7     | 217  | 7/7   | 0.13 | -0.84 | 75,75,75,75                 | 0     |
| 86  | MG   | 6     | 1983 | 1/1   | 0.16 | -0.84 | 36,36,36,36                 | 0     |
| 87  | OHX  | 2     | 2139 | 7/7   | 0.17 | -0.84 | 155,155,155,155             | 0     |
| 86  | MG   | 1     | 3646 | 1/1   | 0.15 | -0.85 | 33,33,33,33                 | 0     |
| 86  | MG   | D3    | 201  | 1/1   | 0.18 | -0.85 | 49,49,49,49                 | 0     |
| 86  | MG   | 2     | 1985 | 1/1   | 0.15 | -0.86 | 57,57,57,57                 | 0     |
| 86  | MG   | M9    | 201  | 1/1   | 0.19 | -0.86 | 59,59,59,59                 | 0     |
| 87  | OHX  | 5     | 4105 | 7/7   | 0.14 | -0.86 | 133,133,133,133             | 0     |
| 87  | OHX  | 5     | 3984 | 7/7   | 0.14 | -0.87 | 78,78,78,78                 | 0     |
| 87  | OHX  | 1     | 3998 | 7/7   | 0.13 | -0.88 | 120,120,120,120             | 0     |
| 87  | OHX  | 3     | 220  | 7/7   | 0.13 | -0.88 | 107,107,107,107             | 0     |
| 87  | OHX  | 2     | 2028 | 7/7   | 0.14 | -0.88 | 87,87,87,87                 | 0     |
| 86  | MG   | 5     | 3415 | 1/1   | 0.12 | -0.89 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | sM    | 301  | 1/1   | 0.13 | -0.89 | 33,33,33,33                 | 0     |
| 86  | MG   | 1     | 3724 | 1/1   | 0.14 | -0.90 | 49,49,49,49                 | 0     |
| 87  | OHX  | c8    | 201  | 7/7   | 0.12 | -0.91 | 131,131,131,131             | 0     |
| 87  | OHX  | 5     | 3976 | 7/7   | 0.15 | -0.91 | 78,78,78,78                 | 0     |
| 88  | ZN   | Q3    | 501  | 1/1   | 0.09 | -0.91 | 48,48,48,48                 | 0     |
| 87  | OHX  | 5     | 4039 | 7/7   | 0.08 | -0.92 | 114,114,114,114             | 0     |
| 88  | ZN   | d9    | 101  | 1/1   | 0.12 | -0.93 | 69,69,69,69                 | 0     |
| 87  | OHX  | 1     | 3893 | 7/7   | 0.13 | -0.93 | 66,66,66,66                 | 0     |
| 87  | OHX  | 1     | 3988 | 7/7   | 0.10 | -0.93 | 100,100,100,100             | 0     |
| 86  | MG   | Q2    | 502  | 1/1   | 0.12 | -0.94 | 51,51,51,51                 | 0     |
| 87  | OHX  | 1     | 3941 | 7/7   | 0.13 | -0.94 | 86,86,86,86                 | 0     |
| 87  | OHX  | 2     | 2112 | 7/7   | 0.15 | -0.95 | 148,148,148,148             | 0     |
| 87  | OHX  | 5     | 3915 | 7/7   | 0.14 | -0.95 | 53,53,53,53                 | 0     |
| 87  | OHX  | 1     | 4110 | 7/7   | 0.14 | -0.96 | 125,125,125,125             | 0     |
| 87  | OHX  | 5     | 4032 | 7/7   | 0.14 | -0.96 | 120,120,120,120             | 0     |
| 86  | MG   | L5    | 302  | 1/1   | 0.20 | -0.96 | 57,57,57,57                 | 0     |
| 87  | OHX  | 1     | 3993 | 7/7   | 0.13 | -0.96 | 92,92,92,92                 | 0     |
| 86  | MG   | 4     | 234  | 1/1   | 0.14 | -0.97 | 41,41,41,41                 | 0     |
| 86  | MG   | 1     | 3446 | 1/1   | 0.12 | -0.97 | 35,35,35,35                 | 0     |
| 87  | OHX  | 1     | 4056 | 7/7   | 0.14 | -1.00 | 119,119,119,119             | 0     |
| 86  | MG   | 3     | 211  | 1/1   | 0.12 | -1.00 | 65,65,65,65                 | 0     |
| 87  | OHX  | 2     | 2041 | 7/7   | 0.11 | -1.01 | 97,97,97,97                 | 0     |
| 87  | OHX  | 2     | 2051 | 7/7   | 0.11 | -1.03 | 119,119,119,119             | 0     |
| 88  | ZN   | Q0    | 500  | 1/1   | 0.11 | -1.03 | 39,39,39,39                 | 0     |
| 87  | OHX  | 6     | 2205 | 7/7   | 0.18 | -1.04 | 187,187,187,187             | 0     |
| 88  | ZN   | q0    | 201  | 1/1   | 0.12 | -1.05 | 21,21,21,21                 | 0     |
| 87  | OHX  | 5     | 4017 | 7/7   | 0.14 | -1.06 | 137,137,137,137             | 0     |
| 87  | OHX  | 1     | 3929 | 7/7   | 0.09 | -1.08 | 69,69,69,69                 | 0     |
| 87  | OHX  | 6     | 2115 | 7/7   | 0.18 | -1.10 | 100,100,100,100             | 0     |
| 86  | MG   | 5     | 3484 | 1/1   | 0.13 | -1.10 | 60,60,60,60                 | 0     |
| 87  | OHX  | 5     | 3983 | 7/7   | 0.14 | -1.10 | 68,68,68,68                 | 0     |
| 87  | OHX  | 2     | 2066 | 7/7   | 0.14 | -1.11 | 145,145,145,145             | 0     |
| 86  | MG   | 5     | 3678 | 1/1   | 0.13 | -1.13 | 27,27,27,27                 | 0     |
| 87  | OHX  | 8     | 217  | 7/7   | 0.06 | -1.13 | 92,92,92,92                 | 0     |
| 87  | OHX  | o3    | 203  | 7/7   | 0.14 | -1.13 | 85,85,85,85                 | 0     |
| 86  | MG   | 6     | 2029 | 1/1   | 0.09 | -1.13 | 77,77,77,77                 | 0     |
| 86  | MG   | sM    | 302  | 1/1   | 0.14 | -1.14 | 33,33,33,33                 | 0     |
| 87  | OHX  | O7    | 103  | 7/7   | 0.08 | -1.16 | 78,78,78,78                 | 0     |
| 86  | MG   | 5     | 3751 | 1/1   | 0.15 | -1.16 | 32,32,32,32                 | 0     |
| 87  | OHX  | 1     | 3962 | 7/7   | 0.10 | -1.17 | 84,84,84,84                 | 0     |
| 87  | OHX  | 5     | 3908 | 7/7   | 0.14 | -1.17 | 50,50,50,50                 | 0     |
| 86  | MG   | 1     | 3742 | 1/1   | 0.12 | -1.18 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 2     | 2181 | 1/1   | 0.12 | -1.18 | 96,96,96,96                 | 0     |
| 86  | MG   | 5     | 3407 | 1/1   | 0.11 | -1.18 | 30,30,30,30                 | 0     |
| 88  | ZN   | Q2    | 501  | 1/1   | 0.14 | -1.19 | 67,67,67,67                 | 0     |
| 87  | OHX  | C8    | 201  | 7/7   | 0.09 | -1.19 | 108,108,108,108             | 0     |
| 87  | OHX  | 2     | 2046 | 7/7   | 0.10 | -1.19 | 98,98,98,98                 | 0     |
| 87  | OHX  | 1     | 3946 | 7/7   | 0.10 | -1.20 | 87,87,87,87                 | 0     |
| 88  | ZN   | e1    | 501  | 1/1   | 0.19 | -1.21 | 174,174,174,174             | 0     |
| 86  | MG   | 1     | 3786 | 1/1   | 0.13 | -1.22 | 56,56,56,56                 | 0     |
| 86  | MG   | 1     | 3443 | 1/1   | 0.12 | -1.23 | 73,73,73,73                 | 0     |
| 86  | MG   | N3    | 203  | 1/1   | 0.12 | -1.23 | 44,44,44,44                 | 0     |
| 87  | OHX  | 1     | 4027 | 7/7   | 0.15 | -1.24 | 94,94,94,94                 | 0     |
