



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2022 – 10:52 AM EDT

PDB ID : 7MHM  
Title : Ensemble refinement structure of SARS-CoV-2 main protease (Mpro) at 240 K  
Authors : Ebrahim, A.; Riley, B.T.; Kumaran, D.; Andi, B.; Fuchs, M.R.; McSweeney, S.; Keedy, D.A.  
Deposited on : 2021-04-15  
Resolution : 1.53 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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                          | : | 1.8.5 (274361), CSD as541be (2020)                                 |
| Xtriage (Phenix)               | : | 1.13   |
| EDS                            | : | <b>FAILED</b>  |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.27   |

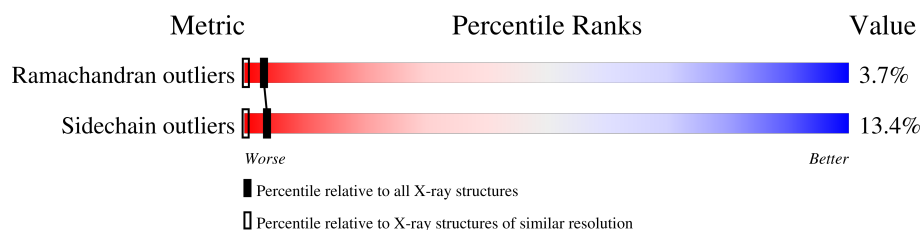
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.53 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)) |
|-----------------------|-----------------------------|---|
| Ramachandran outliers | 138981                      | 2580 (1.56-1.52)                                      |
| Sidechain outliers    | 138945                      | 2577 (1.56-1.52)                                      |


























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

Note EDS failed to run properly.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 1-A   | 306    | 85% 12% .        |
| 1   | 10-A  | 306    | 85% 14% .        |
| 1   | 11-A  | 306    | 83% 14% .        |
| 1   | 12-A  | 306    | 85% 13% .        |
| 1   | 13-A  | 306    | 84% 14% .        |
| 1   | 14-A  | 306    | 85% 13% .        |
| 1   | 15-A  | 306    | 84% 12% . .      |
| 1   | 16-A  | 306    | 85% 12% .        |
| 1   | 17-A  | 306    | 86% 11% .        |










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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | 18-A  | 306    |  85% 14% .    |
| 1   | 19-A  | 306    |  85% 12% .    |
| 1   | 2-A   | 306    |  81% 15% ..   |
| 1   | 20-A  | 306    |  86% 12% .    |
| 1   | 21-A  | 306    |  87% 12% .    |
| 1   | 22-A  | 306    |  92% 7% .     |
| 1   | 23-A  | 306    |  83% 14% ..   |
| 1   | 24-A  | 306    |  83% 13% ..   |
| 1   | 25-A  | 306    |  84% 12% ..   |
| 1   | 26-A  | 306    |  85% 13% .    |
| 1   | 27-A  | 306    |  84% 12% ..   |
| 1   | 28-A  | 306    |  85% 13% ..   |
| 1   | 29-A  | 306    |  79% 18% .  |
| 1   | 3-A   | 306    |  85% 11% .. |
| 1   | 30-A  | 306    |  86% 11% .  |
| 1   | 31-A  | 306    |  83% 15% .  |
| 1   | 32-A  | 306    |  83% 15% .  |
| 1   | 33-A  | 306    |  83% 13% .. |
| 1   | 34-A  | 306    |  83% 13% .  |
| 1   | 35-A  | 306    |  81% 14% .. |
| 1   | 36-A  | 306    |  87% 9% .   |
| 1   | 37-A  | 306    |  83% 14% .. |
| 1   | 38-A  | 306    |  79% 17% .. |
| 1   | 39-A  | 306    |  82% 14% .. |
| 1   | 4-A   | 306    |  82% 14% .. |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | 40-A  | 306    |  86% 12% .   |
| 1   | 41-A  | 306    |  83% 14% .   |
| 1   | 42-A  | 306    |  82% 14% . . |
| 1   | 43-A  | 306    |  79% 17% .   |
| 1   | 5-A   | 306    |  84% 13% .   |
| 1   | 6-A   | 306    |  85% 12% . . |
| 1   | 7-A   | 306    |  82% 16% .   |
| 1   | 8-A   | 306    |  85% 12% .   |
| 1   | 9-A   | 306    |  81% 15% .   |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 210185 atoms, of which 101308 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 3C-like proteinase.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|---------|-------|
| 1   | 1-A   | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 2-A   | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 3-A   | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 4-A   | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 5-A   | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 6-A   | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 7-A   | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 8-A   | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 9-A   | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 10-A  | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 11-A  | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 12-A  | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 13-A  | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 14-A  | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 15-A  | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 16-A  | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |

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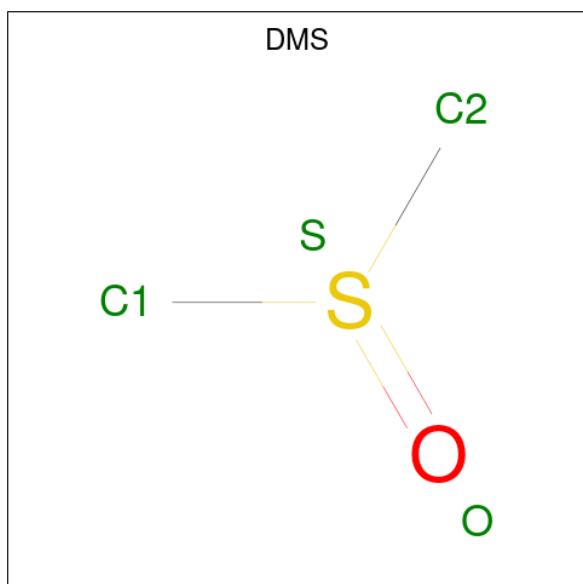
| Mol | Chain | Residues | Atoms         |           |           |          |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|-----------|----------|----------|---------|---------|---------|-------|
| 1   | 17-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 18-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 19-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 20-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 21-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 22-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 23-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 24-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 25-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 26-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 27-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 28-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 29-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 30-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 31-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 32-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 33-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 34-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 35-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 36-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |
| 1   | 37-A  | 306      | Total<br>4681 | C<br>1499 | H<br>2314 | N<br>402 | O<br>444 | S<br>22 | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms |      |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|---------|-------|
| 1   | 38-A  | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 39-A  | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 40-A  | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 41-A  | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 42-A  | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |
| 1   | 43-A  | 306      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4681  | 1499 | 2314 | 402 | 444 | 22 |         |         |       |

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | 1-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 2-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 3-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 4-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 5-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | 6-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 7-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 8-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 9-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 10-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 11-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 12-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 13-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 14-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 15-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 16-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 17-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 18-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 19-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 20-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 21-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 22-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 23-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 24-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 25-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 26-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | 27-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 28-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 29-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 30-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 31-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 32-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 33-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 34-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 35-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 36-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 37-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 38-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 39-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 40-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 41-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 42-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 43-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 1-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 2-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 3-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 4-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | 5-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 6-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 7-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 8-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 9-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 10-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 11-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 12-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 13-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 14-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 15-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 16-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 17-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 18-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 19-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 20-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 21-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 22-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 23-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 24-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 25-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | 26-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 27-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 28-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 29-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 30-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 31-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 32-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 33-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 34-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 35-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 36-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 37-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 38-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 39-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 40-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 41-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 42-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 43-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 1-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 2-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 3-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | 4-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 5-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 6-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 7-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 8-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 9-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 10-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 11-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 12-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 13-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 14-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 15-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 16-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 17-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 18-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 19-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 20-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 21-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 22-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 23-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 24-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | 25-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 26-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 27-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 28-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 29-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 30-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 31-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 32-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 33-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 34-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 35-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 36-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 37-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 38-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 39-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 40-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 41-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 42-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 43-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 1-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 2-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | 3-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 4-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 5-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 6-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 7-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 8-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 9-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 10-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 11-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 12-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 13-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 14-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 15-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 16-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 17-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 18-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 19-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 20-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 21-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 22-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 23-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | 24-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 25-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 26-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 27-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 28-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 29-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 30-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 31-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 32-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 33-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 34-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 35-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 36-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 37-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 38-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 39-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 40-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 41-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 42-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 43-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 1-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | 2-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 3-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 4-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 5-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 6-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 7-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 8-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 9-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 10-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 11-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 12-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 13-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 14-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 15-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 16-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 17-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 18-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 19-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 20-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 21-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 22-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | 23-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 24-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 25-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 26-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 27-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 28-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 29-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 30-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 31-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 32-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 33-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 34-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 35-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 36-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 37-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 38-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 39-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 40-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 41-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 42-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 43-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | 1-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 2-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 3-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 4-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 5-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 6-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 7-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 8-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 9-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 10-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 11-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 12-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 13-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 14-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 15-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 16-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 17-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 18-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 19-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 20-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 21-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | 22-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 23-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 24-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 25-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 26-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 27-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 28-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 29-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 30-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 31-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 32-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 33-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 34-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 35-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 36-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 37-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 38-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 39-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 40-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 41-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 42-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | 43-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 1-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 2-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 3-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 4-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 5-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 6-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 7-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 8-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 9-A   | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 10-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 11-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 12-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 13-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 14-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 15-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 16-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 17-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 18-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 19-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 20-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | 21-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 22-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 23-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 24-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 25-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 26-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 27-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 28-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 29-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 30-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 31-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 32-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 33-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 34-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 35-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 36-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 37-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 38-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 39-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 40-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 41-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 2   | 42-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |
| 2   | 43-A  | 1        | Total | C | H | O | S | 0       | 0       |
|     |       |          | 10    | 2 | 6 | 1 | 1 |         |         |

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | 1-A   | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | 2-A   | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | 3-A   | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | 4-A   | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | 5-A   | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | 6-A   | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | 7-A   | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | 8-A   | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | 9-A   | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | 10-A  | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | 11-A  | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | 12-A  | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | 13-A  | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | 14-A  | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | 15-A  | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | 16-A  | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | 17-A  | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3   | 18-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 19-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 20-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 21-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 22-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 23-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 24-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 25-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 26-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 27-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 28-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 29-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 30-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 31-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 32-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 33-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 34-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 35-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 36-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 37-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 38-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3   | 39-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 40-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 41-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 42-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | 43-A  | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4   | 1-A   | 148      | Total<br>148 | O<br>148 | 0       | 0       |
| 4   | 2-A   | 135      | Total<br>135 | O<br>135 | 0       | 0       |
| 4   | 3-A   | 134      | Total<br>134 | O<br>134 | 0       | 0       |
| 4   | 4-A   | 142      | Total<br>142 | O<br>142 | 0       | 0       |
| 4   | 5-A   | 140      | Total<br>140 | O<br>140 | 0       | 0       |
| 4   | 6-A   | 145      | Total<br>145 | O<br>145 | 0       | 0       |
| 4   | 7-A   | 133      | Total<br>133 | O<br>133 | 0       | 0       |
| 4   | 8-A   | 131      | Total<br>131 | O<br>131 | 0       | 0       |
| 4   | 9-A   | 147      | Total<br>147 | O<br>147 | 0       | 0       |
| 4   | 10-A  | 146      | Total<br>146 | O<br>146 | 0       | 0       |
| 4   | 11-A  | 137      | Total<br>137 | O<br>137 | 0       | 0       |
| 4   | 12-A  | 141      | Total<br>141 | O<br>141 | 0       | 0       |
| 4   | 13-A  | 130      | Total<br>130 | O<br>130 | 0       | 0       |
| 4   | 14-A  | 135      | Total<br>135 | O<br>135 | 0       | 0       |

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*Continued from previous page...*

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4   | 15-A  | 136      | Total<br>136 | O<br>136 | 0       | 0       |
| 4   | 16-A  | 121      | Total<br>121 | O<br>121 | 0       | 0       |
| 4   | 17-A  | 152      | Total<br>152 | O<br>152 | 0       | 0       |
| 4   | 18-A  | 122      | Total<br>122 | O<br>122 | 0       | 0       |
| 4   | 19-A  | 141      | Total<br>141 | O<br>141 | 0       | 0       |
| 4   | 20-A  | 131      | Total<br>131 | O<br>131 | 0       | 0       |
| 4   | 21-A  | 142      | Total<br>142 | O<br>142 | 0       | 0       |
| 4   | 22-A  | 139      | Total<br>139 | O<br>139 | 0       | 0       |
| 4   | 23-A  | 134      | Total<br>134 | O<br>134 | 0       | 0       |
| 4   | 24-A  | 138      | Total<br>138 | O<br>138 | 0       | 0       |
| 4   | 25-A  | 145      | Total<br>145 | O<br>145 | 0       | 0       |
| 4   | 26-A  | 125      | Total<br>125 | O<br>125 | 0       | 0       |
| 4   | 27-A  | 144      | Total<br>144 | O<br>144 | 0       | 0       |
| 4   | 28-A  | 135      | Total<br>135 | O<br>135 | 0       | 0       |
| 4   | 29-A  | 144      | Total<br>144 | O<br>144 | 0       | 0       |
| 4   | 30-A  | 146      | Total<br>146 | O<br>146 | 0       | 0       |
| 4   | 31-A  | 136      | Total<br>136 | O<br>136 | 0       | 0       |
| 4   | 32-A  | 122      | Total<br>122 | O<br>122 | 0       | 0       |
| 4   | 33-A  | 134      | Total<br>134 | O<br>134 | 0       | 0       |
| 4   | 34-A  | 123      | Total<br>123 | O<br>123 | 0       | 0       |
| 4   | 35-A  | 130      | Total<br>130 | O<br>130 | 0       | 0       |

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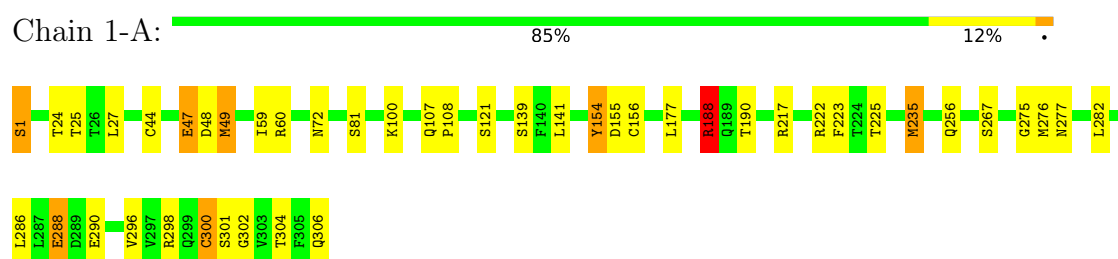
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4   | 36-A  | 139      | Total<br>139 | O<br>139 | 0       | 0       |
| 4   | 37-A  | 140      | Total<br>140 | O<br>140 | 0       | 0       |
| 4   | 38-A  | 120      | Total<br>120 | O<br>120 | 0       | 0       |
| 4   | 39-A  | 145      | Total<br>145 | O<br>145 | 0       | 0       |
| 4   | 40-A  | 121      | Total<br>121 | O<br>121 | 0       | 0       |
| 4   | 41-A  | 127      | Total<br>127 | O<br>127 | 0       | 0       |
| 4   | 42-A  | 133      | Total<br>133 | O<br>133 | 0       | 0       |
| 4   | 43-A  | 140      | Total<br>140 | O<br>140 | 0       | 0       |

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

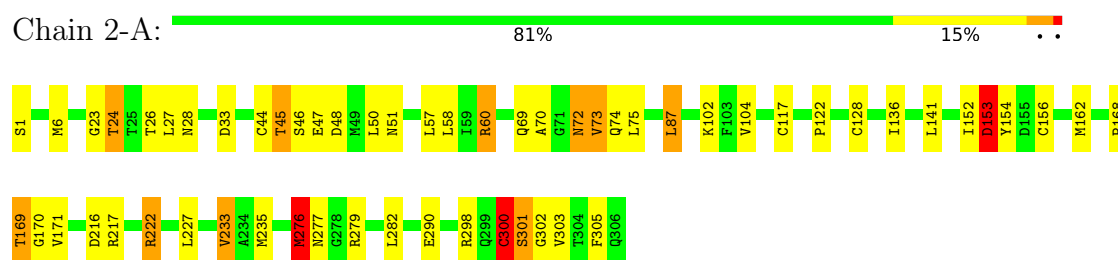
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

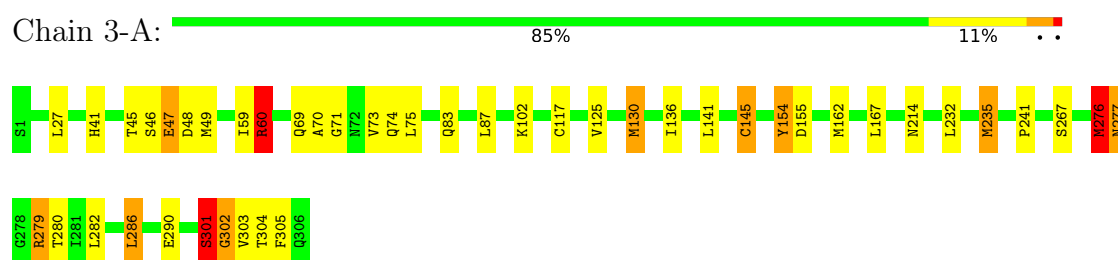
#### • Molecule 1: 3C-like proteinase



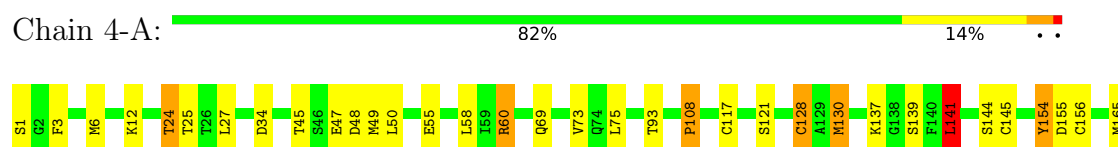
#### • Molecule 1: 3C-like proteinase

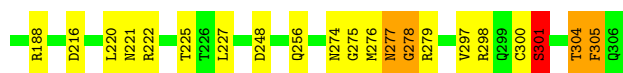


#### • Molecule 1: 3C-like proteinase



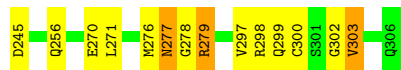
#### • Molecule 1: 3C-like proteinase





- Molecule 1: 3C-like proteinase

Chain 5-A: 84% 13% .



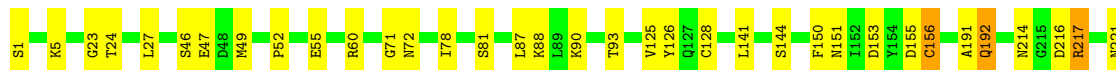
- Molecule 1: 3C-like proteinase

Chain 6-A: 85% 12% . .



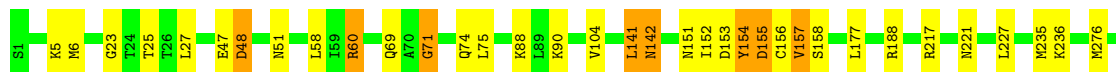
- Molecule 1: 3C-like proteinase

Chain 7-A: 82% 16% .



- Molecule 1: 3C-like proteinase

Chain 8-A: 85% 12% .