| 86  | MG   | l5    | 302  | 1/1   | 0.09 | -1.24 | 53,53,53,53                 | 0     |
| 86  | MG   | 5     | 3851 | 1/1   | 0.15 | -1.25 | 39,39,39,39                 | 0     |
| 87  | OHX  | 5     | 4131 | 7/7   | 0.12 | -1.26 | 124,124,124,124             | 0     |
| 86  | MG   | 5     | 3892 | 1/1   | 0.12 | -1.27 | 52,52,52,52                 | 0     |
| 87  | OHX  | 2     | 2045 | 7/7   | 0.07 | -1.27 | 114,114,114,114             | 0     |
| 86  | MG   | 5     | 3721 | 1/1   | 0.15 | -1.28 | 31,31,31,31                 | 0     |
| 87  | OHX  | n9    | 101  | 7/7   | 0.13 | -1.29 | 54,54,54,54                 | 0     |
| 86  | MG   | q0    | 202  | 1/1   | 0.16 | -1.29 | 37,37,37,37                 | 0     |
| 87  | OHX  | 5     | 3949 | 7/7   | 0.08 | -1.29 | 80,80,80,80                 | 0     |
| 86  | MG   | M6    | 201  | 1/1   | 0.11 | -1.30 | 42,42,42,42                 | 0     |
| 87  | OHX  | 5     | 3999 | 7/7   | 0.11 | -1.31 | 88,88,88,88                 | 0     |
| 87  | OHX  | 2     | 2075 | 7/7   | 0.12 | -1.31 | 103,103,103,103             | 0     |
| 86  | MG   | q1    | 101  | 1/1   | 0.12 | -1.35 | 32,32,32,32                 | 0     |
| 87  | OHX  | 5     | 4133 | 7/7   | 0.16 | -1.35 | 173,173,173,173             | 0     |
| 87  | OHX  | 5     | 3995 | 7/7   | 0.12 | -1.35 | 106,106,106,106             | 0     |
| 87  | OHX  | 5     | 3934 | 7/7   | 0.11 | -1.36 | 79,79,79,79                 | 0     |
| 87  | OHX  | 6     | 2112 | 7/7   | 0.13 | -1.37 | 105,105,105,105             | 0     |
| 87  | OHX  | SR    | 401  | 7/7   | 0.14 | -1.38 | 157,157,157,157             | 0     |
| 87  | OHX  | 8     | 224  | 7/7   | 0.10 | -1.39 | 125,125,125,125             | 0     |
| 87  | OHX  | 5     | 4084 | 7/7   | 0.16 | -1.39 | 90,90,90,90                 | 0     |
| 87  | OHX  | 2     | 2038 | 7/7   | 0.13 | -1.40 | 86,86,86,86                 | 0     |
| 87  | OHX  | 5     | 3989 | 7/7   | 0.10 | -1.40 | 98,98,98,98                 | 0     |
| 87  | OHX  | 1     | 3928 | 7/7   | 0.08 | -1.40 | 82,82,82,82                 | 0     |
| 87  | OHX  | 6     | 2050 | 7/7   | 0.12 | -1.41 | 45,45,45,45                 | 0     |
| 87  | OHX  | 6     | 2105 | 7/7   | 0.12 | -1.41 | 96,96,96,96                 | 0     |
| 87  | OHX  | 1     | 3884 | 7/7   | 0.11 | -1.41 | 53,53,53,53                 | 0     |
| 87  | OHX  | m0    | 301  | 7/7   | 0.07 | -1.43 | 104,104,104,104             | 0     |
| 87  | OHX  | 2     | 2035 | 7/7   | 0.12 | -1.44 | 113,113,113,113             | 0     |
| 88  | ZN   | d6    | 500  | 1/1   | 0.12 | -1.45 | 48,48,48,48                 | 0     |
| 87  | OHX  | 1     | 3875 | 7/7   | 0.14 | -1.46 | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 3817 | 1/1   | 0.10 | -1.47 | 31,31,31,31                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 1     | 3683 | 1/1   | 0.12 | -1.47 | 57,57,57,57                 | 0     |
| 87  | OHX  | 1     | 3939 | 7/7   | 0.08 | -1.48 | 87,87,87,87                 | 0     |
| 88  | ZN   | q3    | 501  | 1/1   | 0.10 | -1.49 | 53,53,53,53                 | 0     |
| 87  | OHX  | 5     | 3902 | 7/7   | 0.12 | -1.50 | 35,35,35,35                 | 0     |
| 87  | OHX  | 5     | 4018 | 7/7   | 0.09 | -1.51 | 110,110,110,110             | 0     |
| 87  | OHX  | 6     | 2052 | 7/7   | 0.14 | -1.53 | 53,53,53,53                 | 0     |
| 88  | ZN   | D9    | 101  | 1/1   | 0.07 | -1.53 | 72,72,72,72                 | 0     |
| 87  | OHX  | 5     | 4243 | 7/7   | 0.25 | -1.54 | 224,224,224,224             | 0     |
| 87  | OHX  | 5     | 3940 | 7/7   | 0.10 | -1.54 | 73,73,73,73                 | 0     |
| 86  | MG   | 6     | 2004 | 1/1   | 0.14 | -1.55 | 66,66,66,66                 | 0     |
| 86  | MG   | N8    | 203  | 1/1   | 0.15 | -1.55 | 26,26,26,26                 | 0     |
| 86  | MG   | 5     | 3819 | 1/1   | 0.05 | -1.55 | 52,52,52,52                 | 0     |
| 87  | OHX  | 5     | 4042 | 7/7   | 0.07 | -1.57 | 144,144,144,144             | 0     |
| 86  | MG   | 5     | 3769 | 1/1   | 0.12 | -1.57 | 35,35,35,35                 | 0     |
| 87  | OHX  | 2     | 2096 | 7/7   | 0.08 | -1.57 | 139,139,139,139             | 0     |
| 88  | ZN   | O7    | 101  | 1/1   | 0.11 | -1.57 | 27,27,27,27                 | 0     |
| 87  | OHX  | 6     | 2098 | 7/7   | 0.14 | -1.57 | 115,115,115,115             | 0     |
| 87  | OHX  | 5     | 3914 | 7/7   | 0.12 | -1.58 | 50,50,50,50                 | 0     |
| 87  | OHX  | C3    | 201  | 7/7   | 0.24 | -1.59 | 145,145,145,145             | 0     |
| 87  | OHX  | 6     | 2167 | 7/7   | 0.17 | -1.59 | 190,190,190,190             | 0     |
| 87  | OHX  | 1     | 4018 | 7/7   | 0.09 | -1.61 | 116,116,116,116             | 0     |
| 87  | OHX  | 5     | 4021 | 7/7   | 0.16 | -1.62 | 79,79,79,79                 | 0     |
| 87  | OHX  | 1     | 4039 | 7/7   | 0.07 | -1.63 | 131,131,131,131             | 0     |
| 87  | OHX  | o7    | 502  | 7/7   | 0.12 | -1.63 | 86,86,86,86                 | 0     |
| 87  | OHX  | 1     | 3954 | 7/7   | 0.10 | -1.64 | 93,93,93,93                 | 0     |
| 86  | MG   | 5     | 3706 | 1/1   | 0.17 | -1.64 | 38,38,38,38                 | 0     |
| 87  | OHX  | 1     | 4070 | 7/7   | 0.09 | -1.65 | 127,127,127,127             | 0     |
| 87  | OHX  | C5    | 201  | 7/7   | 0.17 | -1.66 | 153,153,153,153             | 0     |
| 88  | ZN   | E1    | 501  | 1/1   | 0.05 | -1.66 | 111,111,111,111             | 0     |
| 87  | OHX  | 2     | 2071 | 7/7   | 0.13 | -1.66 | 130,130,130,130             | 0     |
| 86  | MG   | 1     | 3776 | 1/1   | 0.16 | -1.67 | 32,32,32,32                 | 0     |
| 87  | OHX  | 1     | 3934 | 7/7   | 0.12 | -1.67 | 85,85,85,85                 | 0     |
| 87  | OHX  | 5     | 3981 | 7/7   | 0.12 | -1.68 | 89,89,89,89                 | 0     |
| 87  | OHX  | 5     | 4041 | 7/7   | 0.14 | -1.69 | 107,107,107,107             | 0     |
| 87  | OHX  | 3     | 218  | 7/7   | 0.14 | -1.69 | 80,80,80,80                 | 0     |
| 87  | OHX  | 2     | 2092 | 7/7   | 0.08 | -1.69 | 140,140,140,140             | 0     |
| 87  | OHX  | 1     | 3969 | 7/7   | 0.14 | -1.69 | 82,82,82,82                 | 0     |
| 87  | OHX  | 5     | 3957 | 7/7   | 0.10 | -1.70 | 75,75,75,75                 | 0     |
| 88  | ZN   | D6    | 500  | 1/1   | 0.08 | -1.70 | 72,72,72,72                 | 0     |
| 86  | MG   | 5     | 3701 | 1/1   | 0.15 | -1.70 | 48,48,48,48                 | 0     |
| 86  | MG   | 5     | 3473 | 1/1   | 0.10 | -1.70 | 52,52,52,52                 | 0     |
| 87  | OHX  | 5     | 3986 | 7/7   | 0.12 | -1.71 | 67,67,67,67                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 87  | OHX  | 2     | 2080 | 7/7   | 0.10 | -1.72 | 131,131,131,131             | 0     |
| 86  | MG   | 1     | 3759 | 1/1   | 0.12 | -1.72 | 39,39,39,39                 | 0     |
| 86  | MG   | 1     | 3770 | 1/1   | 0.15 | -1.72 | 80,80,80,80                 | 0     |
| 87  | OHX  | 6     | 2055 | 7/7   | 0.13 | -1.73 | 57,57,57,57                 | 0     |
| 86  | MG   | 1     | 3426 | 1/1   | 0.12 | -1.74 | 47,47,47,47                 | 0     |
| 87  | OHX  | 1     | 3983 | 7/7   | 0.14 | -1.74 | 70,70,70,70                 | 0     |
| 86  | MG   | 5     | 3600 | 1/1   | 0.07 | -1.75 | 31,31,31,31                 | 0     |
| 87  | OHX  | 2     | 2102 | 7/7   | 0.14 | -1.76 | 186,186,186,186             | 0     |
| 87  | OHX  | 2     | 2044 | 7/7   | 0.09 | -1.76 | 99,99,99,99                 | 0     |
| 87  | OHX  | 1     | 4025 | 7/7   | 0.16 | -1.77 | 94,94,94,94                 | 0     |
| 87  | OHX  | 2     | 2026 | 7/7   | 0.13 | -1.79 | 83,83,83,83                 | 0     |
| 87  | OHX  | 5     | 4056 | 7/7   | 0.09 | -1.79 | 79,79,79,79                 | 0     |
| 87  | OHX  | 1     | 3892 | 7/7   | 0.14 | -1.80 | 53,53,53,53                 | 0     |
| 87  | OHX  | 1     | 3930 | 7/7   | 0.09 | -1.81 | 73,73,73,73                 | 0     |
| 87  | OHX  | 8     | 220  | 7/7   | 0.13 | -1.82 | 103,103,103,103             | 0     |
| 87  | OHX  | 1     | 3879 | 7/7   | 0.12 | -1.82 | 48,48,48,48                 | 0     |
| 87  | OHX  | 7     | 221  | 7/7   | 0.14 | -1.82 | 76,76,76,76                 | 0     |
| 87  | OHX  | 2     | 2108 | 7/7   | 0.10 | -1.83 | 114,114,114,114             | 0     |
| 87  | OHX  | 2     | 2037 | 7/7   | 0.09 | -1.84 | 82,82,82,82                 | 0     |
| 87  | OHX  | 2     | 2032 | 7/7   | 0.14 | -1.84 | 88,88,88,88                 | 0     |
| 86  | MG   | 1     | 3738 | 1/1   | 0.14 | -1.84 | 27,27,27,27                 | 0     |
| 87  | OHX  | 4     | 223  | 7/7   | 0.12 | -1.84 | 96,96,96,96                 | 0     |
| 86  | MG   | 1     | 3630 | 1/1   | 0.15 | -1.84 | 53,53,53,53                 | 0     |
| 86  | MG   | 5     | 3686 | 1/1   | 0.16 | -1.86 | 53,53,53,53                 | 0     |
| 86  | MG   | 1     | 4219 | 1/1   | 0.14 | -1.87 | 23,23,23,23                 | 0     |
| 87  | OHX  | n3    | 203  | 7/7   | 0.08 | -1.90 | 75,75,75,75                 | 0     |
| 86  | MG   | 6     | 1998 | 1/1   | 0.13 | -1.90 | 44,44,44,44                 | 0     |
| 87  | OHX  | 1     | 3872 | 7/7   | 0.10 | -1.91 | 39,39,39,39                 | 0     |
| 86  | MG   | 5     | 3731 | 1/1   | 0.11 | -1.93 | 45,45,45,45                 | 0     |
| 87  | OHX  | 6     | 2070 | 7/7   | 0.10 | -1.95 | 75,75,75,75                 | 0     |
| 87  | OHX  | 5     | 4025 | 7/7   | 0.07 | -1.97 | 104,104,104,104             | 0     |
| 87  | OHX  | 5     | 4006 | 7/7   | 0.15 | -1.99 | 96,96,96,96                 | 0     |
| 87  | OHX  | O7    | 104  | 7/7   | 0.12 | -2.00 | 82,82,82,82                 | 0     |
| 87  | OHX  | 2     | 2021 | 7/7   | 0.11 | -2.01 | 63,63,63,63                 | 0     |
| 87  | OHX  | 1     | 4160 | 7/7   | 0.13 | -2.01 | 82,82,82,82                 | 0     |
| 87  | OHX  | 1     | 3891 | 7/7   | 0.11 | -2.03 | 57,57,57,57                 | 0     |
| 87  | OHX  | 5     | 3967 | 7/7   | 0.10 | -2.04 | 83,83,83,83                 | 0     |
| 86  | MG   | 5     | 3821 | 1/1   | 0.11 | -2.04 | 48,48,48,48                 | 0     |
| 87  | OHX  | 6     | 2107 | 7/7   | 0.11 | -2.05 | 102,102,102,102             | 0     |
| 86  | MG   | 5     | 3737 | 1/1   | 0.11 | -2.05 | 43,43,43,43                 | 0     |
| 87  | OHX  | 6     | 2125 | 7/7   | 0.11 | -2.06 | 119,119,119,119             | 0     |
| 87  | OHX  | 5     | 3944 | 7/7   | 0.12 | -2.07 | 67,67,67,67                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 87  | OHX  | 5     | 3992 | 7/7   | 0.12 | -2.07 | 76,76,76,76                 | 0     |
| 87  | OHX  | 5     | 3956 | 7/7   | 0.14 | -2.09 | 77,77,77,77                 | 0     |
| 87  | OHX  | 1     | 3888 | 7/7   | 0.14 | -2.09 | 55,55,55,55                 | 0     |
| 86  | MG   | 5     | 3824 | 1/1   | 0.11 | -2.09 | 55,55,55,55                 | 0     |
| 87  | OHX  | 6     | 2057 | 7/7   | 0.13 | -2.10 | 67,67,67,67                 | 0     |
| 87  | OHX  | 6     | 2062 | 7/7   | 0.13 | -2.10 | 81,81,81,81                 | 0     |
| 87  | OHX  | 2     | 2085 | 7/7   | 0.13 | -2.10 | 110,110,110,110             | 0     |
| 87  | OHX  | 1     | 3938 | 7/7   | 0.10 | -2.11 | 85,85,85,85                 | 0     |
| 87  | OHX  | 6     | 2117 | 7/7   | 0.14 | -2.12 | 104,104,104,104             | 0     |
| 87  | OHX  | 5     | 4103 | 7/7   | 0.13 | -2.13 | 123,123,123,123             | 0     |
| 86  | MG   | 1     | 3663 | 1/1   | 0.14 | -2.14 | 25,25,25,25                 | 0     |
| 87  | OHX  | 6     | 2080 | 7/7   | 0.11 | -2.15 | 95,95,95,95                 | 0     |
| 87  | OHX  | 5     | 3978 | 7/7   | 0.12 | -2.15 | 83,83,83,83                 | 0     |
| 87  | OHX  | 1     | 3881 | 7/7   | 0.14 | -2.15 | 54,54,54,54                 | 0     |
| 86  | MG   | 1     | 3558 | 1/1   | 0.09 | -2.16 | 41,41,41,41                 | 0     |
| 87  | OHX  | 1     | 3935 | 7/7   | 0.08 | -2.16 | 87,87,87,87                 | 0     |