- Molecule 1: 3C-like proteinase

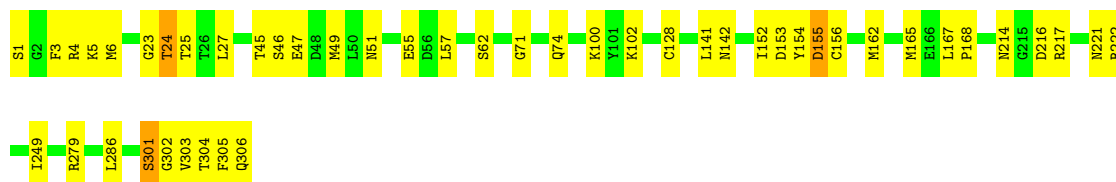
Chain 9-A: 81% 15% .





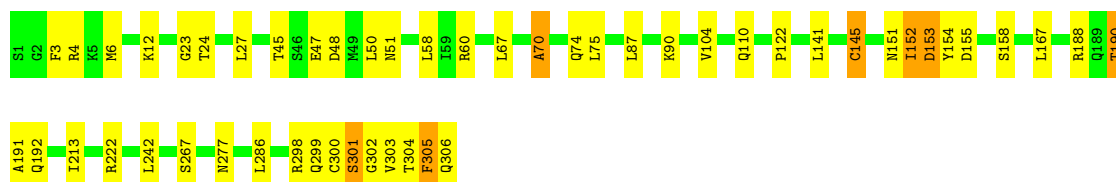
- Molecule 1: 3C-like proteinase

Chain 10-A: 85% 14% .



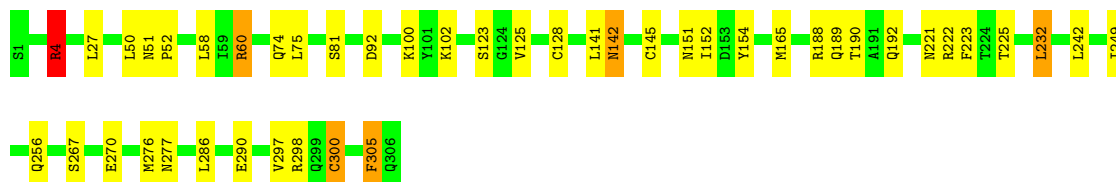
- Molecule 1: 3C-like proteinase

Chain 11-A: 83% 14% .



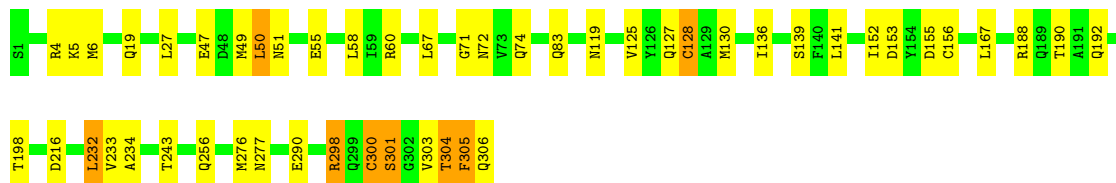
- Molecule 1: 3C-like proteinase

Chain 12-A: 85% 13% .



- Molecule 1: 3C-like proteinase

Chain 13-A: 84% 14% .



- Molecule 1: 3C-like proteinase

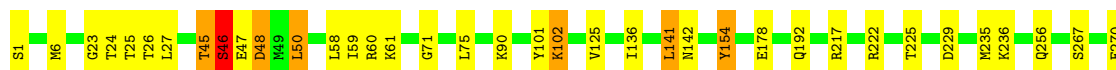
Chain 14-A: 85% 13% .





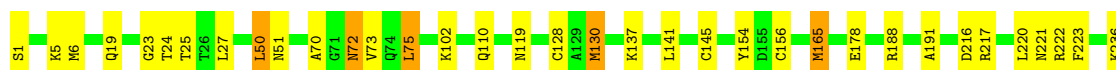
- Molecule 1: 3C-like proteinase

Chain 15-A: 84% 12% . .



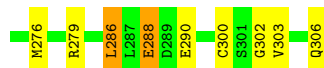
- Molecule 1: 3C-like proteinase

Chain 16-A: 85% 12% .



- Molecule 1: 3C-like proteinase

Chain 17-A: 86% 11% .



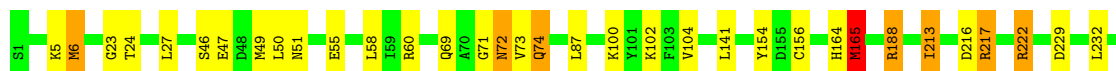
- Molecule 1: 3C-like proteinase

Chain 18-A: 85% 14% .



- Molecule 1: 3C-like proteinase

Chain 19-A: 85% 12% .





- Molecule 1: 3C-like proteinase

Chain 20-A: 86% 12%



- Molecule 1: 3C-like proteinase

Chain 21-A: 87% 12%



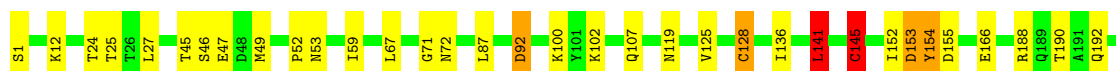
- Molecule 1: 3C-like proteinase

Chain 22-A: 92% 7%



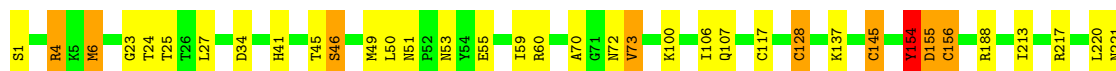
- Molecule 1: 3C-like proteinase

Chain 23-A: 83% 14%




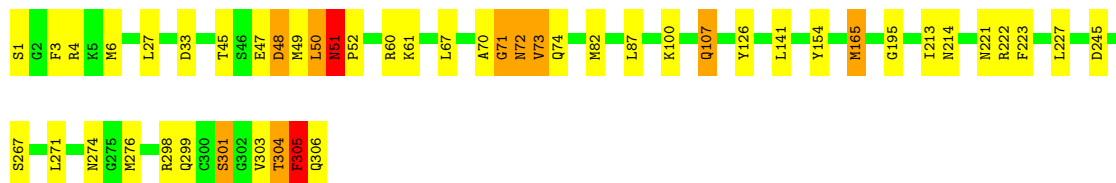
- Molecule 1: 3C-like proteinase

Chain 24-A: 83% 13%




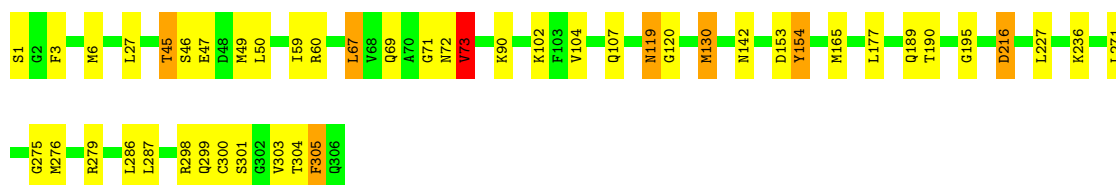
- Molecule 1: 3C-like proteinase

Chain 25-A:  84% 12% ..




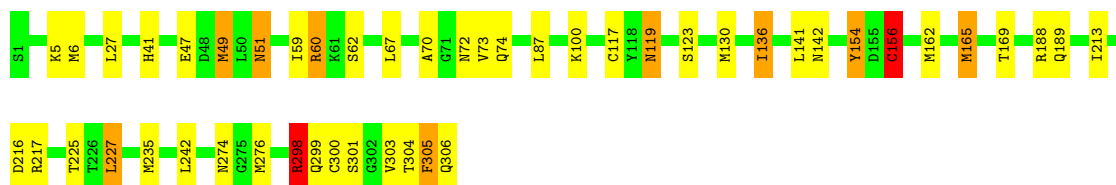
- Molecule 1: 3C-like proteinase

Chain 26-A:  85% 13% .




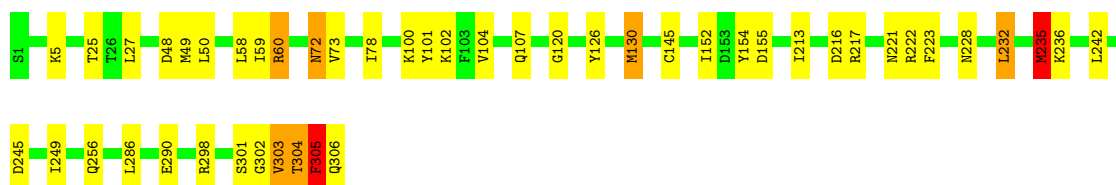
- Molecule 1: 3C-like proteinase

Chain 27-A:  84% 12% ..




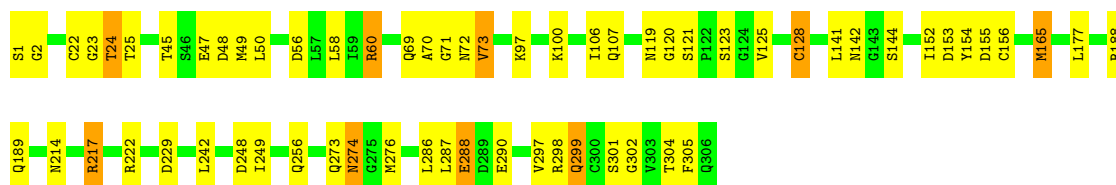
- Molecule 1: 3C-like proteinase

Chain 28-A:  85% 13% ..



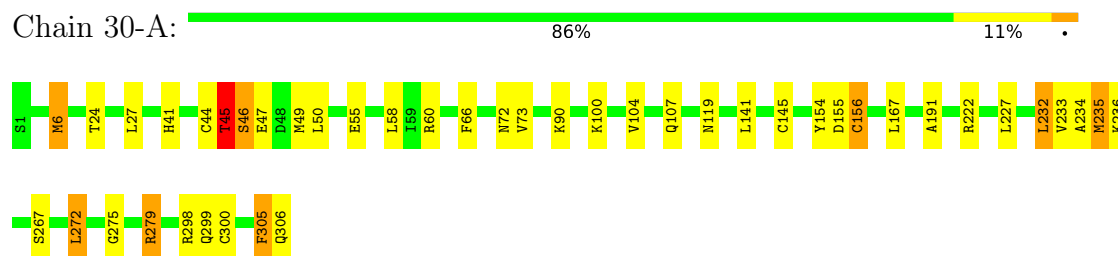
- Molecule 1: 3C-like proteinase

Chain 29-A:  79% 18% .