| 87  | OHX  | 5     | 3917 | 7/7   | 0.11 | -2.17 | 55,55,55,55                 | 0     |
| 87  | OHX  | 2     | 2095 | 7/7   | 0.08 | -2.18 | 153,153,153,153             | 0     |
| 87  | OHX  | 5     | 3959 | 7/7   | 0.11 | -2.19 | 73,73,73,73                 | 0     |
| 86  | MG   | 5     | 3684 | 1/1   | 0.15 | -2.20 | 20,20,20,20                 | 0     |
| 86  | MG   | 5     | 3772 | 1/1   | 0.11 | -2.21 | 58,58,58,58                 | 0     |
| 87  | OHX  | 1     | 3958 | 7/7   | 0.13 | -2.22 | 89,89,89,89                 | 0     |
| 86  | MG   | 5     | 3666 | 1/1   | 0.14 | -2.22 | 43,43,43,43                 | 0     |
| 87  | OHX  | 1     | 3985 | 7/7   | 0.10 | -2.24 | 88,88,88,88                 | 0     |
| 87  | OHX  | 7     | 218  | 7/7   | 0.12 | -2.24 | 73,73,73,73                 | 0     |
| 86  | MG   | 1     | 3743 | 1/1   | 0.10 | -2.25 | 27,27,27,27                 | 0     |
| 87  | OHX  | 6     | 2086 | 7/7   | 0.10 | -2.25 | 99,99,99,99                 | 0     |
| 87  | OHX  | 1     | 3974 | 7/7   | 0.07 | -2.28 | 108,108,108,108             | 0     |
| 86  | MG   | 5     | 3713 | 1/1   | 0.08 | -2.29 | 54,54,54,54                 | 0     |
| 87  | OHX  | 6     | 2148 | 7/7   | 0.12 | -2.29 | 110,110,110,110             | 0     |
| 87  | OHX  | 5     | 3935 | 7/7   | 0.09 | -2.30 | 59,59,59,59                 | 0     |
| 87  | OHX  | 6     | 2088 | 7/7   | 0.08 | -2.30 | 108,108,108,108             | 0     |
| 86  | MG   | 6     | 1915 | 1/1   | 0.13 | -2.32 | 61,61,61,61                 | 0     |
| 87  | OHX  | 1     | 4129 | 7/7   | 0.15 | -2.33 | 126,126,126,126             | 0     |
| 87  | OHX  | 1     | 4090 | 7/7   | 0.12 | -2.33 | 178,178,178,178             | 0     |
| 87  | OHX  | 2     | 2069 | 7/7   | 0.11 | -2.34 | 109,109,109,109             | 0     |
| 87  | OHX  | 1     | 3871 | 7/7   | 0.13 | -2.35 | 40,40,40,40                 | 0     |
| 86  | MG   | 1     | 3730 | 1/1   | 0.15 | -2.38 | 63,63,63,63                 | 0     |
| 87  | OHX  | 6     | 2102 | 7/7   | 0.09 | -2.39 | 145,145,145,145             | 0     |
| 87  | OHX  | 6     | 2077 | 7/7   | 0.09 | -2.39 | 118,118,118,118             | 0     |
| 87  | OHX  | 6     | 2084 | 7/7   | 0.14 | -2.39 | 84,84,84,84                 | 0     |
| 87  | OHX  | 6     | 2069 | 7/7   | 0.10 | -2.40 | 104,104,104,104             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 87  | OHX  | 1     | 3896 | 7/7   | 0.09 | -2.42 | 59,59,59,59                 | 0     |
| 87  | OHX  | 1     | 4183 | 7/7   | 0.22 | -2.43 | 230,230,230,230             | 0     |
| 88  | ZN   | o7    | 501  | 1/1   | 0.09 | -2.43 | 35,35,35,35                 | 0     |
| 87  | OHX  | 2     | 2024 | 7/7   | 0.11 | -2.44 | 73,73,73,73                 | 0     |
| 86  | MG   | 5     | 4260 | 1/1   | 0.14 | -2.45 | 26,26,26,26                 | 0     |
| 86  | MG   | 1     | 3830 | 1/1   | 0.09 | -2.47 | 51,51,51,51                 | 0     |
| 87  | OHX  | 6     | 2091 | 7/7   | 0.11 | -2.48 | 105,105,105,105             | 0     |
| 87  | OHX  | 5     | 3906 | 7/7   | 0.13 | -2.50 | 44,44,44,44                 | 0     |
| 87  | OHX  | 6     | 2103 | 7/7   | 0.10 | -2.50 | 160,160,160,160             | 0     |
| 87  | OHX  | 1     | 4017 | 7/7   | 0.13 | -2.51 | 115,115,115,115             | 0     |
| 87  | OHX  | 5     | 3996 | 7/7   | 0.13 | -2.52 | 88,88,88,88                 | 0     |
| 86  | MG   | 2     | 1963 | 1/1   | 0.14 | -2.52 | 141,141,141,141             | 0     |
| 87  | OHX  | 8     | 215  | 7/7   | 0.12 | -2.52 | 44,44,44,44                 | 0     |
| 87  | OHX  | 6     | 2100 | 7/7   | 0.09 | -2.53 | 141,141,141,141             | 0     |
| 87  | OHX  | 1     | 3932 | 7/7   | 0.07 | -2.55 | 97,97,97,97                 | 0     |
| 87  | OHX  | 5     | 4051 | 7/7   | 0.08 | -2.55 | 113,113,113,113             | 0     |
| 87  | OHX  | 6     | 2059 | 7/7   | 0.12 | -2.55 | 59,59,59,59                 | 0     |
| 87  | OHX  | 1     | 3952 | 7/7   | 0.09 | -2.57 | 84,84,84,84                 | 0     |
| 87  | OHX  | 1     | 3905 | 7/7   | 0.09 | -2.57 | 70,70,70,70                 | 0     |
| 87  | OHX  | 5     | 4009 | 7/7   | 0.12 | -2.58 | 73,73,73,73                 | 0     |
| 87  | OHX  | 6     | 2085 | 7/7   | 0.07 | -2.59 | 83,83,83,83                 | 0     |
| 86  | MG   | 1     | 3677 | 1/1   | 0.08 | -2.60 | 65,65,65,65                 | 0     |
| 86  | MG   | 5     | 3734 | 1/1   | 0.11 | -2.61 | 33,33,33,33                 | 0     |
| 87  | OHX  | 5     | 4004 | 7/7   | 0.10 | -2.62 | 91,91,91,91                 | 0     |
| 87  | OHX  | 2     | 2030 | 7/7   | 0.07 | -2.63 | 92,92,92,92                 | 0     |
| 86  | MG   | 5     | 3841 | 1/1   | 0.09 | -2.63 | 56,56,56,56                 | 0     |
| 86  | MG   | 1     | 3642 | 1/1   | 0.12 | -2.63 | 51,51,51,51                 | 0     |
| 86  | MG   | 5     | 3811 | 1/1   | 0.15 | -2.65 | 61,61,61,61                 | 0     |
| 87  | OHX  | 1     | 4008 | 7/7   | 0.10 | -2.65 | 102,102,102,102             | 0     |
| 86  | MG   | 5     | 3862 | 1/1   | 0.12 | -2.65 | 31,31,31,31                 | 0     |
| 87  | OHX  | 5     | 3938 | 7/7   | 0.06 | -2.67 | 54,54,54,54                 | 0     |
| 87  | OHX  | 1     | 4003 | 7/7   | 0.09 | -2.67 | 129,129,129,129             | 0     |
| 87  | OHX  | s1    | 302  | 7/7   | 0.10 | -2.68 | 72,72,72,72                 | 0     |
| 86  | MG   | 1     | 3754 | 1/1   | 0.11 | -2.68 | 29,29,29,29                 | 0     |
| 87  | OHX  | 1     | 3914 | 7/7   | 0.10 | -2.68 | 79,79,79,79                 | 0     |
| 87  | OHX  | 1     | 4141 | 7/7   | 0.14 | -2.68 | 90,90,90,90                 | 0     |
| 87  | OHX  | 1     | 4002 | 7/7   | 0.08 | -2.69 | 153,153,153,153             | 0     |
| 87  | OHX  | 1     | 3890 | 7/7   | 0.10 | -2.70 | 58,58,58,58                 | 0     |
| 87  | OHX  | 1     | 3951 | 7/7   | 0.11 | -2.70 | 76,76,76,76                 | 0     |
| 87  | OHX  | 1     | 3904 | 7/7   | 0.11 | -2.70 | 74,74,74,74                 | 0     |
| 87  | OHX  | 5     | 4023 | 7/7   | 0.15 | -2.71 | 92,92,92,92                 | 0     |
| 86  | MG   | 1     | 3664 | 1/1   | 0.09 | -2.71 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 1     | 3632 | 1/1   | 0.11 | -2.72 | 21,21,21,21                 | 0     |
| 87  | OHX  | 6     | 2090 | 7/7   | 0.09 | -2.74 | 91,91,91,91                 | 0     |
| 86  | MG   | 5     | 3401 | 1/1   | 0.12 | -2.77 | 54,54,54,54                 | 0     |
| 87  | OHX  | 5     | 3910 | 7/7   | 0.12 | -2.77 | 34,34,34,34                 | 0     |
| 87  | OHX  | 6     | 2081 | 7/7   | 0.10 | -2.78 | 77,77,77,77                 | 0     |
| 87  | OHX  | 2     | 2058 | 7/7   | 0.11 | -2.79 | 87,87,87,87                 | 0     |
| 86  | MG   | 5     | 3831 | 1/1   | 0.09 | -2.81 | 63,63,63,63                 | 0     |
| 87  | OHX  | 5     | 3950 | 7/7   | 0.06 | -2.82 | 83,83,83,83                 | 0     |
| 86  | MG   | 6     | 2009 | 1/1   | 0.10 | -2.83 | 46,46,46,46                 | 0     |
| 86  | MG   | 5     | 3565 | 1/1   | 0.14 | -2.84 | 17,17,17,17                 | 0     |
| 87  | OHX  | 5     | 3923 | 7/7   | 0.11 | -2.86 | 53,53,53,53                 | 0     |
| 87  | OHX  | 1     | 3924 | 7/7   | 0.07 | -2.86 | 80,80,80,80                 | 0     |
| 86  | MG   | 5     | 3679 | 1/1   | 0.09 | -2.86 | 85,85,85,85                 | 0     |
| 87  | OHX  | 2     | 2027 | 7/7   | 0.09 | -2.86 | 95,95,95,95                 | 0     |
| 87  | OHX  | 2     | 2047 | 7/7   | 0.09 | -2.87 | 107,107,107,107             | 0     |
| 87  | OHX  | 6     | 2138 | 7/7   | 0.11 | -2.88 | 116,116,116,116             | 0     |
| 87  | OHX  | 2     | 2156 | 7/7   | 0.17 | -2.88 | 283,283,283,283             | 0     |
| 86  | MG   | 5     | 3787 | 1/1   | 0.08 | -2.90 | 32,32,32,32                 | 0     |
| 87  | OHX  | 6     | 2061 | 7/7   | 0.09 | -2.90 | 77,77,77,77                 | 0     |
| 87  | OHX  | 1     | 3908 | 7/7   | 0.12 | -2.91 | 68,68,68,68                 | 0     |
| 87  | OHX  | 1     | 3942 | 7/7   | 0.10 | -2.91 | 79,79,79,79                 | 0     |
| 87  | OHX  | 1     | 3882 | 7/7   | 0.11 | -2.91 | 46,46,46,46                 | 0     |
| 87  | OHX  | M0    | 303  | 7/7   | 0.14 | -2.93 | 88,88,88,88                 | 0     |
| 86  | MG   | 5     | 3708 | 1/1   | 0.10 | -2.94 | 36,36,36,36                 | 0     |
| 87  | OHX  | 5     | 4078 | 7/7   | 0.07 | -2.95 | 152,152,152,152             | 0     |
| 87  | OHX  | 2     | 2068 | 7/7   | 0.09 | -2.97 | 111,111,111,111             | 0     |
| 87  | OHX  | 1     | 3898 | 7/7   | 0.08 | -2.99 | 60,60,60,60                 | 0     |
| 87  | OHX  | 1     | 3968 | 7/7   | 0.07 | -3.00 | 104,104,104,104             | 0     |
| 87  | OHX  | 3     | 217  | 7/7   | 0.12 | -3.00 | 89,89,89,89                 | 0     |
| 87  | OHX  | 5     | 3948 | 7/7   | 0.07 | -3.01 | 72,72,72,72                 | 0     |
| 87  | OHX  | 5     | 3988 | 7/7   | 0.08 | -3.02 | 82,82,82,82                 | 0     |
| 87  | OHX  | 2     | 2033 | 7/7   | 0.10 | -3.02 | 85,85,85,85                 | 0     |
| 87  | OHX  | 5     | 3937 | 7/7   | 0.13 | -3.04 | 60,60,60,60                 | 0     |
| 87  | OHX  | 1     | 3999 | 7/7   | 0.09 | -3.06 | 102,102,102,102             | 0     |
| 87  | OHX  | 2     | 2025 | 7/7   | 0.12 | -3.08 | 64,64,64,64                 | 0     |
| 87  | OHX  | 1     | 3877 | 7/7   | 0.11 | -3.10 | 36,36,36,36                 | 0     |
| 87  | OHX  | 6     | 2097 | 7/7   | 0.11 | -3.13 | 114,114,114,114             | 0     |
| 87  | OHX  | 6     | 2072 | 7/7   | 0.05 | -3.15 | 84,84,84,84                 | 0     |
| 87  | OHX  | 6     | 2104 | 7/7   | 0.05 | -3.15 | 153,153,153,153             | 0     |
| 87  | OHX  | 5     | 3973 | 7/7   | 0.12 | -3.16 | 67,67,67,67                 | 0     |
| 87  | OHX  | 5     | 3963 | 7/7   | 0.05 | -3.17 | 76,76,76,76                 | 0     |
| 87  | OHX  | 2     | 2076 | 7/7   | 0.14 | -3.18 | 111,111,111,111             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 87  | OHX  | 5     | 3979 | 7/7   | 0.14 | -3.20 | 67,67,67,67                 | 0     |
| 87  | OHX  | 2     | 2154 | 7/7   | 0.20 | -3.21 | 229,229,229,229             | 0     |
| 87  | OHX  | 2     | 2029 | 7/7   | 0.10 | -3.21 | 101,101,101,101             | 0     |
| 87  | OHX  | 6     | 2074 | 7/7   | 0.10 | -3.22 | 93,93,93,93                 | 0     |
| 87  | OHX  | 1     | 4022 | 7/7   | 0.07 | -3.23 | 135,135,135,135             | 0     |
| 86  | MG   | 1     | 3709 | 1/1   | 0.12 | -3.27 | 45,45,45,45                 | 0     |
| 87  | OHX  | 5     | 3958 | 7/7   | 0.06 | -3.30 | 67,67,67,67                 | 0     |
| 87  | OHX  | 2     | 2053 | 7/7   | 0.13 | -3.31 | 95,95,95,95                 | 0     |
| 87  | OHX  | 1     | 3948 | 7/7   | 0.12 | -3.32 | 78,78,78,78                 | 0     |
| 86  | MG   | 5     | 3628 | 1/1   | 0.13 | -3.34 | 41,41,41,41                 | 0     |
| 87  | OHX  | 5     | 4082 | 7/7   | 0.12 | -3.35 | 83,83,83,83                 | 0     |
| 87  | OHX  | 1     | 3976 | 7/7   | 0.10 | -3.37 | 92,92,92,92                 | 0     |
| 87  | OHX  | 1     | 3967 | 7/7   | 0.12 | -3.39 | 78,78,78,78                 | 0     |
| 87  | OHX  | 1     | 4036 | 7/7   | 0.13 | -3.40 | 108,108,108,108             | 0     |
| 87  | OHX  | 1     | 3918 | 7/7   | 0.05 | -3.42 | 69,69,69,69                 | 0     |
| 86  | MG   | 5     | 3764 | 1/1   | 0.11 | -3.43 | 25,25,25,25                 | 0     |
| 87  | OHX  | 1     | 3980 | 7/7   | 0.08 | -3.44 | 105,105,105,105             | 0     |
| 87  | OHX  | 2     | 2064 | 7/7   | 0.08 | -3.45 | 118,118,118,118             | 0     |
| 87  | OHX  | 5     | 4111 | 7/7   | 0.10 | -3.46 | 62,62,62,62                 | 0     |
| 87  | OHX  | 6     | 2092 | 7/7   | 0.06 | -3.49 | 112,112,112,112             | 0     |