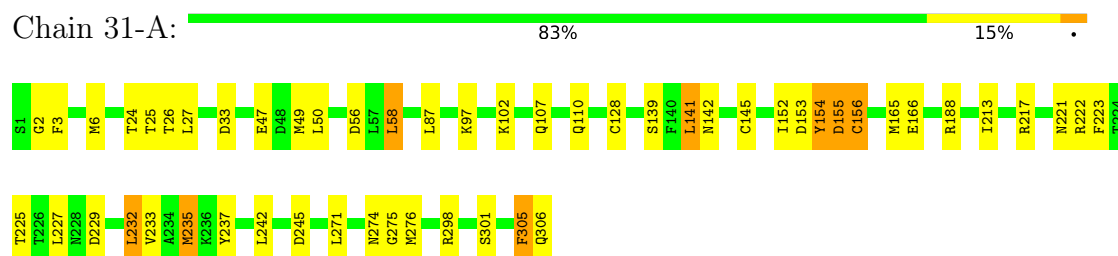




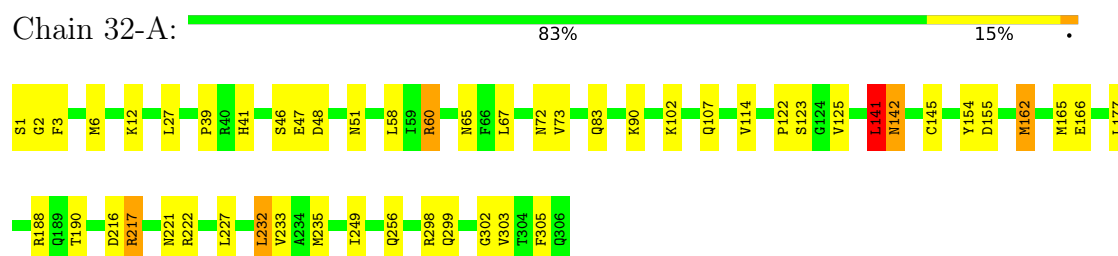
## • Molecule 1: 3C-like proteinase



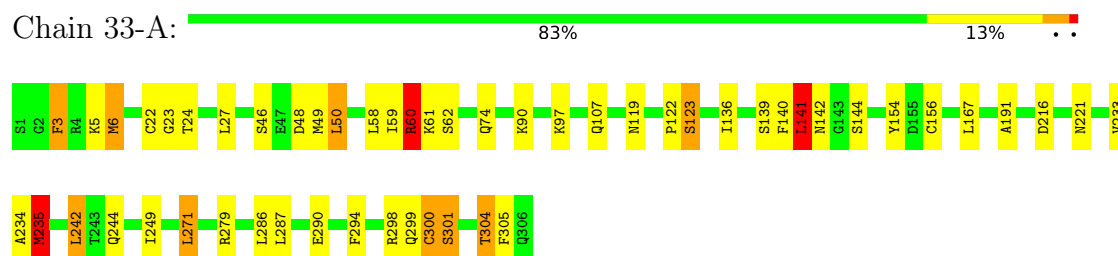
## • Molecule 1: 3C-like proteinase



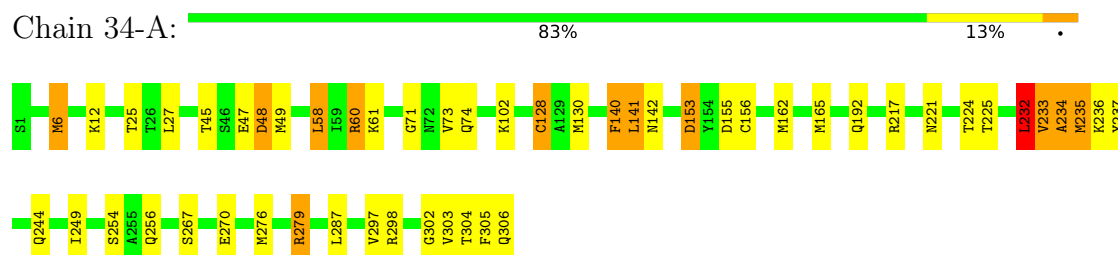
## • Molecule 1: 3C-like proteinase



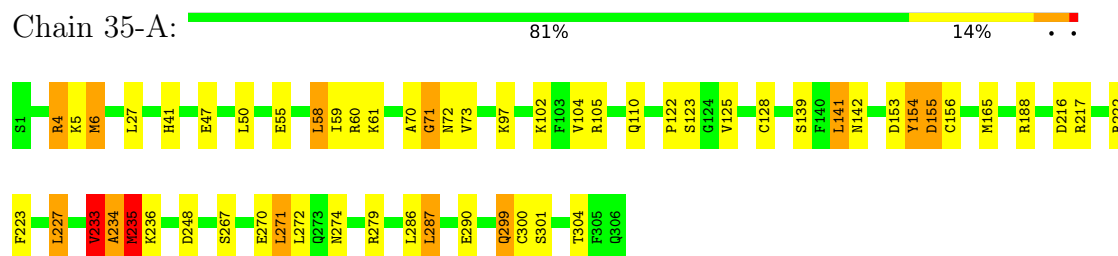
## • Molecule 1: 3C-like proteinase



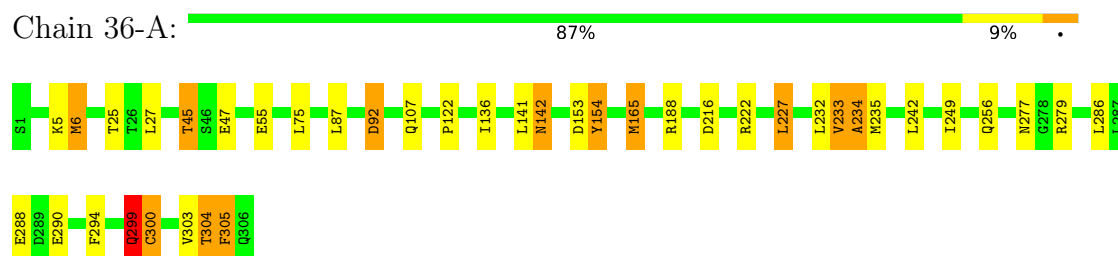
## • Molecule 1: 3C-like proteinase



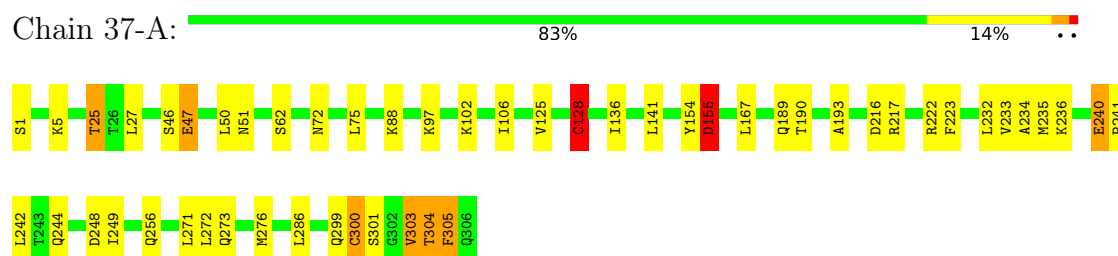
- Molecule 1: 3C-like proteinase



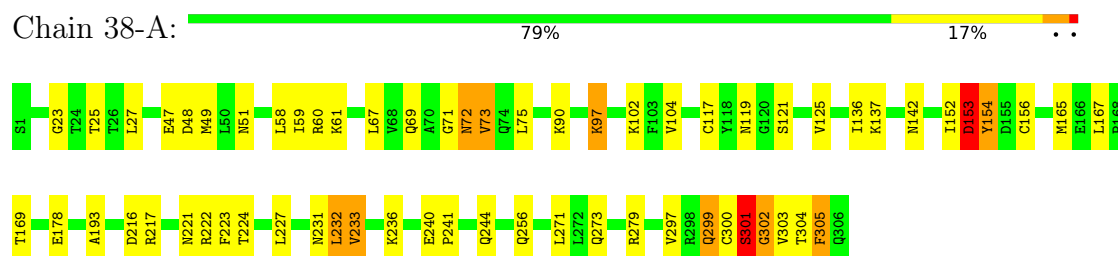
- Molecule 1: 3C-like proteinase



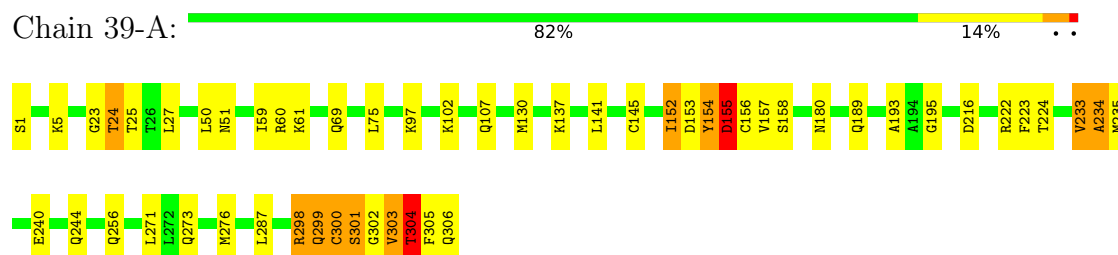
- Molecule 1: 3C-like proteinase



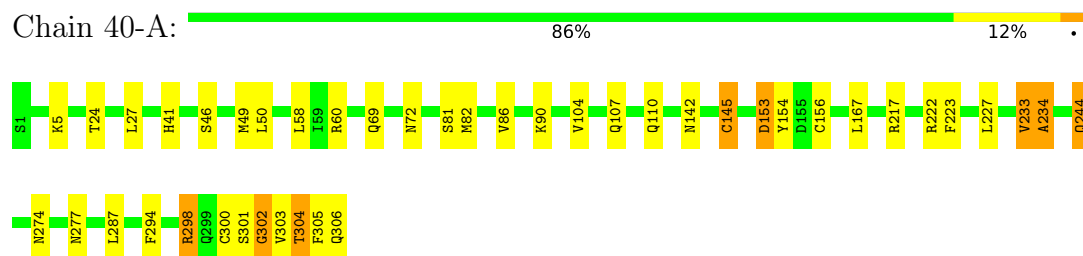
- Molecule 1: 3C-like proteinase



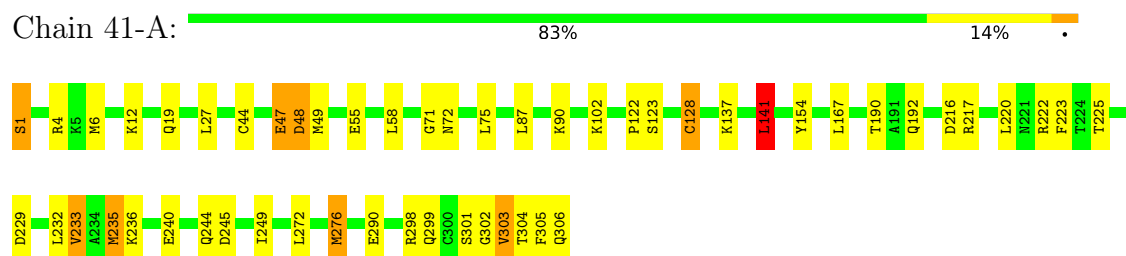
- Molecule 1: 3C-like proteinase



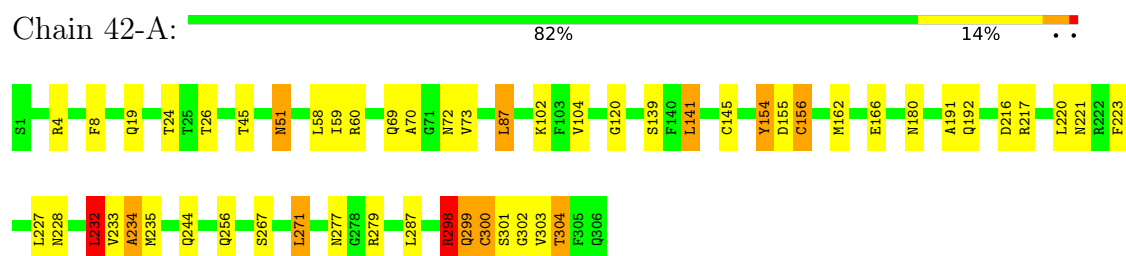
- Molecule 1: 3C-like proteinase



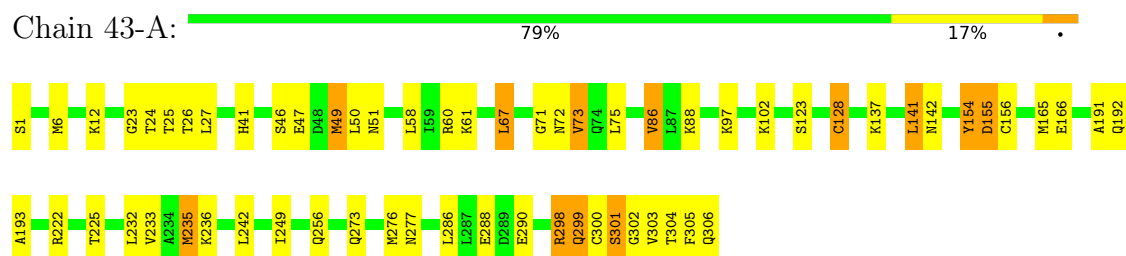
- Molecule 1: 3C-like proteinase



- Molecule 1: 3C-like proteinase



- Molecule 1: 3C-like proteinase



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

| Property   | Value   | Source    |
|--|---|-----------|
| Space group  | C 1 2 1   | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 114.19Å 53.49Å 45.00Å<br>90.00° 103.04° 90.00°              | Depositor |
| Resolution (Å)   | 48.20 – 1.53  | Depositor |
| % Data completeness<br>(in resolution range)             | 99.9 (48.20-1.53)   | Depositor |
| $R_{merge}$  | 0.18  | Depositor |
| $R_{sym}$  | (Not available)   | Depositor |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>               | 0.86 (at 1.53Å)   | Xtriage   |
| Refinement program                                       | PHENIX (phenix.ensemble_refinement:1.19.2_4158)             | Depositor |
| R, $R_{free}$  | 0.158 , 0.197   | Depositor |
| Wilson B-factor (Å <sup>2</sup> )                        | 16.3  | Xtriage   |
| Anisotropy   | 0.260   | Xtriage   |
| L-test for twinning <sup>2</sup>                         | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$ | Xtriage   |
| Estimated twinning fraction                              | No twinning to report.                                      | Xtriage   |
| Total number of atoms                                    | 210185  | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 19.0  | wwPDB-VP  |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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   | 1-A   | 0.78         | 4/2420 (0.2%)  | 0.89        | 2/3289 (0.1%) |
| 1   | 2-A   | 0.81         | 2/2420 (0.1%)  | 0.96        | 7/3289 (0.2%) |
| 1   | 3-A   | 0.77         | 4/2420 (0.2%)  | 0.91        | 3/3289 (0.1%) |
| 1   | 4-A   | 0.80         | 3/2420 (0.1%)  | 0.97        | 7/3289 (0.2%) |
| 1   | 5-A   | 0.74         | 1/2420 (0.0%)  | 0.92        | 3/3289 (0.1%) |
| 1   | 6-A   | 0.79         | 3/2420 (0.1%)  | 0.95        | 8/3289 (0.2%) |
| 1   | 7-A   | 0.77         | 3/2420 (0.1%)  | 0.86        | 3/3289 (0.1%) |
| 1   | 8-A   | 0.73         | 0/2420         | 0.91        | 1/3289 (0.0%) |
| 1   | 9-A   | 0.83         | 6/2420 (0.2%)  | 0.94        | 7/3289 (0.2%) |
| 1   | 10-A  | 0.86         | 3/2420 (0.1%)  | 0.89        | 1/3289 (0.0%) |
| 1   | 11-A  | 0.83         | 1/2420 (0.0%)  | 0.93        | 3/3289 (0.1%) |
| 1   | 12-A  | 0.96         | 2/2420 (0.1%)  | 0.96        | 4/3289 (0.1%) |
| 1   | 13-A  | 0.79         | 4/2420 (0.2%)  | 0.92        | 6/3289 (0.2%) |
| 1   | 14-A  | 0.79         | 3/2420 (0.1%)  | 0.90        | 1/3289 (0.0%) |
| 1   | 15-A  | 0.74         | 0/2420         | 0.88        | 4/3289 (0.1%) |
| 1   | 16-A  | 0.79         | 6/2420 (0.2%)  | 0.93        | 3/3289 (0.1%) |
| 1   | 17-A  | 1.06         | 9/2420 (0.4%)  | 0.93        | 4/3289 (0.1%) |
| 1   | 18-A  | 0.76         | 3/2420 (0.1%)  | 0.91        | 4/3289 (0.1%) |
| 1   | 19-A  | 0.80         | 6/2420 (0.2%)  | 0.91        | 5/3289 (0.2%) |
| 1   | 20-A  | 0.78         | 1/2420 (0.0%)  | 0.89        | 2/3289 (0.1%) |
| 1   | 21-A  | 0.70         | 1/2420 (0.0%)  | 0.87        | 6/3289 (0.2%) |
| 1   | 22-A  | 0.74         | 0/2420         | 0.88        | 3/3289 (0.1%) |
| 1   | 23-A  | 0.82         | 3/2420 (0.1%)  | 0.92        | 6/3289 (0.2%) |
| 1   | 24-A  | 1.36         | 10/2420 (0.4%) | 0.99        | 6/3289 (0.2%) |
| 1   | 25-A  | 0.79         | 3/2420 (0.1%)  | 0.93        | 5/3289 (0.2%) |
| 1   | 26-A  | 0.77         | 3/2420 (0.1%)  | 0.91        | 4/3289 (0.1%) |
| 1   | 27-A  | 0.74         | 5/2420 (0.2%)  | 0.94        | 6/3289 (0.2%) |
| 1   | 28-A  | 0.83         | 2/2420 (0.1%)  | 0.94        | 5/3289 (0.2%) |
| 1   | 29-A  | 0.77         | 6/2420 (0.2%)  | 0.93        | 5/3289 (0.2%) |
| 1   | 30-A  | 0.78         | 4/2420 (0.2%)  | 0.91        | 3/3289 (0.1%) |
| 1   | 31-A  | 0.78         | 4/2420 (0.2%)  | 0.97        | 6/3289 (0.2%) |
| 1   | 32-A  | 0.76         | 1/2420 (0.0%)  | 0.93        | 3/3289 (0.1%) |

| Mol | Chain | Bond lengths |                   | Bond angles |                   |
|-----|-------|--------------|-------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5           | RMSZ        | # Z  >5           |
| 1   | 33-A  | 0.78         | 2/2420 (0.1%)     | 0.94        | 6/3289 (0.2%)     |
| 1   | 34-A  | 0.75         | 3/2420 (0.1%)     | 0.95        | 7/3289 (0.2%)     |
| 1   | 35-A  | 0.82         | 4/2420 (0.2%)     | 0.99        | 11/3289 (0.3%)    |
| 1   | 36-A  | 0.80         | 5/2420 (0.2%)     | 0.98        | 7/3289 (0.2%)     |
| 1   | 37-A  | 0.74         | 3/2420 (0.1%)     | 0.93        | 3/3289 (0.1%)     |
| 1   | 38-A  | 0.76         | 1/2420 (0.0%)     | 0.94        | 3/3289 (0.1%)     |
| 1   | 39-A  | 0.84         | 4/2420 (0.2%)     | 0.91        | 3/3289 (0.1%)     |
| 1   | 40-A  | 0.82         | 5/2420 (0.2%)     | 0.85        | 0/3289            |
| 1   | 41-A  | 0.74         | 1/2420 (0.0%)     | 0.92        | 5/3289 (0.2%)     |
| 1   | 42-A  | 0.89         | 3/2420 (0.1%)     | 0.95        | 7/3289 (0.2%)     |
| 1   | 43-A  | 0.84         | 5/2420 (0.2%)     | 0.94        | 7/3289 (0.2%)     |
| All | All   | 0.82         | 142/104060 (0.1%) | 0.93        | 195/141427 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | 1-A   | 0                   | 5                   |
| 1   | 2-A   | 0                   | 12                  |
| 1   | 3-A   | 0                   | 10                  |
| 1   | 4-A   | 0                   | 8                   |
| 1   | 5-A   | 0                   | 14                  |
| 1   | 6-A   | 0                   | 4                   |
| 1   | 7-A   | 0                   | 7                   |
| 1   | 8-A   | 0                   | 5                   |
| 1   | 9-A   | 0                   | 7                   |
| 1   | 10-A  | 0                   | 4                   |
| 1   | 11-A  | 0                   | 7                   |
| 1   | 12-A  | 0                   | 6                   |
| 1   | 13-A  | 0                   | 5                   |
| 1   | 14-A  | 0                   | 6                   |
| 1   | 15-A  | 0                   | 8                   |
| 1   | 16-A  | 0                   | 6                   |
| 1   | 17-A  | 0                   | 5                   |
| 1   | 18-A  | 0                   | 2                   |
| 1   | 19-A  | 0                   | 11                  |
| 1   | 20-A  | 0                   | 5                   |
| 1   | 21-A  | 0                   | 4                   |
| 1   | 22-A  | 0                   | 1                   |
| 1   | 23-A  | 0                   | 6                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | 24-A  | 0                   | 9                   |
| 1   | 25-A  | 0                   | 8                   |
| 1   | 26-A  | 0                   | 2                   |
| 1   | 27-A  | 0                   | 9                   |
| 1   | 28-A  | 0                   | 8                   |
| 1   | 29-A  | 0                   | 8                   |
| 1   | 30-A  | 0                   | 9                   |
| 1   | 31-A  | 0                   | 3                   |
| 1   | 32-A  | 0                   | 6                   |
| 1   | 33-A  | 0                   | 9                   |
| 1   | 34-A  | 0                   | 9                   |
| 1   | 35-A  | 0                   | 6                   |
| 1   | 36-A  | 0                   | 7                   |
| 1   | 37-A  | 0                   | 3                   |
| 1   | 38-A  | 0                   | 7                   |
| 1   | 39-A  | 0                   | 9                   |
| 1   | 40-A  | 0                   | 4                   |
| 1   | 41-A  | 0                   | 7                   |
| 1   | 42-A  | 0                   | 12                  |
| 1   | 43-A  | 0                   | 9                   |
| All | All   | 0                   | 292                 |

All (142) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | 24-A  | 145 | CYS  | CB-SG | 52.09  | 2.70        | 1.82     |
| 1   | 17-A  | 145 | CYS  | CB-SG | 32.91  | 2.38        | 1.82     |
| 1   | 12-A  | 145 | CYS  | CB-SG | 29.14  | 2.31        | 1.82     |
| 1   | 42-A  | 145 | CYS  | CB-SG | 21.65  | 2.19        | 1.82     |
| 1   | 10-A  | 128 | CYS  | CB-SG | -20.32 | 1.47        | 1.82     |
| 1   | 39-A  | 156 | CYS  | CB-SG | 16.78  | 2.10        | 1.82     |
| 1   | 28-A  | 145 | CYS  | CB-SG | -16.58 | 1.54        | 1.82     |
| 1   | 24-A  | 128 | CYS  | CB-SG | -16.38 | 1.54        | 1.82     |
| 1   | 2-A   | 128 | CYS  | CB-SG | -15.40 | 1.56        | 1.82     |
| 1   | 11-A  | 145 | CYS  | CB-SG | 15.35  | 2.08        | 1.82     |
| 1   | 43-A  | 128 | CYS  | CB-SG | -15.27 | 1.56        | 1.82     |
| 1   | 9-A   | 145 | CYS  | CB-SG | 11.96  | 2.02        | 1.82     |
| 1   | 40-A  | 145 | CYS  | CB-SG | -11.87 | 1.62        | 1.82     |
| 1   | 30-A  | 156 | CYS  | CB-SG | 11.56  | 2.02        | 1.82     |
| 1   | 7-A   | 156 | CYS  | CB-SG | 11.31  | 2.01        | 1.82     |
| 1   | 23-A  | 145 | CYS  | CB-SG | -10.92 | 1.63        | 1.82     |
| 1   | 35-A  | 156 | CYS  | CB-SG | -9.75  | 1.65        | 1.82     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | 34-A  | 128 | CYS  | CB-SG   | -9.71 | 1.65        | 1.82     |
| 1   | 23-A  | 128 | CYS  | CB-SG   | -9.37 | 1.66        | 1.82     |
| 1   | 31-A  | 145 | CYS  | CB-SG   | 9.01  | 1.97        | 1.82     |
| 1   | 26-A  | 300 | CYS  | CB-SG   | -8.96 | 1.67        | 1.82     |
| 1   | 33-A  | 22  | CYS  | CB-SG   | -8.70 | 1.67        | 1.82     |
| 1   | 17-A  | 165 | MET  | CB-CG   | 8.68  | 1.79        | 1.51     |
| 1   | 17-A  | 288 | GLU  | CB-CG   | 8.51  | 1.68        | 1.52     |
| 1   | 9-A   | 47  | GLU  | CB-CG   | 8.48  | 1.68        | 1.52     |
| 1   | 40-A  | 156 | CYS  | CB-SG   | -8.29 | 1.68        | 1.82     |
| 1   | 39-A  | 145 | CYS  | CB-SG   | 8.24  | 1.96        | 1.82     |
| 1   | 37-A  | 128 | CYS  | CB-SG   | -8.24 | 1.68        | 1.82     |
| 1   | 42-A  | 300 | CYS  | CB-SG   | -7.92 | 1.68        | 1.82     |
| 1   | 39-A  | 240 | GLU  | CG-CD   | 7.87  | 1.63        | 1.51     |
| 1   | 18-A  | 300 | CYS  | CB-SG   | -7.86 | 1.68        | 1.82     |
| 1   | 6-A   | 145 | CYS  | CB-SG   | 7.84  | 1.95        | 1.82     |
| 1   | 24-A  | 145 | CYS  | CA-CB   | 7.77  | 1.71        | 1.53     |
| 1   | 29-A  | 128 | CYS  | CB-SG   | 7.62  | 1.95        | 1.82     |
| 1   | 33-A  | 290 | GLU  | CG-CD   | 7.58  | 1.63        | 1.51     |
| 1   | 5-A   | 117 | CYS  | CB-SG   | 7.57  | 1.95        | 1.82     |
| 1   | 40-A  | 300 | CYS  | CB-SG   | 7.50  | 1.95        | 1.82     |
| 1   | 9-A   | 288 | GLU  | CB-CG   | 7.49  | 1.66        | 1.52     |
| 1   | 16-A  | 128 | CYS  | CB-SG   | 7.47  | 1.95        | 1.82     |
| 1   | 36-A  | 55  | GLU  | CB-CG   | 7.36  | 1.66        | 1.52     |
| 1   | 19-A  | 156 | CYS  | CB-SG   | -7.32 | 1.69        | 1.82     |
| 1   | 16-A  | 297 | VAL  | CB-CG2  | -7.26 | 1.37        | 1.52     |
| 1   | 1-A   | 288 | GLU  | CB-CG   | 7.22  | 1.65        | 1.52     |
| 1   | 13-A  | 300 | CYS  | CB-SG   | -7.15 | 1.70        | 1.82     |
| 1   | 36-A  | 6   | MET  | CB-CG   | 6.91  | 1.73        | 1.51     |
| 1   | 24-A  | 156 | CYS  | CB-SG   | 6.85  | 1.93        | 1.82     |
| 1   | 16-A  | 130 | MET  | CB-CG   | 6.83  | 1.73        | 1.51     |
| 1   | 1-A   | 235 | MET  | CB-CG   | 6.83  | 1.73        | 1.51     |
| 1   | 6-A   | 156 | CYS  | CB-SG   | -6.73 | 1.70        | 1.82     |
| 1   | 19-A  | 69  | GLN  | CB-CG   | 6.72  | 1.70        | 1.52     |
| 1   | 7-A   | 128 | CYS  | CB-SG   | 6.64  | 1.93        | 1.82     |
| 1   | 19-A  | 290 | GLU  | CB-CG   | -6.62 | 1.39        | 1.52     |
| 1   | 17-A  | 156 | CYS  | CB-SG   | -6.61 | 1.71        | 1.82     |
| 1   | 24-A  | 237 | TYR  | CD2-CE2 | -6.58 | 1.29        | 1.39     |
| 1   | 43-A  | 290 | GLU  | CG-CD   | 6.57  | 1.61        | 1.51     |
| 1   | 3-A   | 117 | CYS  | CB-SG   | -6.52 | 1.71        | 1.82     |
| 1   | 13-A  | 290 | GLU  | CB-CG   | -6.50 | 1.39        | 1.52     |
| 1   | 24-A  | 290 | GLU  | CG-CD   | 6.47  | 1.61        | 1.51     |
| 1   | 19-A  | 6   | MET  | CB-CG   | 6.44  | 1.72        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | 29-A  | 156 | CYS  | CB-SG   | -6.43 | 1.71        | 1.82     |
| 1   | 36-A  | 154 | TYR  | CB-CG   | 6.33  | 1.61        | 1.51     |
| 1   | 29-A  | 229 | ASP  | CB-CG   | 6.29  | 1.65        | 1.51     |
| 1   | 17-A  | 290 | GLU  | CG-CD   | 6.28  | 1.61        | 1.51     |
| 1   | 4-A   | 130 | MET  | CB-CG   | 6.26  | 1.71        | 1.51     |
| 1   | 31-A  | 237 | TYR  | CD2-CE2 | -6.19 | 1.30        | 1.39     |
| 1   | 17-A  | 217 | ARG  | CB-CG   | 6.16  | 1.69        | 1.52     |
| 1   | 3-A   | 145 | CYS  | CB-SG   | 6.16  | 1.92        | 1.82     |
| 1   | 3-A   | 290 | GLU  | CG-CD   | 6.11  | 1.61        | 1.51     |
| 1   | 13-A  | 290 | GLU  | CG-CD   | -6.08 | 1.42        | 1.51     |
| 1   | 37-A  | 273 | GLN  | CB-CG   | 6.07  | 1.69        | 1.52     |
| 1   | 31-A  | 153 | ASP  | CB-CG   | 5.97  | 1.64        | 1.51     |
| 1   | 17-A  | 256 | GLN  | CB-CG   | 5.92  | 1.68        | 1.52     |
| 1   | 36-A  | 153 | ASP  | CB-CG   | 5.90  | 1.64        | 1.51     |
| 1   | 40-A  | 298 | ARG  | CG-CD   | 5.87  | 1.66        | 1.51     |
| 1   | 30-A  | 145 | CYS  | CB-SG   | 5.86  | 1.92        | 1.82     |
| 1   | 1-A   | 296 | VAL  | CB-CG1  | -5.84 | 1.40        | 1.52     |
| 1   | 25-A  | 305 | PHE  | CD1-CE1 | -5.84 | 1.27        | 1.39     |
| 1   | 27-A  | 117 | CYS  | CB-SG   | -5.81 | 1.72        | 1.81     |
| 1   | 39-A  | 240 | GLU  | CB-CG   | 5.81  | 1.63        | 1.52     |
| 1   | 43-A  | 154 | TYR  | CD2-CE2 | -5.80 | 1.30        | 1.39     |
| 1   | 1-A   | 49  | MET  | CB-CG   | 5.73  | 1.69        | 1.51     |
| 1   | 14-A  | 300 | CYS  | CB-SG   | 5.70  | 1.92        | 1.82     |
| 1   | 28-A  | 290 | GLU  | CB-CG   | -5.69 | 1.41        | 1.52     |
| 1   | 41-A  | 128 | CYS  | CB-SG   | -5.64 | 1.72        | 1.81     |
| 1   | 24-A  | 300 | CYS  | CB-SG   | -5.62 | 1.72        | 1.81     |
| 1   | 17-A  | 145 | CYS  | CA-CB   | 5.57  | 1.66        | 1.53     |
| 1   | 9-A   | 188 | ARG  | CG-CD   | 5.56  | 1.65        | 1.51     |
| 1   | 12-A  | 300 | CYS  | CB-SG   | 5.53  | 1.91        | 1.82     |
| 1   | 34-A  | 140 | PHE  | CB-CG   | -5.53 | 1.42        | 1.51     |
| 1   | 35-A  | 128 | CYS  | CB-SG   | -5.48 | 1.72        | 1.81     |
| 1   | 34-A  | 237 | TYR  | CD2-CE2 | -5.47 | 1.31        | 1.39     |
| 1   | 26-A  | 154 | TYR  | CB-CG   | 5.46  | 1.59        | 1.51     |
| 1   | 42-A  | 156 | CYS  | CB-SG   | -5.45 | 1.73        | 1.81     |
| 1   | 21-A  | 117 | CYS  | CB-SG   | -5.44 | 1.73        | 1.81     |
| 1   | 10-A  | 55  | GLU  | CG-CD   | 5.43  | 1.60        | 1.51     |
| 1   | 30-A  | 300 | CYS  | CB-SG   | -5.43 | 1.73        | 1.81     |
| 1   | 3-A   | 130 | MET  | CB-CG   | 5.42  | 1.68        | 1.51     |
| 1   | 29-A  | 217 | ARG  | CG-CD   | 5.41  | 1.65        | 1.51     |
| 1   | 43-A  | 288 | GLU  | CG-CD   | 5.40  | 1.60        | 1.51     |
| 1   | 27-A  | 298 | ARG  | CG-CD   | 5.39  | 1.65        | 1.51     |
| 1   | 14-A  | 154 | TYR  | CD2-CE2 | -5.39 | 1.31        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | 31-A  | 229 | ASP  | CB-CG   | 5.38  | 1.63        | 1.51     |
| 1   | 37-A  | 240 | GLU  | CB-CG   | 5.38  | 1.62        | 1.52     |
| 1   | 26-A  | 130 | MET  | CB-CG   | 5.37  | 1.68        | 1.51     |
| 1   | 38-A  | 117 | CYS  | CB-SG   | -5.36 | 1.73        | 1.81     |
| 1   | 30-A  | 55  | GLU  | CG-CD   | 5.35  | 1.59        | 1.51     |
| 1   | 6-A   | 154 | TYR  | CD1-CE1 | 5.35  | 1.47        | 1.39     |
| 1   | 29-A  | 288 | GLU  | CB-CG   | 5.33  | 1.62        | 1.52     |
| 1   | 4-A   | 128 | CYS  | CB-SG   | -5.32 | 1.73        | 1.81     |
| 1   | 18-A  | 290 | GLU  | CB-CG   | -5.32 | 1.42        | 1.52     |
| 1   | 20-A  | 165 | MET  | CB-CG   | 5.31  | 1.68        | 1.51     |
| 1   | 25-A  | 214 | ASN  | CB-CG   | 5.30  | 1.63        | 1.51     |
| 1   | 14-A  | 189 | GLN  | CG-CD   | 5.27  | 1.63        | 1.51     |
| 1   | 16-A  | 110 | GLN  | CB-CG   | 5.27  | 1.66        | 1.52     |
| 1   | 43-A  | 86  | VAL  | CB-CG2  | -5.26 | 1.41        | 1.52     |
| 1   | 35-A  | 290 | GLU  | CB-CG   | -5.24 | 1.42        | 1.52     |
| 1   | 19-A  | 290 | GLU  | CD-OE1  | 5.22  | 1.31        | 1.25     |
| 1   | 40-A  | 244 | GLN  | CB-CG   | 5.22  | 1.66        | 1.52     |
| 1   | 16-A  | 145 | CYS  | CB-SG   | 5.21  | 1.91        | 1.82     |
| 1   | 9-A   | 156 | CYS  | CB-SG   | 5.21  | 1.91        | 1.82     |
| 1   | 25-A  | 107 | GLN  | CG-CD   | 5.20  | 1.63        | 1.51     |
| 1   | 24-A  | 55  | GLU  | CG-CD   | -5.20 | 1.44        | 1.51     |
| 1   | 32-A  | 145 | CYS  | CB-SG   | -5.18 | 1.73        | 1.81     |
| 1   | 27-A  | 298 | ARG  | CB-CG   | 5.17  | 1.66        | 1.52     |
| 1   | 23-A  | 279 | ARG  | CB-CG   | 5.14  | 1.66        | 1.52     |
| 1   | 10-A  | 55  | GLU  | CB-CG   | 5.12  | 1.61        | 1.52     |
| 1   | 4-A   | 156 | CYS  | CB-SG   | -5.12 | 1.73        | 1.81     |
| 1   | 17-A  | 1   | SER  | N-CA    | -5.12 | 1.36        | 1.46     |
| 1   | 18-A  | 279 | ARG  | CG-CD   | 5.11  | 1.64        | 1.51     |
| 1   | 24-A  | 6   | MET  | CB-CG   | -5.11 | 1.35        | 1.51     |
| 1   | 29-A  | 107 | GLN  | CB-CG   | 5.11  | 1.66        | 1.52     |
| 1   | 19-A  | 165 | MET  | CB-CG   | 5.10  | 1.67        | 1.51     |
| 1   | 36-A  | 290 | GLU  | CB-CG   | -5.10 | 1.42        | 1.52     |
| 1   | 27-A  | 136 | ILE  | CG1-CD1 | 5.10  | 1.85        | 1.50     |
| 1   | 27-A  | 156 | CYS  | CB-SG   | -5.09 | 1.73        | 1.81     |
| 1   | 9-A   | 47  | GLU  | CG-CD   | 5.08  | 1.59        | 1.51     |
| 1   | 7-A   | 55  | GLU  | CB-CG   | 5.08  | 1.61        | 1.52     |
| 1   | 13-A  | 128 | CYS  | CB-SG   | 5.08  | 1.90        | 1.82     |
| 1   | 24-A  | 117 | CYS  | CB-SG   | -5.07 | 1.73        | 1.81     |
| 1   | 2-A   | 290 | GLU  | CD-OE1  | 5.05  | 1.31        | 1.25     |
| 1   | 35-A  | 55  | GLU  | CB-CG   | 5.05  | 1.61        | 1.52     |
| 1   | 16-A  | 300 | CYS  | CB-SG   | 5.03  | 1.90        | 1.82     |