| 87  | OHX  | 1     | 3944 | 7/7   | 0.10 | -3.51 | 78,78,78,78                 | 0     |
| 87  | OHX  | m6    | 202  | 7/7   | 0.10 | -3.52 | 77,77,77,77                 | 0     |
| 87  | OHX  | 1     | 4093 | 7/7   | 0.11 | -3.55 | 60,60,60,60                 | 0     |
| 87  | OHX  | 6     | 2082 | 7/7   | 0.08 | -3.57 | 88,88,88,88                 | 0     |
| 87  | OHX  | 1     | 3887 | 7/7   | 0.09 | -3.58 | 52,52,52,52                 | 0     |
| 87  | OHX  | 5     | 4029 | 7/7   | 0.11 | -3.58 | 73,73,73,73                 | 0     |
| 87  | OHX  | 1     | 3950 | 7/7   | 0.07 | -3.58 | 89,89,89,89                 | 0     |
| 87  | OHX  | 5     | 4035 | 7/7   | 0.09 | -3.59 | 88,88,88,88                 | 0     |
| 87  | OHX  | 5     | 3955 | 7/7   | 0.08 | -3.59 | 81,81,81,81                 | 0     |
| 87  | OHX  | 2     | 2034 | 7/7   | 0.04 | -3.60 | 78,78,78,78                 | 0     |
| 87  | OHX  | 1     | 3921 | 7/7   | 0.07 | -3.62 | 85,85,85,85                 | 0     |
| 87  | OHX  | 5     | 3953 | 7/7   | 0.08 | -3.62 | 85,85,85,85                 | 0     |
| 86  | MG   | 5     | 3732 | 1/1   | 0.12 | -3.63 | 35,35,35,35                 | 0     |
| 87  | OHX  | 5     | 3968 | 7/7   | 0.10 | -3.63 | 78,78,78,78                 | 0     |
| 86  | MG   | 5     | 3613 | 1/1   | 0.12 | -3.63 | 26,26,26,26                 | 0     |
| 87  | OHX  | 1     | 3987 | 7/7   | 0.10 | -3.66 | 63,63,63,63                 | 0     |
| 87  | OHX  | 1     | 3911 | 7/7   | 0.06 | -3.66 | 60,60,60,60                 | 0     |
| 87  | OHX  | 2     | 2054 | 7/7   | 0.11 | -3.66 | 115,115,115,115             | 0     |
| 87  | OHX  | 5     | 3991 | 7/7   | 0.12 | -3.69 | 83,83,83,83                 | 0     |
| 87  | OHX  | N1    | 201  | 7/7   | 0.08 | -3.69 | 53,53,53,53                 | 0     |
| 87  | OHX  | 5     | 3951 | 7/7   | 0.12 | -3.70 | 69,69,69,69                 | 0     |
| 87  | OHX  | 4     | 221  | 7/7   | 0.12 | -3.74 | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 87  | OHX  | 1     | 3955 | 7/7   | 0.07 | -3.75 | 112,112,112,112             | 0     |
| 87  | OHX  | 5     | 3924 | 7/7   | 0.12 | -3.76 | 59,59,59,59                 | 0     |
| 87  | OHX  | 5     | 3970 | 7/7   | 0.07 | -3.79 | 84,84,84,84                 | 0     |
| 86  | MG   | 5     | 3766 | 1/1   | 0.12 | -3.79 | 50,50,50,50                 | 0     |
| 87  | OHX  | 2     | 2081 | 7/7   | 0.08 | -3.81 | 119,119,119,119             | 0     |
| 87  | OHX  | 5     | 3913 | 7/7   | 0.09 | -3.81 | 44,44,44,44                 | 0     |
| 87  | OHX  | 5     | 3912 | 7/7   | 0.10 | -3.85 | 43,43,43,43                 | 0     |
| 87  | OHX  | 1     | 3906 | 7/7   | 0.07 | -3.87 | 56,56,56,56                 | 0     |
| 86  | MG   | 1     | 3747 | 1/1   | 0.09 | -3.88 | 28,28,28,28                 | 0     |
| 86  | MG   | 5     | 3855 | 1/1   | 0.06 | -3.88 | 46,46,46,46                 | 0     |
| 87  | OHX  | 1     | 3986 | 7/7   | 0.11 | -3.88 | 84,84,84,84                 | 0     |
| 87  | OHX  | 5     | 4013 | 7/7   | 0.06 | -3.90 | 136,136,136,136             | 0     |
| 87  | OHX  | 1     | 3915 | 7/7   | 0.12 | -3.91 | 57,57,57,57                 | 0     |
| 87  | OHX  | 5     | 4008 | 7/7   | 0.08 | -3.91 | 53,53,53,53                 | 0     |
| 86  | MG   | 1     | 3751 | 1/1   | 0.12 | -3.92 | 53,53,53,53                 | 0     |
| 87  | OHX  | 2     | 2057 | 7/7   | 0.10 | -3.93 | 109,109,109,109             | 0     |
| 86  | MG   | 5     | 3726 | 1/1   | 0.07 | -3.95 | 46,46,46,46                 | 0     |
| 87  | OHX  | M6    | 202  | 7/7   | 0.11 | -4.02 | 89,89,89,89                 | 0     |
| 87  | OHX  | 1     | 4198 | 7/7   | 0.09 | -4.03 | 167,167,167,167             | 0     |
| 87  | OHX  | 5     | 3960 | 7/7   | 0.10 | -4.04 | 56,56,56,56                 | 0     |
| 87  | OHX  | 6     | 2076 | 7/7   | 0.07 | -4.08 | 116,116,116,116             | 0     |
| 87  | OHX  | 1     | 3925 | 7/7   | 0.06 | -4.09 | 72,72,72,72                 | 0     |
| 87  | OHX  | 5     | 4001 | 7/7   | 0.08 | -4.10 | 95,95,95,95                 | 0     |
| 87  | OHX  | 6     | 2060 | 7/7   | 0.07 | -4.11 | 68,68,68,68                 | 0     |
| 87  | OHX  | 1     | 4000 | 7/7   | 0.08 | -4.12 | 117,117,117,117             | 0     |
| 87  | OHX  | 5     | 4007 | 7/7   | 0.06 | -4.13 | 109,109,109,109             | 0     |
| 87  | OHX  | 5     | 4010 | 7/7   | 0.11 | -4.14 | 88,88,88,88                 | 0     |
| 87  | OHX  | 1     | 3913 | 7/7   | 0.10 | -4.15 | 69,69,69,69                 | 0     |
| 87  | OHX  | 6     | 2068 | 7/7   | 0.05 | -4.19 | 87,87,87,87                 | 0     |
| 87  | OHX  | 1     | 3966 | 7/7   | 0.08 | -4.20 | 89,89,89,89                 | 0     |
| 87  | OHX  | 1     | 3907 | 7/7   | 0.06 | -4.22 | 65,65,65,65                 | 0     |
| 87  | OHX  | 5     | 3993 | 7/7   | 0.10 | -4.24 | 85,85,85,85                 | 0     |
| 87  | OHX  | 5     | 3971 | 7/7   | 0.06 | -4.32 | 87,87,87,87                 | 0     |
| 87  | OHX  | 6     | 2073 | 7/7   | 0.12 | -4.34 | 73,73,73,73                 | 0     |
| 87  | OHX  | 5     | 3990 | 7/7   | 0.06 | -4.39 | 69,69,69,69                 | 0     |
| 87  | OHX  | 1     | 3917 | 7/7   | 0.07 | -4.41 | 76,76,76,76                 | 0     |
| 87  | OHX  | 5     | 3998 | 7/7   | 0.05 | -4.41 | 101,101,101,101             | 0     |
| 87  | OHX  | 5     | 3942 | 7/7   | 0.09 | -4.47 | 68,68,68,68                 | 0     |
| 87  | OHX  | 5     | 4022 | 7/7   | 0.10 | -4.52 | 98,98,98,98                 | 0     |
| 87  | OHX  | 5     | 3945 | 7/7   | 0.10 | -4.53 | 71,71,71,71                 | 0     |
| 87  | OHX  | 5     | 3921 | 7/7   | 0.10 | -4.54 | 56,56,56,56                 | 0     |
| 87  | OHX  | 6     | 2099 | 7/7   | 0.07 | -4.61 | 107,107,107,107             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 86  | MG   | 5     | 3760 | 1/1   | 0.06 | -4.75 | 30,30,30,30                 | 0     |