All (195) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | 24-A  | 145 | CYS  | CA-CB-SG  | 18.24  | 146.83      | 114.00   |
| 1   | 12-A  | 145 | CYS  | CA-CB-SG  | 14.00  | 139.19      | 114.00   |
| 1   | 31-A  | 145 | CYS  | CA-CB-SG  | 13.24  | 137.83      | 114.00   |
| 1   | 17-A  | 145 | CYS  | CA-CB-SG  | 13.01  | 137.43      | 114.00   |
| 1   | 36-A  | 227 | LEU  | CA-CB-CG  | 12.38  | 143.77      | 115.30   |
| 1   | 11-A  | 145 | CYS  | CA-CB-SG  | 12.33  | 136.20      | 114.00   |
| 1   | 16-A  | 50  | LEU  | CA-CB-CG  | 11.74  | 142.30      | 115.30   |
| 1   | 9-A   | 141 | LEU  | CA-CB-CG  | 10.46  | 139.37      | 115.30   |
| 1   | 35-A  | 58  | LEU  | CA-CB-CG  | 10.33  | 139.05      | 115.30   |
| 1   | 34-A  | 128 | CYS  | CA-CB-SG  | -10.18 | 95.68       | 114.00   |
| 1   | 34-A  | 232 | LEU  | CA-CB-CG  | 10.13  | 138.60      | 115.30   |
| 1   | 31-A  | 153 | ASP  | CB-CG-OD1 | 10.06  | 127.35      | 118.30   |
| 1   | 9-A   | 145 | CYS  | CA-CB-SG  | 9.25   | 130.64      | 114.00   |
| 1   | 4-A   | 145 | CYS  | CA-CB-SG  | -9.20  | 97.43       | 114.00   |
| 1   | 39-A  | 156 | CYS  | CA-CB-SG  | 9.16   | 130.48      | 114.00   |
| 1   | 42-A  | 156 | CYS  | CA-CB-SG  | -9.15  | 97.53       | 114.00   |
| 1   | 27-A  | 227 | LEU  | CA-CB-CG  | 9.13   | 136.30      | 115.30   |
| 1   | 36-A  | 87  | LEU  | CA-CB-CG  | 8.88   | 135.71      | 115.30   |
| 1   | 4-A   | 130 | MET  | CG-SD-CE  | -8.65  | 86.36       | 100.20   |
| 1   | 33-A  | 50  | LEU  | CA-CB-CG  | 8.65   | 135.20      | 115.30   |
| 1   | 42-A  | 145 | CYS  | CA-CB-SG  | 8.56   | 129.40      | 114.00   |
| 1   | 41-A  | 240 | GLU  | CA-CB-CG  | 8.52   | 132.15      | 113.40   |
| 1   | 17-A  | 165 | MET  | CG-SD-CE  | 8.47   | 113.76      | 100.20   |
| 1   | 6-A   | 155 | ASP  | CB-CG-OD2 | 8.43   | 125.88      | 118.30   |
| 1   | 35-A  | 227 | LEU  | CA-CB-CG  | 8.26   | 134.31      | 115.30   |
| 1   | 4-A   | 117 | CYS  | CA-CB-SG  | 8.12   | 128.62      | 114.00   |
| 1   | 35-A  | 141 | LEU  | CA-CB-CG  | -8.06  | 96.75       | 115.30   |
| 1   | 13-A  | 232 | LEU  | CA-CB-CG  | 7.64   | 132.87      | 115.30   |
| 1   | 36-A  | 165 | MET  | CA-CB-CG  | 7.55   | 126.14      | 113.30   |
| 1   | 35-A  | 227 | LEU  | CB-CG-CD1 | 7.50   | 123.75      | 111.00   |
| 1   | 4-A   | 141 | LEU  | CB-CG-CD2 | 7.44   | 123.65      | 111.00   |
| 1   | 21-A  | 130 | MET  | CA-CB-CG  | 7.44   | 125.95      | 113.30   |
| 1   | 21-A  | 128 | CYS  | CA-CB-SG  | 7.38   | 127.28      | 114.00   |
| 1   | 23-A  | 154 | TYR  | CA-CB-CG  | 7.31   | 127.29      | 113.40   |
| 1   | 27-A  | 165 | MET  | CG-SD-CE  | 7.29   | 111.87      | 100.20   |
| 1   | 24-A  | 156 | CYS  | CA-CB-SG  | 7.24   | 127.04      | 114.00   |
| 1   | 3-A   | 49  | MET  | CG-SD-CE  | 7.19   | 111.70      | 100.20   |
| 1   | 27-A  | 227 | LEU  | CB-CG-CD2 | 7.19   | 123.22      | 111.00   |
| 1   | 36-A  | 6   | MET  | CB-CG-SD  | 7.18   | 133.95      | 112.40   |
| 1   | 6-A   | 128 | CYS  | CA-CB-SG  | -7.12  | 101.18      | 114.00   |
| 1   | 32-A  | 222 | ARG  | NE-CZ-NH1 | 7.00   | 123.80      | 120.30   |
| 1   | 6-A   | 235 | MET  | CG-SD-CE  | 6.98   | 111.37      | 100.20   |
| 1   | 43-A  | 155 | ASP  | CB-CG-OD1 | -6.98  | 112.02      | 118.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | 25-A  | 51  | ASN  | C-N-CD     | -6.83 | 105.56      | 120.60   |
| 1   | 31-A  | 58  | LEU  | CA-CB-CG   | 6.80  | 130.95      | 115.30   |
| 1   | 8-A   | 141 | LEU  | CA-CB-CG   | 6.77  | 130.87      | 115.30   |
| 1   | 27-A  | 305 | PHE  | CB-CG-CD1  | 6.74  | 125.52      | 120.80   |
| 1   | 6-A   | 235 | MET  | CB-CG-SD   | 6.73  | 132.58      | 112.40   |
| 1   | 2-A   | 290 | GLU  | OE1-CD-OE2 | 6.66  | 131.29      | 123.30   |
| 1   | 31-A  | 156 | CYS  | CA-CB-SG   | 6.62  | 125.91      | 114.00   |
| 1   | 28-A  | 145 | CYS  | CA-CB-SG   | -6.61 | 102.10      | 114.00   |
| 1   | 24-A  | 6   | MET  | CB-CG-SD   | -6.55 | 92.76       | 112.40   |
| 1   | 28-A  | 232 | LEU  | CA-CB-CG   | -6.53 | 100.28      | 115.30   |
| 1   | 38-A  | 302 | GLY  | N-CA-C     | 6.49  | 129.32      | 113.10   |
| 1   | 43-A  | 235 | MET  | CA-CB-CG   | 6.42  | 124.21      | 113.30   |
| 1   | 16-A  | 165 | MET  | CB-CG-SD   | -6.40 | 93.20       | 112.40   |
| 1   | 15-A  | 50  | LEU  | CB-CG-CD2  | 6.39  | 121.86      | 111.00   |
| 1   | 35-A  | 41  | HIS  | N-CA-CB    | 6.37  | 122.06      | 110.60   |
| 1   | 38-A  | 232 | LEU  | CA-CB-CG   | 6.37  | 129.95      | 115.30   |
| 1   | 42-A  | 232 | LEU  | CB-CG-CD1  | 6.37  | 121.82      | 111.00   |
| 1   | 3-A   | 286 | LEU  | CA-CB-CG   | 6.35  | 129.90      | 115.30   |
| 1   | 29-A  | 56  | ASP  | CB-CG-OD1  | 6.31  | 123.98      | 118.30   |
| 1   | 25-A  | 165 | MET  | CG-SD-CE   | -6.30 | 90.12       | 100.20   |
| 1   | 21-A  | 130 | MET  | CB-CG-SD   | 6.28  | 131.23      | 112.40   |
| 1   | 1-A   | 235 | MET  | CB-CG-SD   | 6.26  | 131.19      | 112.40   |
| 1   | 23-A  | 300 | CYS  | CA-CB-SG   | 6.20  | 125.16      | 114.00   |
| 1   | 19-A  | 165 | MET  | CB-CG-SD   | 6.18  | 130.94      | 112.40   |
| 1   | 34-A  | 58  | LEU  | CA-CB-CG   | 6.17  | 129.49      | 115.30   |
| 1   | 17-A  | 286 | LEU  | CA-CB-CG   | 6.16  | 129.46      | 115.30   |
| 1   | 20-A  | 286 | LEU  | CA-CB-CG   | 6.14  | 129.43      | 115.30   |
| 1   | 13-A  | 128 | CYS  | CA-CB-SG   | 6.13  | 125.03      | 114.00   |
| 1   | 23-A  | 227 | LEU  | CB-CG-CD2  | 6.12  | 121.41      | 111.00   |
| 1   | 29-A  | 128 | CYS  | CA-CB-SG   | 6.11  | 124.99      | 114.00   |
| 1   | 9-A   | 188 | ARG  | CB-CG-CD   | 6.09  | 127.43      | 111.60   |
| 1   | 16-A  | 279 | ARG  | NE-CZ-NH1  | 6.06  | 123.33      | 120.30   |
| 1   | 35-A  | 6   | MET  | CB-CG-SD   | 6.06  | 130.58      | 112.40   |
| 1   | 37-A  | 248 | ASP  | CB-CG-OD1  | 6.04  | 123.73      | 118.30   |
| 1   | 14-A  | 286 | LEU  | CA-CB-CG   | 6.03  | 129.16      | 115.30   |
| 1   | 43-A  | 298 | ARG  | NE-CZ-NH1  | 6.02  | 123.31      | 120.30   |
| 1   | 35-A  | 287 | LEU  | CA-CB-CG   | 6.02  | 129.14      | 115.30   |
| 1   | 4-A   | 156 | CYS  | CA-CB-SG   | -6.01 | 103.17      | 114.00   |
| 1   | 32-A  | 162 | MET  | CG-SD-CE   | 5.99  | 109.78      | 100.20   |
| 1   | 15-A  | 48  | ASP  | CB-CG-OD2  | -5.97 | 112.92      | 118.30   |
| 1   | 35-A  | 71  | GLY  | C-N-CA     | 5.97  | 136.62      | 121.70   |
| 1   | 30-A  | 272 | LEU  | CB-CG-CD1  | 5.94  | 121.10      | 111.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | 2-A   | 153 | ASP  | CB-CG-OD1  | -5.92 | 112.97      | 118.30   |
| 1   | 43-A  | 128 | CYS  | CB-CA-C    | -5.92 | 98.57       | 110.40   |
| 1   | 36-A  | 300 | CYS  | CA-CB-SG   | 5.90  | 124.62      | 114.00   |
| 1   | 27-A  | 162 | MET  | CG-SD-CE   | 5.88  | 109.61      | 100.20   |
| 1   | 34-A  | 140 | PHE  | C-N-CA     | 5.88  | 136.39      | 121.70   |
| 1   | 33-A  | 141 | LEU  | CB-CG-CD2  | 5.85  | 120.94      | 111.00   |
| 1   | 41-A  | 240 | GLU  | CB-CG-CD   | -5.85 | 98.41       | 114.20   |
| 1   | 2-A   | 276 | MET  | CG-SD-CE   | 5.84  | 109.55      | 100.20   |
| 1   | 27-A  | 305 | PHE  | CB-CG-CD2  | -5.84 | 116.71      | 120.80   |
| 1   | 7-A   | 49  | MET  | CA-CB-CG   | -5.84 | 103.38      | 113.30   |
| 1   | 42-A  | 271 | LEU  | CA-CB-CG   | 5.84  | 128.73      | 115.30   |
| 1   | 23-A  | 92  | ASP  | CB-CG-OD2  | 5.83  | 123.55      | 118.30   |
| 1   | 19-A  | 6   | MET  | CB-CG-SD   | 5.83  | 129.88      | 112.40   |
| 1   | 2-A   | 57  | LEU  | CB-CG-CD1  | -5.82 | 101.11      | 111.00   |
| 1   | 33-A  | 22  | CYS  | CA-CB-SG   | -5.82 | 103.53      | 114.00   |
| 1   | 28-A  | 130 | MET  | CG-SD-CE   | 5.80  | 109.49      | 100.20   |
| 1   | 39-A  | 300 | CYS  | CA-CB-SG   | 5.78  | 124.39      | 114.00   |
| 1   | 30-A  | 6   | MET  | CG-SD-CE   | -5.76 | 90.99       | 100.20   |
| 1   | 23-A  | 155 | ASP  | CB-CG-OD1  | 5.74  | 123.47      | 118.30   |
| 1   | 12-A  | 232 | LEU  | CA-CB-CG   | 5.73  | 128.47      | 115.30   |
| 1   | 12-A  | 4   | ARG  | CB-CG-CD   | 5.70  | 126.43      | 111.60   |
| 1   | 29-A  | 165 | MET  | CB-CG-SD   | -5.70 | 95.29       | 112.40   |
| 1   | 41-A  | 276 | MET  | CG-SD-CE   | -5.70 | 91.09       | 100.20   |
| 1   | 18-A  | 6   | MET  | CG-SD-CE   | -5.67 | 91.12       | 100.20   |
| 1   | 33-A  | 6   | MET  | CG-SD-CE   | 5.63  | 109.20      | 100.20   |
| 1   | 13-A  | 50  | LEU  | CA-CB-CG   | 5.61  | 128.21      | 115.30   |
| 1   | 41-A  | 6   | MET  | CG-SD-CE   | 5.61  | 109.18      | 100.20   |
| 1   | 20-A  | 130 | MET  | CG-SD-CE   | -5.59 | 91.25       | 100.20   |
| 1   | 2-A   | 87  | LEU  | CA-CB-CG   | 5.59  | 128.15      | 115.30   |
| 1   | 6-A   | 235 | MET  | CA-CB-CG   | 5.59  | 122.80      | 113.30   |
| 1   | 25-A  | 213 | ILE  | CG1-CB-CG2 | -5.58 | 99.13       | 111.40   |
| 1   | 22-A  | 276 | MET  | CA-CB-CG   | 5.57  | 122.78      | 113.30   |
| 1   | 4-A   | 50  | LEU  | CB-CG-CD2  | -5.55 | 101.56      | 111.00   |
| 1   | 29-A  | 56  | ASP  | CB-CG-OD2  | -5.54 | 113.31      | 118.30   |
| 1   | 33-A  | 271 | LEU  | CA-CB-CG   | 5.53  | 128.01      | 115.30   |
| 1   | 43-A  | 288 | GLU  | OE1-CD-OE2 | -5.52 | 116.67      | 123.30   |
| 1   | 15-A  | 141 | LEU  | CB-CG-CD1  | 5.52  | 120.38      | 111.00   |
| 1   | 9-A   | 300 | CYS  | CA-CB-SG   | -5.51 | 104.08      | 114.00   |
| 1   | 6-A   | 75  | LEU  | CA-CB-CG   | 5.51  | 127.97      | 115.30   |
| 1   | 11-A  | 48  | ASP  | CB-CG-OD1  | -5.50 | 113.35      | 118.30   |
| 1   | 26-A  | 216 | ASP  | CB-CG-OD1  | -5.50 | 113.35      | 118.30   |
| 1   | 6-A   | 145 | CYS  | CA-CB-SG   | 5.50  | 123.89      | 114.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | 5-A   | 229 | ASP  | CB-CG-OD2  | 5.49  | 123.24      | 118.30   |
| 1   | 19-A  | 165 | MET  | N-CA-CB    | 5.48  | 120.46      | 110.60   |
| 1   | 7-A   | 128 | CYS  | CA-CB-SG   | -5.46 | 104.17      | 114.00   |
| 1   | 12-A  | 4   | ARG  | CA-CB-CG   | 5.46  | 125.41      | 113.40   |
| 1   | 21-A  | 88  | LYS  | CD-CE-NZ   | 5.46  | 124.25      | 111.70   |
| 1   | 42-A  | 73  | VAL  | CA-CB-CG2  | -5.45 | 102.73      | 110.90   |
| 1   | 37-A  | 88  | LYS  | CD-CE-NZ   | 5.45  | 124.23      | 111.70   |
| 1   | 28-A  | 126 | TYR  | CA-CB-CG   | 5.45  | 123.75      | 113.40   |
| 1   | 2-A   | 87  | LEU  | CB-CG-CD1  | 5.44  | 120.25      | 111.00   |
| 1   | 19-A  | 229 | ASP  | CB-CG-OD1  | 5.42  | 123.17      | 118.30   |
| 1   | 30-A  | 232 | LEU  | CA-CB-CG   | 5.40  | 127.71      | 115.30   |
| 1   | 34-A  | 6   | MET  | CG-SD-CE   | 5.39  | 108.82      | 100.20   |
| 1   | 23-A  | 227 | LEU  | CA-CB-CG   | 5.39  | 127.69      | 115.30   |
| 1   | 34-A  | 48  | ASP  | CB-CG-OD2  | -5.37 | 113.47      | 118.30   |
| 1   | 13-A  | 156 | CYS  | CA-CB-SG   | 5.36  | 123.64      | 114.00   |
| 1   | 25-A  | 82  | MET  | CG-SD-CE   | 5.34  | 108.75      | 100.20   |
| 1   | 21-A  | 49  | MET  | CG-SD-CE   | -5.34 | 91.66       | 100.20   |
| 1   | 24-A  | 271 | LEU  | CA-CB-CG   | 5.34  | 127.58      | 115.30   |
| 1   | 5-A   | 271 | LEU  | CB-CG-CD1  | -5.33 | 101.94      | 111.00   |
| 1   | 10-A  | 57  | LEU  | CB-CG-CD1  | -5.32 | 101.96      | 111.00   |
| 1   | 15-A  | 286 | LEU  | CA-CB-CG   | 5.29  | 127.46      | 115.30   |
| 1   | 28-A  | 235 | MET  | CG-SD-CE   | -5.28 | 91.75       | 100.20   |
| 1   | 35-A  | 271 | LEU  | CA-CB-CG   | 5.28  | 127.44      | 115.30   |
| 1   | 13-A  | 49  | MET  | CB-CG-SD   | -5.28 | 96.57       | 112.40   |
| 1   | 32-A  | 141 | LEU  | CA-CB-CG   | 5.28  | 127.43      | 115.30   |
| 1   | 35-A  | 41  | HIS  | CA-CB-CG   | 5.26  | 122.55      | 113.60   |
| 1   | 38-A  | 165 | MET  | CG-SD-CE   | 5.25  | 108.61      | 100.20   |
| 1   | 29-A  | 229 | ASP  | CB-CG-OD1  | 5.25  | 123.03      | 118.30   |
| 1   | 24-A  | 154 | TYR  | CA-CB-CG   | 5.25  | 123.37      | 113.40   |
| 1   | 4-A   | 277 | ASN  | CB-CA-C    | 5.25  | 120.89      | 110.40   |
| 1   | 42-A  | 87  | LEU  | CA-CB-CG   | 5.24  | 127.35      | 115.30   |
| 1   | 3-A   | 235 | MET  | CA-CB-CG   | 5.24  | 122.20      | 113.30   |
| 1   | 24-A  | 155 | ASP  | CB-CG-OD1  | -5.23 | 113.59      | 118.30   |
| 1   | 6-A   | 89  | LEU  | CA-CB-CG   | 5.22  | 127.31      | 115.30   |
| 1   | 18-A  | 188 | ARG  | CB-CG-CD   | 5.22  | 125.18      | 111.60   |
| 1   | 36-A  | 92  | ASP  | CB-CG-OD1  | 5.22  | 123.00      | 118.30   |
| 1   | 35-A  | 248 | ASP  | CB-CG-OD1  | 5.21  | 122.99      | 118.30   |
| 1   | 39-A  | 298 | ARG  | CA-CB-CG   | 5.21  | 124.87      | 113.40   |
| 1   | 33-A  | 242 | LEU  | CB-CG-CD2  | 5.20  | 119.83      | 111.00   |
| 1   | 7-A   | 276 | MET  | CG-SD-CE   | -5.19 | 91.89       | 100.20   |
| 1   | 43-A  | 299 | GLN  | C-N-CA     | 5.19  | 134.68      | 121.70   |
| 1   | 41-A  | 290 | GLU  | OE1-CD-OE2 | 5.17  | 129.51      | 123.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | 26-A  | 67  | LEU  | CA-CB-CG  | 5.17  | 127.19      | 115.30   |
| 1   | 11-A  | 48  | ASP  | CB-CG-OD2 | 5.16  | 122.94      | 118.30   |
| 1   | 17-A  | 232 | LEU  | CB-CG-CD2 | 5.16  | 119.77      | 111.00   |
| 1   | 22-A  | 153 | ASP  | CB-CG-OD2 | 5.15  | 122.94      | 118.30   |
| 1   | 22-A  | 155 | ASP  | CB-CG-OD1 | 5.15  | 122.93      | 118.30   |
| 1   | 2-A   | 300 | CYS  | CA-CB-SG  | 5.14  | 123.26      | 114.00   |
| 1   | 21-A  | 298 | ARG  | NE-CZ-NH1 | 5.14  | 122.87      | 120.30   |
| 1   | 37-A  | 155 | ASP  | CB-CG-OD2 | 5.14  | 122.92      | 118.30   |
| 1   | 13-A  | 305 | PHE  | CB-CG-CD1 | 5.14  | 124.39      | 120.80   |
| 1   | 18-A  | 6   | MET  | CB-CG-SD  | 5.13  | 127.79      | 112.40   |
| 1   | 34-A  | 12  | LYS  | CB-CG-CD  | 5.13  | 124.94      | 111.60   |
| 1   | 42-A  | 298 | ARG  | CG-CD-NE  | 5.13  | 122.57      | 111.80   |
| 1   | 26-A  | 49  | MET  | CB-CG-SD  | 5.12  | 127.76      | 112.40   |
| 1   | 31-A  | 141 | LEU  | CA-CB-CG  | 5.12  | 127.07      | 115.30   |
| 1   | 1-A   | 188 | ARG  | NE-CZ-NH1 | 5.09  | 122.85      | 120.30   |
| 1   | 5-A   | 92  | ASP  | CB-CG-OD2 | 5.07  | 122.86      | 118.30   |
| 1   | 43-A  | 67  | LEU  | CA-CB-CG  | 5.06  | 126.94      | 115.30   |
| 1   | 18-A  | 300 | CYS  | CA-CB-SG  | -5.04 | 104.92      | 114.00   |
| 1   | 26-A  | 287 | LEU  | CB-CG-CD1 | -5.04 | 102.43      | 111.00   |
| 1   | 9-A   | 235 | MET  | CB-CG-SD  | 5.04  | 127.52      | 112.40   |
| 1   | 19-A  | 156 | CYS  | CA-CB-SG  | -5.03 | 104.95      | 114.00   |
| 1   | 36-A  | 305 | PHE  | CB-CG-CD1 | -5.02 | 117.28      | 120.80   |
| 1   | 9-A   | 242 | LEU  | CA-CB-CG  | 5.02  | 126.85      | 115.30   |
| 1   | 9-A   | 97  | LYS  | CD-CE-NZ  | 5.02  | 123.24      | 111.70   |
| 1   | 25-A  | 304 | THR  | C-N-CA    | -5.00 | 109.19      | 121.70   |
| 1   | 31-A  | 56  | ASP  | CB-CG-OD2 | -5.00 | 113.80      | 118.30   |

There are no chirality outliers.