| 87  | OHX  | 5     | 3977 | 7/7   | 0.08 | -4.77 | 84,84,84,84                 | 0     |
| 87  | OHX  | 1     | 3927 | 7/7   | 0.07 | -4.77 | 72,72,72,72                 | 0     |
| 87  | OHX  | 5     | 3961 | 7/7   | 0.10 | -4.80 | 61,61,61,61                 | 0     |
| 87  | OHX  | 6     | 2079 | 7/7   | 0.10 | -4.86 | 92,92,92,92                 | 0     |
| 87  | OHX  | 1     | 3899 | 7/7   | 0.07 | -4.87 | 55,55,55,55                 | 0     |
| 87  | OHX  | 5     | 3932 | 7/7   | 0.09 | -4.87 | 49,49,49,49                 | 0     |
| 87  | OHX  | 5     | 3903 | 7/7   | 0.10 | -4.87 | 37,37,37,37                 | 0     |
| 87  | OHX  | 7     | 222  | 7/7   | 0.08 | -4.93 | 83,83,83,83                 | 0     |
| 87  | OHX  | 2     | 2040 | 7/7   | 0.06 | -5.09 | 86,86,86,86                 | 0     |
| 87  | OHX  | 5     | 3920 | 7/7   | 0.07 | -5.09 | 56,56,56,56                 | 0     |
| 87  | OHX  | 2     | 2036 | 7/7   | 0.08 | -5.14 | 86,86,86,86                 | 0     |
| 87  | OHX  | 7     | 220  | 7/7   | 0.11 | -5.18 | 73,73,73,73                 | 0     |
| 87  | OHX  | 2     | 2059 | 7/7   | 0.06 | -5.23 | 114,114,114,114             | 0     |
| 87  | OHX  | 2     | 2039 | 7/7   | 0.06 | -5.27 | 83,83,83,83                 | 0     |
| 87  | OHX  | 5     | 3947 | 7/7   | 0.08 | -5.30 | 58,58,58,58                 | 0     |
| 87  | OHX  | 2     | 2022 | 7/7   | 0.17 | -5.33 | 73,73,73,73                 | 0     |
| 87  | OHX  | 1     | 3919 | 7/7   | 0.07 | -5.35 | 71,71,71,71                 | 0     |
| 87  | OHX  | 2     | 2042 | 7/7   | 0.06 | -5.45 | 86,86,86,86                 | 0     |
| 87  | OHX  | 1     | 3933 | 7/7   | 0.07 | -5.57 | 72,72,72,72                 | 0     |
| 87  | OHX  | 1     | 3922 | 7/7   | 0.10 | -5.57 | 67,67,67,67                 | 0     |
| 87  | OHX  | 6     | 2087 | 7/7   | 0.08 | -5.62 | 96,96,96,96                 | 0     |
| 87  | OHX  | 2     | 2043 | 7/7   | 0.06 | -5.62 | 88,88,88,88                 | 0     |
| 86  | MG   | 1     | 3804 | 1/1   | 0.11 | -5.62 | 45,45,45,45                 | 0     |
| 87  | OHX  | 1     | 3903 | 7/7   | 0.07 | -5.71 | 63,63,63,63                 | 0     |
| 87  | OHX  | 5     | 3954 | 7/7   | 0.09 | -5.72 | 56,56,56,56                 | 0     |
| 86  | MG   | 5     | 3750 | 1/1   | 0.11 | -5.73 | 39,39,39,39                 | 0     |
| 87  | OHX  | 5     | 3964 | 7/7   | 0.09 | -5.75 | 82,82,82,82                 | 0     |
| 87  | OHX  | 1     | 3982 | 7/7   | 0.08 | -5.78 | 80,80,80,80                 | 0     |
| 86  | MG   | 1     | 3607 | 1/1   | 0.11 | -5.78 | 47,47,47,47                 | 0     |
| 86  | MG   | N5    | 201  | 1/1   | 0.14 | -5.91 | 63,63,63,63                 | 0     |
| 87  | OHX  | 5     | 3969 | 7/7   | 0.10 | -5.99 | 76,76,76,76                 | 0     |
| 87  | OHX  | 1     | 3912 | 7/7   | 0.07 | -6.04 | 78,78,78,78                 | 0     |
| 87  | OHX  | 5     | 3982 | 7/7   | 0.08 | -6.05 | 67,67,67,67                 | 0     |
| 87  | OHX  | 1     | 3897 | 7/7   | 0.08 | -6.05 | 51,51,51,51                 | 0     |
| 86  | MG   | 5     | 3833 | 1/1   | 0.06 | -6.14 | 59,59,59,59                 | 0     |
| 87  | OHX  | 6     | 2078 | 7/7   | 0.06 | -6.17 | 69,69,69,69                 | 0     |
| 87  | OHX  | 6     | 2066 | 7/7   | 0.05 | -6.25 | 74,74,74,74                 | 0     |
| 87  | OHX  | 5     | 3972 | 7/7   | 0.10 | -6.47 | 74,74,74,74                 | 0     |
| 87  | OHX  | 1     | 3943 | 7/7   | 0.12 | -6.48 | 82,82,82,82                 | 0     |
| 87  | OHX  | 6     | 2064 | 7/7   | 0.06 | -6.50 | 67,67,67,67                 | 0     |
| 86  | MG   | 5     | 3860 | 1/1   | 0.11 | -6.52 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|-------|-----------------------------|-------|
| 87  | OHX  | 5     | 4044 | 7/7   | 0.13 | -6.52 | 94,94,94,94                 | 0     |
| 87  | OHX  | 5     | 3943 | 7/7   | 0.07 | -6.53 | 74,74,74,74                 | 0     |
| 86  | MG   | 5     | 3818 | 1/1   | 0.11 | -6.54 | 25,25,25,25                 | 0     |
| 87  | OHX  | 5     | 3926 | 7/7   | 0.05 | -6.55 | 52,52,52,52                 | 0     |
| 86  | MG   | 6     | 2002 | 1/1   | 0.07 | -6.61 | 89,89,89,89                 | 0     |
| 87  | OHX  | 5     | 3929 | 7/7   | 0.05 | -6.66 | 64,64,64,64                 | 0     |
| 86  | MG   | 1     | 3772 | 1/1   | 0.09 | -6.68 | 57,57,57,57                 | 0     |
| 87  | OHX  | 6     | 2114 | 7/7   | 0.13 | -6.69 | 109,109,109,109             | 0     |
| 87  | OHX  | 8     | 216  | 7/7   | 0.07 | -6.70 | 59,59,59,59                 | 0     |
| 87  | OHX  | 3     | 215  | 7/7   | 0.08 | -6.75 | 85,85,85,85                 | 0     |
| 87  | OHX  | 1     | 3909 | 7/7   | 0.08 | -6.77 | 52,52,52,52                 | 0     |
| 86  | MG   | 6     | 2022 | 1/1   | 0.10 | -6.78 | 111,111,111,111             | 0     |
| 87  | OHX  | 2     | 2048 | 7/7   | 0.09 | -6.85 | 100,100,100,100             | 0     |
| 87  | OHX  | 6     | 2095 | 7/7   | 0.08 | -6.86 | 97,97,97,97                 | 0     |
| 87  | OHX  | 1     | 3886 | 7/7   | 0.06 | -6.92 | 50,50,50,50                 | 0     |
| 86  | MG   | 5     | 3652 | 1/1   | 0.14 | -6.97 | 85,85,85,85                 | 0     |
| 87  | OHX  | 5     | 3933 | 7/7   | 0.10 | -6.99 | 57,57,57,57                 | 0     |
| 87  | OHX  | 6     | 2096 | 7/7   | 0.10 | -7.03 | 87,87,87,87                 | 0     |
| 87  | OHX  | 5     | 3927 | 7/7   | 0.06 | -7.17 | 47,47,47,47                 | 0     |
| 87  | OHX  | 1     | 3940 | 7/7   | 0.06 | -7.25 | 66,66,66,66                 | 0     |
| 87  | OHX  | 5     | 3962 | 7/7   | 0.04 | -7.32 | 80,80,80,80                 | 0     |
| 86  | MG   | 5     | 3837 | 1/1   | 0.12 | -7.35 | 55,55,55,55                 | 0     |
| 87  | OHX  | 1     | 3889 | 7/7   | 0.07 | -7.35 | 46,46,46,46                 | 0     |
| 87  | OHX  | 2     | 2079 | 7/7   | 0.13 | -7.52 | 116,116,116,116             | 0     |
| 86  | MG   | 6     | 1989 | 1/1   | 0.13 | -7.57 | 35,35,35,35                 | 0     |