All (292) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | 1-A   | 1   | SER  | Peptide   |
| 1   | 1-A   | 188 | ARG  | Sidechain |
| 1   | 1-A   | 25  | THR  | Peptide   |
| 1   | 1-A   | 300 | CYS  | Peptide   |
| 1   | 1-A   | 44  | CYS  | Peptide   |
| 1   | 10-A  | 1   | SER  | Peptide   |
| 1   | 10-A  | 23  | GLY  | Peptide   |
| 1   | 10-A  | 24  | THR  | Peptide   |
| 1   | 10-A  | 71  | GLY  | Peptide   |
| 1   | 11-A  | 151 | ASN  | Peptide   |
| 1   | 11-A  | 188 | ARG  | Sidechain |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Group</b>      |
|------------|--------------|------------|-------------|-------------------|
| 1          | 11-A         | 191        | ALA         | Peptide           |
| 1          | 11-A         | 192        | GLN         | Peptide           |
| 1          | 11-A         | 301        | SER         | Peptide           |
| 1          | 11-A         | 303        | VAL         | Peptide           |
| 1          | 11-A         | 70         | ALA         | Peptide           |
| 1          | 12-A         | 142        | ASN         | Peptide           |
| 1          | 12-A         | 300        | CYS         | Peptide           |
| 1          | 12-A         | 305        | PHE         | Peptide           |
| 1          | 12-A         | 4          | ARG         | Sidechain         |
| 1          | 12-A         | 52         | PRO         | Peptide           |
| 1          | 12-A         | 60         | ARG         | Peptide           |
| 1          | 13-A         | 298        | ARG         | Sidechain         |
| 1          | 13-A         | 300        | CYS         | Peptide           |
| 1          | 13-A         | 301        | SER         | Peptide           |
| 1          | 13-A         | 4          | ARG         | Sidechain         |
| 1          | 13-A         | 71         | GLY         | Peptide           |
| 1          | 14-A         | 153        | ASP         | Peptide           |
| 1          | 14-A         | 300        | CYS         | Mainchain,Peptide |
| 1          | 14-A         | 303        | VAL         | Peptide           |
| 1          | 14-A         | 304        | THR         | Peptide           |
| 1          | 14-A         | 4          | ARG         | Sidechain         |
| 1          | 15-A         | 1          | SER         | Peptide           |
| 1          | 15-A         | 278        | GLY         | Peptide           |
| 1          | 15-A         | 300        | CYS         | Peptide           |
| 1          | 15-A         | 301        | SER         | Peptide           |
| 1          | 15-A         | 303        | VAL         | Peptide           |
| 1          | 15-A         | 45         | THR         | Peptide           |
| 1          | 15-A         | 46         | SER         | Peptide           |
| 1          | 15-A         | 71         | GLY         | Peptide           |
| 1          | 16-A         | 1          | SER         | Peptide           |
| 1          | 16-A         | 220        | LEU         | Peptide           |
| 1          | 16-A         | 276        | MET         | Peptide           |
| 1          | 16-A         | 279        | ARG         | Sidechain         |
| 1          | 16-A         | 300        | CYS         | Peptide           |
| 1          | 16-A         | 70         | ALA         | Peptide           |
| 1          | 17-A         | 217        | ARG         | Peptide           |
| 1          | 17-A         | 24         | THR         | Peptide           |
| 1          | 17-A         | 302        | GLY         | Peptide           |
| 1          | 17-A         | 48         | ASP         | Peptide           |
| 1          | 17-A         | 72         | ASN         | Peptide           |
| 1          | 18-A         | 22         | CYS         | Peptide           |
| 1          | 18-A         | 302        | GLY         | Peptide           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Group</b> |
|------------|--------------|------------|-------------|--------------|
| 1          | 19-A         | 164        | HIS         | Peptide      |
| 1          | 19-A         | 165        | MET         | Peptide      |
| 1          | 19-A         | 188        | ARG         | Sidechain    |
| 1          | 19-A         | 213        | ILE         | Peptide      |
| 1          | 19-A         | 217        | ARG         | Sidechain    |
| 1          | 19-A         | 222        | ARG         | Sidechain    |
| 1          | 19-A         | 276        | MET         | Peptide      |
| 1          | 19-A         | 303        | VAL         | Peptide      |
| 1          | 19-A         | 49         | MET         | Peptide      |
| 1          | 19-A         | 72         | ASN         | Peptide      |
| 1          | 19-A         | 74         | GLN         | Peptide      |
| 1          | 2-A          | 152        | ILE         | Peptide      |
| 1          | 2-A          | 156        | CYS         | Peptide      |
| 1          | 2-A          | 217        | ARG         | Sidechain    |
| 1          | 2-A          | 24         | THR         | Peptide      |
| 1          | 2-A          | 276        | MET         | Peptide      |
| 1          | 2-A          | 279        | ARG         | Sidechain    |
| 1          | 2-A          | 298        | ARG         | Peptide      |
| 1          | 2-A          | 301        | SER         | Peptide      |
| 1          | 2-A          | 302        | GLY         | Peptide      |
| 1          | 2-A          | 44         | CYS         | Peptide      |
| 1          | 2-A          | 48         | ASP         | Peptide      |
| 1          | 2-A          | 60         | ARG         | Peptide      |
| 1          | 20-A         | 188        | ARG         | Sidechain    |
| 1          | 20-A         | 302        | GLY         | Peptide      |
| 1          | 20-A         | 303        | VAL         | Peptide      |
| 1          | 20-A         | 45         | THR         | Peptide      |
| 1          | 20-A         | 73         | VAL         | Peptide      |
| 1          | 21-A         | 188        | ARG         | Sidechain    |
| 1          | 21-A         | 69         | GLN         | Peptide      |
| 1          | 21-A         | 71         | GLY         | Peptide      |
| 1          | 21-A         | 73         | VAL         | Peptide      |
| 1          | 22-A         | 298        | ARG         | Sidechain    |
| 1          | 23-A         | 128        | CYS         | Peptide      |
| 1          | 23-A         | 141        | LEU         | Peptide      |
| 1          | 23-A         | 153        | ASP         | Peptide      |
| 1          | 23-A         | 303        | VAL         | Peptide      |
| 1          | 23-A         | 52         | PRO         | Peptide      |
| 1          | 23-A         | 92         | ASP         | Peptide      |
| 1          | 24-A         | 128        | CYS         | Peptide      |
| 1          | 24-A         | 154        | TYR         | Peptide      |
| 1          | 24-A         | 156        | CYS         | Peptide      |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | 24-A  | 241 | PRO  | Peptide   |
| 1   | 24-A  | 298 | ARG  | Sidechain |
| 1   | 24-A  | 4   | ARG  | Sidechain |
| 1   | 24-A  | 45  | THR  | Peptide   |
| 1   | 24-A  | 70  | ALA  | Peptide   |
| 1   | 24-A  | 73  | VAL  | Peptide   |
| 1   | 25-A  | 301 | SER  | Peptide   |
| 1   | 25-A  | 305 | PHE  | Peptide   |
| 1   | 25-A  | 4   | ARG  | Sidechain |
| 1   | 25-A  | 50  | LEU  | Peptide   |
| 1   | 25-A  | 60  | ARG  | Peptide   |
| 1   | 25-A  | 70  | ALA  | Peptide   |
| 1   | 25-A  | 71  | GLY  | Peptide   |
| 1   | 25-A  | 73  | VAL  | Peptide   |
| 1   | 26-A  | 153 | ASP  | Peptide   |
| 1   | 26-A  | 73  | VAL  | Peptide   |
| 1   | 27-A  | 119 | ASN  | Peptide   |
| 1   | 27-A  | 141 | LEU  | Peptide   |
| 1   | 27-A  | 154 | TYR  | Peptide   |
| 1   | 27-A  | 188 | ARG  | Sidechain |
| 1   | 27-A  | 298 | ARG  | Sidechain |
| 1   | 27-A  | 299 | GLN  | Peptide   |
| 1   | 27-A  | 304 | THR  | Peptide   |
| 1   | 27-A  | 60  | ARG  | Peptide   |
| 1   | 27-A  | 73  | VAL  | Peptide   |
| 1   | 28-A  | 101 | TYR  | Peptide   |
| 1   | 28-A  | 120 | GLY  | Peptide   |
| 1   | 28-A  | 217 | ARG  | Sidechain |
| 1   | 28-A  | 235 | MET  | Peptide   |
| 1   | 28-A  | 305 | PHE  | Peptide   |
| 1   | 28-A  | 59  | ILE  | Peptide   |
| 1   | 28-A  | 60  | ARG  | Peptide   |
| 1   | 28-A  | 72  | ASN  | Peptide   |
| 1   | 29-A  | 120 | GLY  | Peptide   |
| 1   | 29-A  | 23  | GLY  | Peptide   |
| 1   | 29-A  | 24  | THR  | Peptide   |
| 1   | 29-A  | 274 | ASN  | Peptide   |
| 1   | 29-A  | 302 | GLY  | Peptide   |
| 1   | 29-A  | 60  | ARG  | Peptide   |
| 1   | 29-A  | 70  | ALA  | Peptide   |
| 1   | 29-A  | 73  | VAL  | Peptide   |
| 1   | 3-A   | 276 | MET  | Peptide   |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Group</b> |
|------------|--------------|------------|-------------|--------------|
| 1          | 3-A          | 277        | ASN         | Peptide      |
| 1          | 3-A          | 301        | SER         | Peptide      |
| 1          | 3-A          | 302        | GLY         | Peptide      |
| 1          | 3-A          | 305        | PHE         | Peptide      |
| 1          | 3-A          | 45         | THR         | Peptide      |
| 1          | 3-A          | 47         | GLU         | Peptide      |
| 1          | 3-A          | 59         | ILE         | Peptide      |
| 1          | 3-A          | 60         | ARG         | Peptide      |
| 1          | 3-A          | 70         | ALA         | Peptide      |
| 1          | 30-A         | 232        | LEU         | Peptide      |
| 1          | 30-A         | 235        | MET         | Peptide      |
| 1          | 30-A         | 275        | GLY         | Peptide      |
| 1          | 30-A         | 279        | ARG         | Sidechain    |
| 1          | 30-A         | 298        | ARG         | Sidechain    |
| 1          | 30-A         | 305        | PHE         | Peptide      |
| 1          | 30-A         | 44         | CYS         | Peptide      |
| 1          | 30-A         | 45         | THR         | Peptide      |
| 1          | 30-A         | 49         | MET         | Peptide      |
| 1          | 31-A         | 235        | MET         | Peptide      |
| 1          | 31-A         | 274        | ASN         | Peptide      |
| 1          | 31-A         | 275        | GLY         | Peptide      |
| 1          | 32-A         | 190        | THR         | Peptide      |
| 1          | 32-A         | 217        | ARG         | Sidechain    |
| 1          | 32-A         | 232        | LEU         | Peptide      |
| 1          | 32-A         | 302        | GLY         | Peptide      |
| 1          | 32-A         | 60         | ARG         | Sidechain    |
| 1          | 32-A         | 73         | VAL         | Peptide      |
| 1          | 33-A         | 139        | SER         | Peptide      |
| 1          | 33-A         | 141        | LEU         | Peptide      |
| 1          | 33-A         | 234        | ALA         | Peptide      |
| 1          | 33-A         | 235        | MET         | Peptide      |
| 1          | 33-A         | 298        | ARG         | Sidechain    |
| 1          | 33-A         | 300        | CYS         | Peptide      |
| 1          | 33-A         | 304        | THR         | Peptide      |
| 1          | 33-A         | 46         | SER         | Peptide      |
| 1          | 33-A         | 60         | ARG         | Peptide      |
| 1          | 34-A         | 140        | PHE         | Mainchain    |
| 1          | 34-A         | 153        | ASP         | Peptide      |
| 1          | 34-A         | 232        | LEU         | Peptide      |
| 1          | 34-A         | 233        | VAL         | Peptide      |
| 1          | 34-A         | 234        | ALA         | Peptide      |
| 1          | 34-A         | 279        | ARG         | Sidechain    |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | 34-A  | 297 | VAL  | Peptide   |
| 1   | 34-A  | 304 | THR  | Peptide   |
| 1   | 34-A  | 60  | ARG  | Sidechain |
| 1   | 35-A  | 105 | ARG  | Sidechain |
| 1   | 35-A  | 233 | VAL  | Peptide   |
| 1   | 35-A  | 234 | ALA  | Peptide   |
| 1   | 35-A  | 235 | MET  | Peptide   |
| 1   | 35-A  | 299 | GLN  | Peptide   |
| 1   | 35-A  | 4   | ARG  | Sidechain |
| 1   | 36-A  | 216 | ASP  | Peptide   |
| 1   | 36-A  | 233 | VAL  | Peptide   |
| 1   | 36-A  | 234 | ALA  | Peptide   |
| 1   | 36-A  | 299 | GLN  | Peptide   |
| 1   | 36-A  | 304 | THR  | Peptide   |
| 1   | 36-A  | 45  | THR  | Peptide   |
| 1   | 36-A  | 92  | ASP  | Peptide   |
| 1   | 37-A  | 128 | CYS  | Peptide   |
| 1   | 37-A  | 234 | ALA  | Peptide   |
| 1   | 37-A  | 304 | THR  | Peptide   |
| 1   | 38-A  | 152 | ILE  | Peptide   |
| 1   | 38-A  | 153 | ASP  | Peptide   |
| 1   | 38-A  | 231 | ASN  | Peptide   |
| 1   | 38-A  | 301 | SER  | Peptide   |
| 1   | 38-A  | 72  | ASN  | Peptide   |
| 1   | 38-A  | 73  | VAL  | Peptide   |
| 1   | 38-A  | 97  | LYS  | Peptide   |
| 1   | 39-A  | 152 | ILE  | Peptide   |
| 1   | 39-A  | 155 | ASP  | Peptide   |
| 1   | 39-A  | 23  | GLY  | Peptide   |
| 1   | 39-A  | 233 | VAL  | Peptide   |
| 1   | 39-A  | 234 | ALA  | Peptide   |
| 1   | 39-A  | 25  | THR  | Peptide   |
| 1   | 39-A  | 299 | GLN  | Peptide   |
| 1   | 39-A  | 303 | VAL  | Peptide   |
| 1   | 39-A  | 304 | THR  | Peptide   |
| 1   | 4-A   | 221 | ASN  | Peptide   |
| 1   | 4-A   | 275 | GLY  | Peptide   |
| 1   | 4-A   | 278 | GLY  | Peptide   |
| 1   | 4-A   | 279 | ARG  | Sidechain |
| 1   | 4-A   | 298 | ARG  | Sidechain |
| 1   | 4-A   | 300 | CYS  | Peptide   |
| 1   | 4-A   | 301 | SER  | Peptide   |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | 4-A   | 305 | PHE  | Peptide   |
| 1   | 40-A  | 233 | VAL  | Peptide   |
| 1   | 40-A  | 234 | ALA  | Peptide   |
| 1   | 40-A  | 302 | GLY  | Peptide   |
| 1   | 40-A  | 304 | THR  | Peptide   |
| 1   | 41-A  | 1   | SER  | Peptide   |
| 1   | 41-A  | 141 | LEU  | Peptide   |
| 1   | 41-A  | 190 | THR  | Peptide   |
| 1   | 41-A  | 233 | VAL  | Peptide   |
| 1   | 41-A  | 235 | MET  | Peptide   |
| 1   | 41-A  | 303 | VAL  | Peptide   |
| 1   | 41-A  | 44  | CYS  | Peptide   |
| 1   | 42-A  | 120 | GLY  | Peptide   |
| 1   | 42-A  | 141 | LEU  | Peptide   |
| 1   | 42-A  | 155 | ASP  | Peptide   |
| 1   | 42-A  | 220 | LEU  | Peptide   |
| 1   | 42-A  | 232 | LEU  | Peptide   |
| 1   | 42-A  | 233 | VAL  | Peptide   |
| 1   | 42-A  | 234 | ALA  | Peptide   |
| 1   | 42-A  | 279 | ARG  | Sidechain |
| 1   | 42-A  | 298 | ARG  | Sidechain |
| 1   | 42-A  | 304 | THR  | Peptide   |
| 1   | 42-A  | 4   | ARG  | Sidechain |
| 1   | 42-A  | 70  | ALA  | Peptide   |
| 1   | 43-A  | 1   | SER  | Peptide   |
| 1   | 43-A  | 128 | CYS  | Peptide   |
| 1   | 43-A  | 141 | LEU  | Peptide   |
| 1   | 43-A  | 142 | ASN  | Peptide   |
| 1   | 43-A  | 156 | CYS  | Peptide   |
| 1   | 43-A  | 300 | CYS  | Peptide   |
| 1   | 43-A  | 302 | GLY  | Peptide   |
| 1   | 43-A  | 50  | LEU  | Peptide   |
| 1   | 43-A  | 72  | ASN  | Peptide   |
| 1   | 5-A   | 141 | LEU  | Peptide   |
| 1   | 5-A   | 154 | TYR  | Peptide   |
| 1   | 5-A   | 220 | LEU  | Peptide   |
| 1   | 5-A   | 23  | GLY  | Peptide   |
| 1   | 5-A   | 24  | THR  | Peptide   |
| 1   | 5-A   | 278 | GLY  | Peptide   |
| 1   | 5-A   | 279 | ARG  | Sidechain |
| 1   | 5-A   | 302 | GLY  | Peptide   |
| 1   | 5-A   | 303 | VAL  | Peptide   |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | 5-A   | 48  | ASP  | Peptide   |
| 1   | 5-A   | 60  | ARG  | Peptide   |
| 1   | 5-A   | 70  | ALA  | Peptide   |
| 1   | 5-A   | 71  | GLY  | Peptide   |
| 1   | 5-A   | 72  | ASN  | Peptide   |
| 1   | 6-A   | 23  | GLY  | Peptide   |
| 1   | 6-A   | 24  | THR  | Peptide   |
| 1   | 6-A   | 277 | ASN  | Peptide   |
| 1   | 6-A   | 61  | LYS  | Peptide   |
| 1   | 7-A   | 141 | LEU  | Peptide   |
| 1   | 7-A   | 150 | PHE  | Peptide   |
| 1   | 7-A   | 217 | ARG  | Sidechain |
| 1   | 7-A   | 275 | GLY  | Peptide   |
| 1   | 7-A   | 278 | GLY  | Peptide   |
| 1   | 7-A   | 280 | THR  | Peptide   |
| 1   | 7-A   | 302 | GLY  | Peptide   |
| 1   | 8-A   | 157 | VAL  | Peptide   |
| 1   | 8-A   | 298 | ARG  | Sidechain |
| 1   | 8-A   | 300 | CYS  | Peptide   |
| 1   | 8-A   | 60  | ARG  | Sidechain |
| 1   | 8-A   | 71  | GLY  | Peptide   |
| 1   | 9-A   | 142 | ASN  | Peptide   |
| 1   | 9-A   | 152 | ILE  | Peptide   |
| 1   | 9-A   | 153 | ASP  | Peptide   |
| 1   | 9-A   | 155 | ASP  | Peptide   |
| 1   | 9-A   | 23  | GLY  | Peptide   |
| 1   | 9-A   | 24  | THR  | Peptide   |
| 1   | 9-A   | 275 | GLY  | Peptide   |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1-A   | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 2-A   | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 3-A   | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 4-A   | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 5-A   | 2367  | 2314     | 2313     | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 6-A   | 2367  | 2314     | 2314     | 0       | 0            |
| 1   | 7-A   | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 8-A   | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 9-A   | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 10-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 11-A  | 2367  | 2314     | 2314     | 0       | 0            |
| 1   | 12-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 13-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 14-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 15-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 16-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 17-A  | 2367  | 2314     | 2314     | 0       | 0            |
| 1   | 18-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 19-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 20-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 21-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 22-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 23-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 24-A  | 2367  | 2314     | 2314     | 0       | 0            |
| 1   | 25-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 26-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 27-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 28-A  | 2367  | 2314     | 2314     | 0       | 0            |
| 1   | 29-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 30-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 31-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 32-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 33-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 34-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 35-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 36-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 37-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 38-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 39-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 40-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 41-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 1   | 42-A  | 2367  | 2314     | 2314     | 0       | 0            |
| 1   | 43-A  | 2367  | 2314     | 2313     | 0       | 0            |
| 2   | 1-A   | 28    | 42       | 42       | 0       | 0            |
| 2   | 2-A   | 28    | 42       | 42       | 0       | 0            |
| 2   | 3-A   | 28    | 42       | 42       | 0       | 0            |
| 2   | 4-A   | 28    | 42       | 42       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | 5-A   | 28    | 42       | 42       | 0       | 0            |
| 2   | 6-A   | 28    | 42       | 42       | 0       | 0            |
| 2   | 7-A   | 28    | 42       | 42       | 0       | 0            |
| 2   | 8-A   | 28    | 42       | 42       | 0       | 0            |
| 2   | 9-A   | 28    | 42       | 42       | 0       | 0            |
| 2   | 10-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 11-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 12-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 13-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 14-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 15-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 16-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 17-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 18-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 19-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 20-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 21-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 22-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 23-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 24-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 25-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 26-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 27-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 28-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 29-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 30-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 31-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 32-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 33-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 34-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 35-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 36-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 37-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 38-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 39-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 40-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 41-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 42-A  | 28    | 42       | 42       | 0       | 0            |
| 2   | 43-A  | 28    | 42       | 42       | 0       | 0            |
| 3   | 1-A   | 1     | 0        | 0        | 0       | 0            |
| 3   | 2-A   | 1     | 0        | 0        | 0       | 0            |
| 3   | 3-A   | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | 4-A   | 1     | 0        | 0        | 0       | 0            |
| 3   | 5-A   | 1     | 0        | 0        | 0       | 0            |
| 3   | 6-A   | 1     | 0        | 0        | 0       | 0            |
| 3   | 7-A   | 1     | 0        | 0        | 0       | 0            |
| 3   | 8-A   | 1     | 0        | 0        | 0       | 0            |
| 3   | 9-A   | 1     | 0        | 0        | 0       | 0            |
| 3   | 10-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 11-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 12-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 13-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 14-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 15-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 16-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 17-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 18-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 19-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 20-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 21-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 22-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 23-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 24-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 25-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 26-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 27-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 28-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 29-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 30-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 31-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 32-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 33-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 34-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 35-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 36-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 37-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 38-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 39-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 40-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 41-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 42-A  | 1     | 0        | 0        | 0       | 0            |
| 3   | 43-A  | 1     | 0        | 0        | 0       | 0            |
| 4   | 1-A   | 148   | 0        | 0        | 0       | 0            |
| 4   | 2-A   | 135   | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 4   | 3-A   | 134    | 0        | 0        | 0       | 0            |
| 4   | 4-A   | 142    | 0        | 0        | 0       | 0            |
| 4   | 5-A   | 140    | 0        | 0        | 0       | 0            |
| 4   | 6-A   | 145    | 0        | 0        | 0       | 0            |
| 4   | 7-A   | 133    | 0        | 0        | 0       | 0            |
| 4   | 8-A   | 131    | 0        | 0        | 0       | 0            |
| 4   | 9-A   | 147    | 0        | 0        | 0       | 0            |
| 4   | 10-A  | 146    | 0        | 0        | 0       | 0            |
| 4   | 11-A  | 137    | 0        | 0        | 0       | 0            |
| 4   | 12-A  | 141    | 0        | 0        | 0       | 0            |
| 4   | 13-A  | 130    | 0        | 0        | 0       | 0            |
| 4   | 14-A  | 135    | 0        | 0        | 0       | 0            |
| 4   | 15-A  | 136    | 0        | 0        | 0       | 0            |
| 4   | 16-A  | 121    | 0        | 0        | 0       | 0            |
| 4   | 17-A  | 152    | 0        | 0        | 0       | 0            |
| 4   | 18-A  | 122    | 0        | 0        | 0       | 0            |
| 4   | 19-A  | 141    | 0        | 0        | 0       | 0            |
| 4   | 20-A  | 131    | 0        | 0        | 0       | 0            |
| 4   | 21-A  | 142    | 0        | 0        | 0       | 0            |
| 4   | 22-A  | 139    | 0        | 0        | 0       | 0            |
| 4   | 23-A  | 134    | 0        | 0        | 0       | 0            |
| 4   | 24-A  | 138    | 0        | 0        | 0       | 0            |
| 4   | 25-A  | 145    | 0        | 0        | 0       | 0            |
| 4   | 26-A  | 125    | 0        | 0        | 0       | 0            |
| 4   | 27-A  | 144    | 0        | 0        | 0       | 0            |
| 4   | 28-A  | 135    | 0        | 0        | 0       | 0            |
| 4   | 29-A  | 144    | 0        | 0        | 0       | 0            |
| 4   | 30-A  | 146    | 0        | 0        | 0       | 0            |
| 4   | 31-A  | 136    | 0        | 0        | 0       | 0            |
| 4   | 32-A  | 122    | 0        | 0        | 0       | 0            |
| 4   | 33-A  | 134    | 0        | 0        | 0       | 0            |
| 4   | 34-A  | 123    | 0        | 0        | 0       | 0            |
| 4   | 35-A  | 130    | 0        | 0        | 0       | 0            |
| 4   | 36-A  | 139    | 0        | 0        | 0       | 0            |
| 4   | 37-A  | 140    | 0        | 0        | 0       | 0            |
| 4   | 38-A  | 120    | 0        | 0        | 0       | 0            |
| 4   | 39-A  | 145    | 0        | 0        | 0       | 0            |
| 4   | 40-A  | 121    | 0        | 0        | 0       | 0            |
| 4   | 41-A  | 127    | 0        | 0        | 0       | 0            |
| 4   | 42-A  | 133    | 0        | 0        | 0       | 0            |
| 4   | 43-A  | 140    | 0        | 0        | 0       | 0            |
| All | All   | 108877 | 101308   | 101271   | 0       | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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 |   |
|-----|-------|---------------|-----------|---------|----------|-------------|---|
| 1   | 1-A   | 304/306 (99%) | 274 (90%) | 21 (7%) | 9 (3%)   | 4           | 0 |
| 1   | 2-A   | 304/306 (99%) | 269 (88%) | 15 (5%) | 20 (7%)  | 1           | 0 |
| 1   | 3-A   | 304/306 (99%) | 274 (90%) | 20 (7%) | 10 (3%)  | 4           | 0 |
| 1   | 4-A   | 304/306 (99%) | 269 (88%) | 20 (7%) | 15 (5%)  | 2           | 0 |
| 1   | 5-A   | 304/306 (99%) | 274 (90%) | 21 (7%) | 9 (3%)   | 4           | 0 |
| 1   | 6-A   | 304/306 (99%) | 277 (91%) | 12 (4%) | 15 (5%)  | 2           | 0 |
| 1   | 7-A   | 304/306 (99%) | 272 (90%) | 21 (7%) | 11 (4%)  | 3           | 0 |
| 1   | 8-A   | 304/306 (99%) | 275 (90%) | 15 (5%) | 14 (5%)  | 2           | 0 |
| 1   | 9-A   | 304/306 (99%) | 275 (90%) | 17 (6%) | 12 (4%)  | 3           | 0 |
| 1   | 10-A  | 304/306 (99%) | 281 (92%) | 13 (4%) | 10 (3%)  | 4           | 0 |
| 1   | 11-A  | 304/306 (99%) | 274 (90%) | 19 (6%) | 11 (4%)  | 3           | 0 |
| 1   | 12-A  | 304/306 (99%) | 282 (93%) | 17 (6%) | 5 (2%)   | 9           | 1 |
| 1   | 13-A  | 304/306 (99%) | 288 (95%) | 13 (4%) | 3 (1%)   | 15          | 3 |
| 1   | 14-A  | 304/306 (99%) | 289 (95%) | 9 (3%)  | 6 (2%)   | 7           | 1 |
| 1   | 15-A  | 304/306 (99%) | 274 (90%) | 16 (5%) | 14 (5%)  | 2           | 0 |
| 1   | 16-A  | 304/306 (99%) | 285 (94%) | 10 (3%) | 9 (3%)   | 4           | 0 |
| 1   | 17-A  | 304/306 (99%) | 282 (93%) | 16 (5%) | 6 (2%)   | 7           | 1 |
| 1   | 18-A  | 304/306 (99%) | 276 (91%) | 19 (6%) | 9 (3%)   | 4           | 0 |
| 1   | 19-A  | 304/306 (99%) | 274 (90%) | 19 (6%) | 11 (4%)  | 3           | 0 |
| 1   | 20-A  | 304/306 (99%) | 288 (95%) | 8 (3%)  | 8 (3%)   | 5           | 0 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |   |
|-----|-------|-------------------|-------------|----------|----------|-------------|---|
| 1   | 21-A  | 304/306 (99%)     | 281 (92%)   | 12 (4%)  | 11 (4%)  | 3           | 0 |
| 1   | 22-A  | 304/306 (99%)     | 277 (91%)   | 20 (7%)  | 7 (2%)   | 6           | 0 |
| 1   | 23-A  | 304/306 (99%)     | 271 (89%)   | 23 (8%)  | 10 (3%)  | 4           | 0 |
| 1   | 24-A  | 304/306 (99%)     | 272 (90%)   | 19 (6%)  | 13 (4%)  | 2           | 0 |
| 1   | 25-A  | 304/306 (99%)     | 279 (92%)   | 15 (5%)  | 10 (3%)  | 4           | 0 |
| 1   | 26-A  | 304/306 (99%)     | 268 (88%)   | 19 (6%)  | 17 (6%)  | 2           | 0 |
| 1   | 27-A  | 304/306 (99%)     | 279 (92%)   | 14 (5%)  | 11 (4%)  | 3           | 0 |
| 1   | 28-A  | 304/306 (99%)     | 277 (91%)   | 17 (6%)  | 10 (3%)  | 4           | 0 |
| 1   | 29-A  | 304/306 (99%)     | 271 (89%)   | 21 (7%)  | 12 (4%)  | 3           | 0 |
| 1   | 30-A  | 304/306 (99%)     | 279 (92%)   | 16 (5%)  | 9 (3%)   | 4           | 0 |
| 1   | 31-A  | 304/306 (99%)     | 268 (88%)   | 27 (9%)  | 9 (3%)   | 4           | 0 |
| 1   | 32-A  | 304/306 (99%)     | 273 (90%)   | 19 (6%)  | 12 (4%)  | 3           | 0 |
| 1   | 33-A  | 304/306 (99%)     | 268 (88%)   | 16 (5%)  | 20 (7%)  | 1           | 0 |
| 1   | 34-A  | 304/306 (99%)     | 275 (90%)   | 17 (6%)  | 12 (4%)  | 3           | 0 |
| 1   | 35-A  | 304/306 (99%)     | 278 (91%)   | 14 (5%)  | 12 (4%)  | 3           | 0 |
| 1   | 36-A  | 304/306 (99%)     | 277 (91%)   | 18 (6%)  | 9 (3%)   | 4           | 0 |
| 1   | 37-A  | 304/306 (99%)     | 272 (90%)   | 18 (6%)  | 14 (5%)  | 2           | 0 |
| 1   | 38-A  | 304/306 (99%)     | 268 (88%)   | 20 (7%)  | 16 (5%)  | 2           | 0 |
| 1   | 39-A  | 304/306 (99%)     | 270 (89%)   | 19 (6%)  | 15 (5%)  | 2           | 0 |
| 1   | 40-A  | 304/306 (99%)     | 287 (94%)   | 10 (3%)  | 7 (2%)   | 6           | 0 |
| 1   | 41-A  | 304/306 (99%)     | 273 (90%)   | 15 (5%)  | 16 (5%)  | 2           | 0 |
| 1   | 42-A  | 304/306 (99%)     | 275 (90%)   | 17 (6%)  | 12 (4%)  | 3           | 0 |
| 1   | 43-A  | 304/306 (99%)     | 270 (89%)   | 21 (7%)  | 13 (4%)  | 2           | 0 |
| All | All   | 13072/13158 (99%) | 11860 (91%) | 728 (6%) | 484 (4%) | 3           | 0 |

All (484) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-A   | 24  | THR  |
| 1   | 1-A   | 47  | GLU  |
| 1   | 1-A   | 154 | TYR  |
| 1   | 1-A   | 304 | THR  |
| 1   | 2-A   | 24  | THR  |
| 1   | 2-A   | 45  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2-A   | 47  | GLU  |
| 1   | 2-A   | 72  | ASN  |
| 1   | 2-A   | 169 | THR  |
| 1   | 2-A   | 222 | ARG  |
| 1   | 2-A   | 300 | CYS  |
| 1   | 2-A   | 301 | SER  |
| 1   | 2-A   | 303 | VAL  |
| 1   | 2-A   | 305 | PHE  |
| 1   | 3-A   | 46  | SER  |
| 1   | 3-A   | 60  | ARG  |
| 1   | 3-A   | 71  | GLY  |
| 1   | 3-A   | 276 | MET  |
| 1   | 3-A   | 277 | ASN  |
| 1   | 3-A   | 302 | GLY  |
| 1   | 4-A   | 24  | THR  |
| 1   | 4-A   | 48  | ASP  |
| 1   | 4-A   | 60  | ARG  |
| 1   | 4-A   | 220 | LEU  |
| 1   | 4-A   | 301 | SER  |
| 1   | 4-A   | 305 | PHE  |
| 1   | 5-A   | 3   | PHE  |
| 1   | 5-A   | 49  | MET  |
| 1   | 5-A   | 142 | ASN  |
| 1   | 5-A   | 155 | ASP  |
| 1   | 5-A   | 303 | VAL  |
| 1   | 6-A   | 24  | THR  |
| 1   | 6-A   | 59  | ILE  |
| 1   | 6-A   | 60  | ARG  |
| 1   | 6-A   | 71  | GLY  |
| 1   | 6-A   | 155 | ASP  |
| 1   | 6-A   | 299 | GLN  |
| 1   | 6-A   | 300 | CYS  |
| 1   | 6-A   | 301 | SER  |
| 1   | 7-A   | 192 | GLN  |
| 1   | 7-A   | 305 | PHE  |
| 1   | 8-A   | 25  | THR  |
| 1   | 8-A   | 48  | ASP  |
| 1   | 8-A   | 51  | ASN  |
| 1   | 8-A   | 142 | ASN  |
| 1   | 8-A   | 152 | ILE  |
| 1   | 8-A   | 154 | TYR  |
| 1   | 8-A   | 155 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 8-A   | 156 | CYS  |
| 1   | 8-A   | 301 | SER  |
| 1   | 8-A   | 304 | THR  |
| 1   | 8-A   | 305 | PHE  |
| 1   | 9-A   | 24  | THR  |
| 1   | 9-A   | 154 | TYR  |
| 1   | 9-A   | 301 | SER  |
| 1   | 9-A   | 302 | GLY  |
| 1   | 10-A  | 155 | ASP  |
| 1   | 10-A  | 303 | VAL  |
| 1   | 11-A  | 70  | ALA  |
| 1   | 11-A  | 152 | ILE  |
| 1   | 11-A  | 153 | ASP  |
| 1   | 11-A  | 154 | TYR  |
| 1   | 11-A  | 155 | ASP  |
| 1   | 11-A  | 277 | ASN  |
| 1   | 12-A  | 50  | LEU  |
| 1   | 12-A  | 152 | ILE  |
| 1   | 13-A  | 152 | ILE  |
| 1   | 13-A  | 304 | THR  |
| 1   | 14-A  | 72  | ASN  |
| 1   | 15-A  | 23  | GLY  |
| 1   | 15-A  | 47  | GLU  |
| 1   | 15-A  | 102 | LYS  |
| 1   | 15-A  | 276 | MET  |
| 1   | 15-A  | 279 | ARG  |
| 1   | 15-A  | 300 | CYS  |
| 1   | 15-A  | 301 | SER  |
| 1   | 15-A  | 303 | VAL  |
| 1   | 15-A  | 304 | THR  |
| 1   | 16-A  | 23  | GLY  |
| 1   | 16-A  | 24  | THR  |
| 1   | 16-A  | 72  | ASN  |
| 1   | 16-A  | 73  | VAL  |
| 1   | 16-A  | 75  | LEU  |
| 1   | 16-A  | 191 | ALA  |
| 1   | 17-A  | 24  | THR  |
| 1   | 17-A  | 276 | MET  |
| 1   | 17-A  | 279 | ARG  |
| 1   | 18-A  | 51  | ASN  |
| 1   | 18-A  | 70  | ALA  |
| 1   | 18-A  | 72  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 18-A  | 153 | ASP  |
| 1   | 18-A  | 301 | SER  |
| 1   | 18-A  | 303 | VAL  |
| 1   | 19-A  | 154 | TYR  |
| 1   | 19-A  | 165 | MET  |
| 1   | 19-A  | 279 | ARG  |
| 1   | 19-A  | 302 | GLY  |
| 1   | 20-A  | 46  | SER  |
| 1   | 20-A  | 61  | LYS  |
| 1   | 20-A  | 73  | VAL  |
| 1   | 20-A  | 74  | GLN  |
| 1   | 20-A  | 155 | ASP  |
| 1   | 20-A  | 301 | SER  |
| 1   | 21-A  | 23  | GLY  |
| 1   | 21-A  | 25  | THR  |
| 1   | 21-A  | 70  | ALA  |
| 1   | 21-A  | 301 | SER  |
| 1   | 21-A  | 303 | VAL  |
| 1   | 22-A  | 48  | ASP  |
| 1   | 22-A  | 301 | SER  |
| 1   | 23-A  | 49  | MET  |
| 1   | 23-A  | 300 | CYS  |
| 1   | 23-A  | 302 | GLY  |
| 1   | 23-A  | 303 | VAL  |
| 1   | 23-A  | 305 | PHE  |
| 1   | 24-A  | 25  | THR  |
| 1   | 24-A  | 46  | SER  |
| 1   | 24-A  | 72  | ASN  |
| 1   | 24-A  | 155 | ASP  |
| 1   | 24-A  | 220 | LEU  |
| 1   | 24-A  | 241 | PRO  |
| 1   | 24-A  | 303 | VAL  |
| 1   | 25-A  | 51  | ASN  |
| 1   | 25-A  | 52  | PRO  |
| 1   | 25-A  | 71  | GLY  |
| 1   | 25-A  | 301 | SER  |
| 1   | 26-A  | 46  | SER  |
| 1   | 26-A  | 47  | GLU  |
| 1   | 26-A  | 59  | ILE  |
| 1   | 26-A  | 72  | ASN  |
| 1   | 26-A  | 73  | VAL  |
| 1   | 26-A  | 120 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 26-A  | 154 | TYR  |
| 1   | 26-A  | 304 | THR  |
| 1   | 26-A  | 305 | PHE  |
| 1   | 27-A  | 60  | ARG  |
| 1   | 27-A  | 300 | CYS  |
| 1   | 28-A  | 60  | ARG  |
| 1   | 28-A  | 72  | ASN  |
| 1   | 28-A  | 301 | SER  |
| 1   | 28-A  | 303 | VAL  |
| 1   | 28-A  | 304 | THR  |
| 1   | 28-A  | 305 | PHE  |
| 1   | 29-A  | 60  | ARG  |
| 1   | 29-A  | 119 | ASN  |
| 1   | 29-A  | 273 | GLN  |
| 1   | 29-A  | 274 | ASN  |
| 1   | 29-A  | 298 | ARG  |
| 1   | 29-A  | 299 | GLN  |
| 1   | 29-A  | 301 | SER  |
| 1   | 30-A  | 46  | SER  |
| 1   | 30-A  | 50  | LEU  |
| 1   | 30-A  | 233 | VAL  |
| 1   | 30-A  | 235 | MET  |
| 1   | 30-A  | 236 | LYS  |
| 1   | 31-A  | 3   | PHE  |
| 1   | 31-A  | 155 | ASP  |
| 1   | 31-A  | 232 | LEU  |
| 1   | 31-A  | 235 | MET  |
| 1   | 31-A  | 301 | SER  |
| 1   | 31-A  | 305 | PHE  |
| 1   | 32-A  | 48  | ASP  |
| 1   | 32-A  | 299 | GLN  |
| 1   | 32-A  | 303 | VAL  |
| 1   | 33-A  | 48  | ASP  |
| 1   | 33-A  | 59  | ILE  |
| 1   | 33-A  | 61  | LYS  |
| 1   | 33-A  | 62  | SER  |
| 1   | 33-A  | 122 | PRO  |
| 1   | 33-A  | 142 | ASN  |
| 1   | 33-A  | 233 | VAL  |
| 1   | 33-A  | 235 | MET  |
| 1   | 33-A  | 299 | GLN  |
| 1   | 33-A  | 305 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 34-A  | 71  | GLY  |
| 1   | 34-A  | 73  | VAL  |
| 1   | 34-A  | 142 | ASN  |
| 1   | 34-A  | 233 | VAL  |
| 1   | 34-A  | 235 | MET  |
| 1   | 34-A  | 303 | VAL  |
| 1   | 35-A  | 50  | LEU  |
| 1   | 35-A  | 141 | LEU  |
| 1   | 35-A  | 154 | TYR  |
| 1   | 35-A  | 155 | ASP  |
| 1   | 35-A  | 233 | VAL  |
| 1   | 35-A  | 234 | ALA  |
| 1   | 35-A  | 235 | MET  |
| 1   | 35-A  | 301 | SER  |
| 1   | 36-A  | 300 | CYS  |
| 1   | 36-A  | 303 | VAL  |
| 1   | 36-A  | 304 | THR  |
| 1   | 37-A  | 25  | THR  |
| 1   | 37-A  | 193 | ALA  |
| 1   | 37-A  | 300 | CYS  |
| 1   | 37-A  | 303 | VAL  |
| 1   | 37-A  | 304 | THR  |
| 1   | 38-A  | 23  | GLY  |
| 1   | 38-A  | 51  | ASN  |
| 1   | 38-A  | 73  | VAL  |
| 1   | 38-A  | 153 | ASP  |
| 1   | 38-A  | 154 | TYR  |
| 1   | 38-A  | 193 | ALA  |
| 1   | 38-A  | 233 | VAL  |
| 1   | 38-A  | 304 | THR  |
| 1   | 39-A  | 24  | THR  |
| 1   | 39-A  | 51  | ASN  |
| 1   | 39-A  | 193 | ALA  |
| 1   | 39-A  | 233 | VAL  |
| 1   | 39-A  | 234 | ALA  |
| 1   | 39-A  | 302 | GLY  |
| 1   | 39-A  | 303 | VAL  |
| 1   | 39-A  | 305 | PHE  |
| 1   | 40-A  | 153 | ASP  |
| 1   | 40-A  | 234 | ALA  |
| 1   | 40-A  | 301 | SER  |
| 1   | 40-A  | 303 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 41-A  | 47  | GLU  |
| 1   | 41-A  | 48  | ASP  |
| 1   | 41-A  | 71  | GLY  |
| 1   | 41-A  | 220 | LEU  |
| 1   | 41-A  | 232 | LEU  |
| 1   | 41-A  | 233 | VAL  |
| 1   | 41-A  | 236 | LYS  |
| 1   | 41-A  | 301 | SER  |
| 1   | 42-A  | 45  | THR  |
| 1   | 42-A  | 141 | LEU  |
| 1   | 42-A  | 191 | ALA  |
| 1   | 42-A  | 192 | GLN  |
| 1   | 42-A  | 221 | ASN  |
| 1   | 42-A  | 299 | GLN  |
| 1   | 42-A  | 301 | SER  |
| 1   | 42-A  | 303 | VAL  |
| 1   | 43-A  | 46  | SER  |
| 1   | 43-A  | 49  | MET  |
| 1   | 43-A  | 73  | VAL  |
| 1   | 43-A  | 154 | TYR  |
| 1   | 43-A  | 193 | ALA  |
| 1   | 43-A  | 301 | SER  |
| 1   | 43-A  | 304 | THR  |
| 1   | 1-A   | 48  | ASP  |
| 1   | 1-A   | 223 | PHE  |
| 1   | 1-A   | 302 | GLY  |
| 1   | 2-A   | 23  | GLY  |
| 1   | 2-A   | 70  | ALA  |
| 1   | 3-A   | 279 | ARG  |
| 1   | 3-A   | 301 | SER  |
| 1   | 4-A   | 47  | GLU  |
| 1   | 5-A   | 24  | THR  |
| 1   | 5-A   | 70  | ALA  |
| 1   | 5-A   | 154 | TYR  |
| 1   | 5-A   | 277 | ASN  |
| 1   | 6-A   | 102 | LYS  |
| 1   | 6-A   | 142 | ASN  |
| 1   | 6-A   | 278 | GLY  |
| 1   | 7-A   | 71  | GLY  |
| 1   | 7-A   | 191 | ALA  |
| 1   | 7-A   | 278 | GLY  |
| 1   | 7-A   | 279 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 8-A   | 23  | GLY  |
| 1   | 9-A   | 156 | CYS  |
| 1   | 9-A   | 192 | GLN  |
| 1   | 9-A   | 235 | MET  |
| 1   | 9-A   | 277 | ASN  |
| 1   | 9-A   | 303 | VAL  |
| 1   | 9-A   | 304 | THR  |
| 1   | 9-A   | 305 | PHE  |
| 1   | 10-A  | 24  | THR  |
| 1   | 10-A  | 301 | SER  |
| 1   | 10-A  | 304 | THR  |
| 1   | 12-A  | 154 | TYR  |
| 1   | 12-A  | 305 | PHE  |
| 1   | 13-A  | 234 | ALA  |
| 1   | 14-A  | 23  | GLY  |
| 1   | 14-A  | 154 | TYR  |
| 1   | 15-A  | 24  | THR  |
| 1   | 15-A  | 48  | ASP  |
| 1   | 15-A  | 154 | TYR  |
| 1   | 15-A  | 278 | GLY  |
| 1   | 16-A  | 277 | ASN  |
| 1   | 17-A  | 23  | GLY  |
| 1   | 17-A  | 72  | ASN  |
| 1   | 18-A  | 23  | GLY  |
| 1   | 18-A  | 277 | ASN  |
| 1   | 18-A  | 279 | ARG  |
| 1   | 19-A  | 46  | SER  |
| 1   | 21-A  | 24  | THR  |
| 1   | 21-A  | 71  | GLY  |
| 1   | 22-A  | 46  | SER  |
| 1   | 22-A  | 154 | TYR  |
| 1   | 22-A  | 192 | GLN  |
| 1   | 22-A  | 303 | VAL  |
| 1   | 24-A  | 51  | ASN  |
| 1   | 24-A  | 73  | VAL  |
| 1   | 24-A  | 301 | SER  |
| 1   | 25-A  | 3   | PHE  |
| 1   | 25-A  | 48  | ASP  |
| 1   | 25-A  | 73  | VAL  |
| 1   | 26-A  | 119 | ASN  |
| 1   | 26-A  | 195 | GLY  |
| 1   | 26-A  | 301 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 27-A  | 72  | ASN  |
| 1   | 27-A  | 142 | ASN  |
| 1   | 27-A  | 301 | SER  |
| 1   | 29-A  | 2   | GLY  |
| 1   | 29-A  | 71  | GLY  |
| 1   | 30-A  | 305 | PHE  |
| 1   | 31-A  | 233 | VAL  |
| 1   | 32-A  | 47  | GLU  |
| 1   | 32-A  | 141 | LEU  |
| 1   | 32-A  | 154 | TYR  |
| 1   | 32-A  | 256 | GLN  |
| 1   | 33-A  | 23  | GLY  |
| 1   | 33-A  | 60  | ARG  |
| 1   | 33-A  | 141 | LEU  |
| 1   | 33-A  | 156 | CYS  |
| 1   | 34-A  | 155 | ASP  |
| 1   | 34-A  | 236 | LYS  |
| 1   | 35-A  | 71  | GLY  |
| 1   | 36-A  | 233 | VAL  |
| 1   | 36-A  | 234 | ALA  |
| 1   | 36-A  | 235 | MET  |
| 1   | 36-A  | 299 | GLN  |
| 1   | 37-A  | 46  | SER  |
| 1   | 37-A  | 154 | TYR  |
| 1   | 37-A  | 216 | ASP  |
| 1   | 37-A  | 233 | VAL  |
| 1   | 37-A  | 299 | GLN  |
| 1   | 37-A  | 305 | PHE  |
| 1   | 38-A  | 71  | GLY  |
| 1   | 38-A  | 72  | ASN  |
| 1   | 38-A  | 223 | PHE  |
| 1   | 38-A  | 299 | GLN  |
| 1   | 38-A  | 301 | SER  |
| 1   | 38-A  | 303 | VAL  |
| 1   | 39-A  | 301 | SER  |
| 1   | 39-A  | 304 | THR  |
| 1   | 40-A  | 233 | VAL  |
| 1   | 40-A  | 302 | GLY  |
| 1   | 41-A  | 49  | MET  |
| 1   | 41-A  | 154 | TYR  |
| 1   | 41-A  | 192 | GLN  |
| 1   | 41-A  | 303 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 43-A  | 71  | GLY  |
| 1   | 43-A  | 191 | ALA  |
| 1   | 1-A   | 108 | PRO  |
| 1   | 2-A   | 46  | SER  |
| 1   | 2-A   | 73  | VAL  |
| 1   | 2-A   | 153 | ASP  |
| 1   | 2-A   | 168 | PRO  |
| 1   | 2-A   | 233 | VAL  |
| 1   | 3-A   | 154 | TYR  |
| 1   | 4-A   | 3   | PHE  |
| 1   | 4-A   | 154 | TYR  |
| 1   | 6-A   | 277 | ASN  |
| 1   | 7-A   | 153 | ASP  |
| 1   | 10-A  | 45  | THR  |
| 1   | 10-A  | 305 | PHE  |
| 1   | 11-A  | 4   | ARG  |
| 1   | 11-A  | 190 | THR  |
| 1   | 14-A  | 45  | THR  |
| 1   | 14-A  | 46  | SER  |
| 1   | 14-A  | 152 | ILE  |
| 1   | 15-A  | 46  | SER  |
| 1   | 16-A  | 154 | TYR  |
| 1   | 17-A  | 303 | VAL  |
| 1   | 19-A  | 72  | ASN  |
| 1   | 19-A  | 74  | GLN  |
| 1   | 20-A  | 154 | TYR  |
| 1   | 24-A  | 23  | GLY  |
| 1   | 24-A  | 302 | GLY  |
| 1   | 25-A  | 72  | ASN  |
| 1   | 26-A  | 45  | THR  |
| 1   | 26-A  | 275 | GLY  |
| 1   | 26-A  | 299 | GLN  |
| 1   | 27-A  | 156 | CYS  |
| 1   | 28-A  | 302 | GLY  |
| 1   | 29-A  | 305 | PHE  |
| 1   | 30-A  | 45  | THR  |
| 1   | 30-A  | 191 | ALA  |
| 1   | 30-A  | 234 | ALA  |
| 1   | 31-A  | 154 | TYR  |
| 1   | 32-A  | 3   | PHE  |
| 1   | 32-A  | 142 | ASN  |
| 1   | 33-A  | 154 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 33-A  | 301 | SER  |
| 1   | 33-A  | 304 | THR  |
| 1   | 34-A  | 192 | GLN  |
| 1   | 34-A  | 234 | ALA  |
| 1   | 36-A  | 142 | ASN  |
| 1   | 37-A  | 47  | GLU  |
| 1   | 38-A  | 305 | PHE  |
| 1   | 39-A  | 154 | TYR  |
| 1   | 39-A  | 195 | GLY  |
| 1   | 41-A  | 141 | LEU  |
| 1   | 41-A  | 304 | THR  |
| 1   | 41-A  | 305 | PHE  |
| 1   | 42-A  | 154 | TYR  |
| 1   | 42-A  | 234 | ALA  |
| 1   | 43-A  | 192 | GLN  |
| 1   | 1-A   | 275 | GLY  |
| 1   | 2-A   | 170 | GLY  |
| 1   | 4-A   | 45  | THR  |
| 1   | 4-A   | 49  | MET  |
| 1   | 4-A   | 304 | THR  |
| 1   | 6-A   | 154 | TYR  |
| 1   | 9-A   | 70  | ALA  |
| 1   | 20-A  | 60  | ARG  |
| 1   | 21-A  | 277 | ASN  |
| 1   | 23-A  | 145 | CYS  |
| 1   | 23-A  | 277 | ASN  |
| 1   | 25-A  | 195 | GLY  |
| 1   | 26-A  | 3   | PHE  |
| 1   | 28-A  | 48  | ASP  |
| 1   | 28-A  | 154 | TYR  |
| 1   | 29-A  | 297 | VAL  |
| 1   | 32-A  | 51  | ASN  |
| 1   | 33-A  | 123 | SER  |
| 1   | 34-A  | 141 | LEU  |
| 1   | 35-A  | 70  | ALA  |
| 1   | 35-A  | 299 | GLN  |
| 1   | 36-A  | 154 | TYR  |
| 1   | 37-A  | 51  | ASN  |
| 1   | 38-A  | 302 | GLY  |
| 1   | 40-A  | 305 | PHE  |
| 1   | 42-A  | 302 | GLY  |
| 1   | 2-A   | 277 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 3-A   | 303 | VAL  |
| 1   | 4-A   | 141 | LEU  |
| 1   | 4-A   | 278 | GLY  |
| 1   | 7-A   | 24  | THR  |
| 1   | 7-A   | 303 | VAL  |
| 1   | 8-A   | 303 | VAL  |
| 1   | 10-A  | 51  | ASN  |
| 1   | 10-A  | 154 | TYR  |
| 1   | 10-A  | 302 | GLY  |
| 1   | 11-A  | 302 | GLY  |
| 1   | 11-A  | 305 | PHE  |
| 1   | 12-A  | 256 | GLN  |
| 1   | 19-A  | 23  | GLY  |
| 1   | 21-A  | 72  | ASN  |
| 1   | 21-A  | 298 | ARG  |
| 1   | 23-A  | 141 | LEU  |
| 1   | 24-A  | 298 | ARG  |
| 1   | 25-A  | 305 | PHE  |
| 1   | 27-A  | 51  | ASN  |
| 1   | 27-A  | 119 | ASN  |
| 1   | 29-A  | 154 | TYR  |
| 1   | 33-A  | 3   | PHE  |
| 1   | 35-A  | 72  | ASN  |
| 1   | 37-A  | 155 | ASP  |
| 1   | 39-A  | 155 | ASP  |
| 1   | 39-A  | 300 | CYS  |
| 1   | 42-A  | 51  | ASN  |
| 1   | 43-A  | 299 | GLN  |
| 1   | 16-A  | 276 | MET  |
| 1   | 19-A  | 277 | ASN  |
| 1   | 22-A  | 155 | ASP  |
| 1   | 23-A  | 278 | GLY  |
| 1   | 27-A  | 49  | MET  |
| 1   | 27-A  | 70  | ALA  |
| 1   | 27-A  | 154 | TYR  |
| 1   | 28-A  | 152 | ILE  |
| 1   | 31-A  | 2   | GLY  |
| 1   | 32-A  | 233 | VAL  |
| 1   | 33-A  | 191 | ALA  |
| 1   | 39-A  | 153 | ASP  |
| 1   | 43-A  | 23  | GLY  |
| 1   | 43-A  | 277 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 4-A   | 108 | PRO  |
| 1   | 7-A   | 52  | PRO  |
| 1   | 26-A  | 71  | GLY  |
| 1   | 32-A  | 2   | GLY  |
| 1   | 21-A  | 73  | VAL  |
| 1   | 34-A  | 302 | GLY  |
| 1   | 11-A  | 23  | GLY  |
| 1   | 19-A  | 51  | ASN  |
| 1   | 23-A  | 71  | GLY  |
| 1   | 41-A  | 302 | GLY  |
| 1   | 2-A   | 171 | VAL  |
| 1   | 6-A   | 106 | ILE  |
| 1   | 6-A   | 303 | VAL  |
| 1   | 7-A   | 23  | GLY  |
| 1   | 8-A   | 71  | GLY  |
| 1   | 19-A  | 71  | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |   |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1   | 1-A   | 263/263 (100%) | 228 (87%) | 35 (13%) | 4           | 0 |
| 1   | 2-A   | 263/263 (100%) | 228 (87%) | 35 (13%) | 4           | 0 |
| 1   | 3-A   | 263/263 (100%) | 230 (88%) | 33 (12%) | 4           | 0 |
| 1   | 4-A   | 263/263 (100%) | 225 (86%) | 38 (14%) | 3           | 0 |
| 1   | 5-A   | 263/263 (100%) | 231 (88%) | 32 (12%) | 5           | 0 |
| 1   | 6-A   | 263/263 (100%) | 232 (88%) | 31 (12%) | 5           | 0 |
| 1   | 7-A   | 263/263 (100%) | 227 (86%) | 36 (14%) | 3           | 0 |
| 1   | 8-A   | 263/263 (100%) | 230 (88%) | 33 (12%) | 4           | 0 |
| 1   | 9-A   | 263/263 (100%) | 224 (85%) | 39 (15%) | 3           | 0 |
| 1   | 10-A  | 263/263 (100%) | 230 (88%) | 33 (12%) | 4           | 0 |
| 1   | 11-A  | 263/263 (100%) | 225 (86%) | 38 (14%) | 3           | 0 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |   |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1   | 12-A  | 263/263 (100%) | 226 (86%) | 37 (14%) | 3           | 0 |
| 1   | 13-A  | 263/263 (100%) | 221 (84%) | 42 (16%) | 2           | 0 |
| 1   | 14-A  | 263/263 (100%) | 225 (86%) | 38 (14%) | 3           | 0 |
| 1   | 15-A  | 263/263 (100%) | 224 (85%) | 39 (15%) | 3           | 0 |
| 1   | 16-A  | 263/263 (100%) | 233 (89%) | 30 (11%) | 5           | 0 |
| 1   | 17-A  | 263/263 (100%) | 231 (88%) | 32 (12%) | 5           | 0 |
| 1   | 18-A  | 263/263 (100%) | 230 (88%) | 33 (12%) | 4           | 0 |
| 1   | 19-A  | 263/263 (100%) | 234 (89%) | 29 (11%) | 6           | 0 |
| 1   | 20-A  | 263/263 (100%) | 231 (88%) | 32 (12%) | 5           | 0 |
| 1   | 21-A  | 263/263 (100%) | 237 (90%) | 26 (10%) | 8           | 0 |
| 1   | 22-A  | 263/263 (100%) | 244 (93%) | 19 (7%)  | 14          | 1 |
| 1   | 23-A  | 263/263 (100%) | 223 (85%) | 40 (15%) | 3           | 0 |
| 1   | 24-A  | 263/263 (100%) | 228 (87%) | 35 (13%) | 4           | 0 |
| 1   | 25-A  | 263/263 (100%) | 228 (87%) | 35 (13%) | 4           | 0 |
| 1   | 26-A  | 263/263 (100%) | 233 (89%) | 30 (11%) | 5           | 0 |
| 1   | 27-A  | 263/263 (100%) | 230 (88%) | 33 (12%) | 4           | 0 |
| 1   | 28-A  | 263/263 (100%) | 230 (88%) | 33 (12%) | 4           | 0 |
| 1   | 29-A  | 263/263 (100%) | 219 (83%) | 44 (17%) | 2           | 0 |
| 1   | 30-A  | 263/263 (100%) | 234 (89%) | 29 (11%) | 6           | 0 |
| 1   | 31-A  | 263/263 (100%) | 222 (84%) | 41 (16%) | 2           | 0 |
| 1   | 32-A  | 263/263 (100%) | 226 (86%) | 37 (14%) | 3           | 0 |
| 1   | 33-A  | 263/263 (100%) | 230 (88%) | 33 (12%) | 4           | 0 |
| 1   | 34-A  | 263/263 (100%) | 226 (86%) | 37 (14%) | 3           | 0 |
| 1   | 35-A  | 263/263 (100%) | 221 (84%) | 42 (16%) | 2           | 0 |
| 1   | 36-A  | 263/263 (100%) | 236 (90%) | 27 (10%) | 7           | 0 |
| 1   | 37-A  | 263/263 (100%) | 223 (85%) | 40 (15%) | 3           | 0 |
| 1   | 38-A  | 263/263 (100%) | 214 (81%) | 49 (19%) | 1           | 0 |
| 1   | 39-A  | 263/263 (100%) | 224 (85%) | 39 (15%) | 3           | 0 |
| 1   | 40-A  | 263/263 (100%) | 227 (86%) | 36 (14%) | 3           | 0 |
| 1   | 41-A  | 263/263 (100%) | 228 (87%) | 35 (13%) | 4           | 0 |
| 1   | 42-A  | 263/263 (100%) | 227 (86%) | 36 (14%) | 3           | 0 |