| 87  | OHX  | 6     | 2065 | 7/7   | 0.04 | -7.58 | 73,73,73,73                 | 0     |
| 87  | OHX  | 5     | 3930 | 7/7   | 0.05 | -7.58 | 65,65,65,65                 | 0     |
| 87  | OHX  | 6     | 2063 | 7/7   | 0.06 | -7.63 | 69,69,69,69                 | 0     |
| 86  | MG   | 1     | 3734 | 1/1   | 0.06 | -7.65 | 50,50,50,50                 | 0     |
| 87  | OHX  | 1     | 3883 | 7/7   | 0.07 | -7.85 | 46,46,46,46                 | 0     |
| 86  | MG   | 1     | 3803 | 1/1   | 0.05 | -8.05 | 80,80,80,80                 | 0     |
| 87  | OHX  | 5     | 3980 | 7/7   | 0.13 | -8.13 | 74,74,74,74                 | 0     |
| 87  | OHX  | 1     | 3937 | 7/7   | 0.07 | -8.23 | 70,70,70,70                 | 0     |
| 87  | OHX  | 1     | 3931 | 7/7   | 0.07 | -8.59 | 61,61,61,61                 | 0     |
| 87  | OHX  | 6     | 2083 | 7/7   | 0.11 | -8.63 | 87,87,87,87                 | 0     |
| 87  | OHX  | 5     | 3907 | 7/7   | 0.13 | -8.78 | 44,44,44,44                 | 0     |
| 87  | OHX  | 5     | 3918 | 7/7   | 0.07 | -8.81 | 51,51,51,51                 | 0     |
| 87  | OHX  | 1     | 3947 | 7/7   | 0.08 | -9.24 | 80,80,80,80                 | 0     |
| 87  | OHX  | 5     | 3922 | 7/7   | 0.07 | -9.37 | 56,56,56,56                 | 0     |
| 87  | OHX  | 1     | 3970 | 7/7   | 0.06 | -9.40 | 54,54,54,54                 | 0     |
| 87  | OHX  | 1     | 3923 | 7/7   | 0.09 | -9.48 | 79,79,79,79                 | 0     |
| 87  | OHX  | 5     | 3965 | 7/7   | 0.09 | -9.55 | 63,63,63,63                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF   | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|--------|-----------------------------|-------|
| 87  | OHX  | 5     | 3936 | 7/7   | 0.05 | -10.34 | 67,67,67,67                 | 0     |
| 86  | MG   | 5     | 3680 | 1/1   | 0.11 | -10.50 | 30,30,30,30                 | 0     |
| 87  | OHX  | 5     | 3946 | 7/7   | 0.06 | -11.58 | 63,63,63,63                 | 0     |
| 86  | MG   | 5     | 3806 | 1/1   | 0.20 | -11.67 | 160,160,160,160             | 0     |
| 86  | MG   | 5     | 3783 | 1/1   | 0.07 | -12.00 | 49,49,49,49                 | 0     |
| 87  | OHX  | 1     | 3936 | 7/7   | 0.05 | -12.01 | 65,65,65,65                 | 0     |
| 86  | MG   | 6     | 1975 | 1/1   | 0.07 | -12.26 | 47,47,47,47                 | 0     |
| 87  | OHX  | 1     | 3894 | 7/7   | 0.08 | -12.28 | 58,58,58,58                 | 0     |
| 87  | OHX  | 1     | 3957 | 7/7   | 0.06 | -12.32 | 78,78,78,78                 | 0     |
| 86  | MG   | 1     | 3494 | 1/1   | 0.08 | -12.71 | 73,73,73,73                 | 0     |
| 87  | OHX  | 1     | 3965 | 7/7   | 0.07 | -13.08 | 90,90,90,90                 | 0     |
| 87  | OHX  | 1     | 3910 | 7/7   | 0.08 | -14.54 | 71,71,71,71                 | 0     |
| 87  | OHX  | 1     | 3920 | 7/7   | 0.07 | -14.82 | 74,74,74,74                 | 0     |
| 87  | OHX  | 5     | 3919 | 7/7   | 0.08 | -16.41 | 48,48,48,48                 | 0     |
| 86  | MG   | 1     | 3491 | 1/1   | 0.68 | -      | 48,48,48,48                 | 0     |
| 86  | MG   | 4     | 216  | 1/1   | 0.24 | -      | 46,46,46,46                 | 0     |
| 86  | MG   | 1     | 3792 | 1/1   | 0.09 | -      | 59,59,59,59                 | 0     |
| 86  | MG   | 5     | 3876 | 1/1   | 0.36 | -      | 38,38,38,38                 | 0     |
| 86  | MG   | 4     | 201  | 1/1   | 0.55 | -      | 51,51,51,51                 | 0     |
| 86  | MG   | 2     | 1993 | 1/1   | 0.59 | -      | 62,62,62,62                 | 0     |
| 86  | MG   | 1     | 3594 | 1/1   | 0.38 | -      | 49,49,49,49                 | 0     |
| 86  | MG   | 6     | 2000 | 1/1   | 0.34 | -      | 92,92,92,92                 | 0     |
| 86  | MG   | 1     | 3842 | 1/1   | 0.56 | -      | 32,32,32,32                 | 0     |
| 86  | MG   | 1     | 3756 | 1/1   | 0.32 | -      | 81,81,81,81                 | 0     |
| 86  | MG   | 2     | 2018 | 1/1   | 0.51 | -      | 50,50,50,50                 | 0     |
| 86  | MG   | 1     | 3752 | 1/1   | 0.35 | -      | 41,41,41,41                 | 0     |
| 86  | MG   | 1     | 3853 | 1/1   | 0.56 | -      | 53,53,53,53                 | 0     |
| 86  | MG   | 5     | 3733 | 1/1   | 0.14 | -      | 51,51,51,51                 | 0     |
| 86  | MG   | 2     | 1953 | 1/1   | 0.17 | -      | 92,92,92,92                 | 0     |
| 86  | MG   | 1     | 3464 | 1/1   | 0.23 | -      | 38,38,38,38                 | 0     |
| 86  | MG   | 5     | 3801 | 1/1   | 0.15 | -      | 32,32,32,32                 | 0     |
| 86  | MG   | 6     | 2047 | 1/1   | 0.50 | -      | 50,50,50,50                 | 0     |
| 86  | MG   | 6     | 2016 | 1/1   | 0.19 | -      | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 3420 | 1/1   | 0.42 | -      | 91,91,91,91                 | 0     |
| 86  | MG   | 5     | 3873 | 1/1   | 0.51 | -      | 51,51,51,51                 | 0     |
| 86  | MG   | 5     | 3774 | 1/1   | 0.26 | -      | 103,103,103,103             | 0     |
| 86  | MG   | 1     | 3404 | 1/1   | 0.61 | -      | 59,59,59,59                 | 0     |
| 86  | MG   | 6     | 2042 | 1/1   | 0.51 | -      | 83,83,83,83                 | 0     |
| 86  | MG   | 3     | 208  | 1/1   | 0.23 | -      | 75,75,75,75                 | 0     |
| 86  | MG   | 2     | 1904 | 1/1   | 0.52 | -      | 63,63,63,63                 | 0     |
| 86  | MG   | 5     | 3617 | 1/1   | 0.25 | -      | 21,21,21,21                 | 0     |
| 86  | MG   | 6     | 2031 | 1/1   | 0.11 | -      | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 2     | 1969 | 1/1   | 0.34 | -    | 82,82,82,82                 | 0     |
| 86  | MG   | 1     | 3796 | 1/1   | 0.09 | -    | 47,47,47,47                 | 0     |
| 86  | MG   | 1     | 3828 | 1/1   | 0.45 | -    | 37,37,37,37                 | 0     |
| 86  | MG   | 5     | 3494 | 1/1   | 0.18 | -    | 18,18,18,18                 | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.