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| Mol | Chain | Analysed           | Rotameric  | Outliers   | Percentiles |   |
|-----|-------|--------------------|------------|------------|-------------|---|
| 1   | 43-A  | 263/263 (100%)     | 220 (84%)  | 43 (16%)   | 2           | 0 |
| All | All   | 11309/11309 (100%) | 9795 (87%) | 1514 (13%) | 4           | 0 |

All (1514) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-A   | 1   | SER  |
| 1   | 1-A   | 27  | LEU  |
| 1   | 1-A   | 47  | GLU  |
| 1   | 1-A   | 49  | MET  |
| 1   | 1-A   | 59  | ILE  |
| 1   | 1-A   | 60  | ARG  |
| 1   | 1-A   | 72  | ASN  |
| 1   | 1-A   | 81  | SER  |
| 1   | 1-A   | 100 | LYS  |
| 1   | 1-A   | 107 | GLN  |
| 1   | 1-A   | 121 | SER  |
| 1   | 1-A   | 139 | SER  |
| 1   | 1-A   | 141 | LEU  |
| 1   | 1-A   | 154 | TYR  |
| 1   | 1-A   | 155 | ASP  |
| 1   | 1-A   | 156 | CYS  |
| 1   | 1-A   | 177 | LEU  |
| 1   | 1-A   | 188 | ARG  |
| 1   | 1-A   | 190 | THR  |
| 1   | 1-A   | 217 | ARG  |
| 1   | 1-A   | 222 | ARG  |
| 1   | 1-A   | 225 | THR  |
| 1   | 1-A   | 235 | MET  |
| 1   | 1-A   | 256 | GLN  |
| 1   | 1-A   | 267 | SER  |
| 1   | 1-A   | 276 | MET  |
| 1   | 1-A   | 277 | ASN  |
| 1   | 1-A   | 282 | LEU  |
| 1   | 1-A   | 286 | LEU  |
| 1   | 1-A   | 288 | GLU  |
| 1   | 1-A   | 290 | GLU  |
| 1   | 1-A   | 298 | ARG  |
| 1   | 1-A   | 300 | CYS  |
| 1   | 1-A   | 301 | SER  |
| 1   | 1-A   | 306 | GLN  |
| 1   | 2-A   | 1   | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2-A   | 6   | MET  |
| 1   | 2-A   | 26  | THR  |
| 1   | 2-A   | 27  | LEU  |
| 1   | 2-A   | 28  | ASN  |
| 1   | 2-A   | 33  | ASP  |
| 1   | 2-A   | 45  | THR  |
| 1   | 2-A   | 50  | LEU  |
| 1   | 2-A   | 51  | ASN  |
| 1   | 2-A   | 58  | LEU  |
| 1   | 2-A   | 60  | ARG  |
| 1   | 2-A   | 69  | GLN  |
| 1   | 2-A   | 72  | ASN  |
| 1   | 2-A   | 73  | VAL  |
| 1   | 2-A   | 74  | GLN  |
| 1   | 2-A   | 75  | LEU  |
| 1   | 2-A   | 87  | LEU  |
| 1   | 2-A   | 102 | LYS  |
| 1   | 2-A   | 104 | VAL  |
| 1   | 2-A   | 117 | CYS  |
| 1   | 2-A   | 122 | PRO  |
| 1   | 2-A   | 136 | ILE  |
| 1   | 2-A   | 141 | LEU  |
| 1   | 2-A   | 153 | ASP  |
| 1   | 2-A   | 154 | TYR  |
| 1   | 2-A   | 162 | MET  |
| 1   | 2-A   | 169 | THR  |
| 1   | 2-A   | 216 | ASP  |
| 1   | 2-A   | 222 | ARG  |
| 1   | 2-A   | 227 | LEU  |
| 1   | 2-A   | 233 | VAL  |
| 1   | 2-A   | 235 | MET  |
| 1   | 2-A   | 276 | MET  |
| 1   | 2-A   | 282 | LEU  |
| 1   | 2-A   | 300 | CYS  |
| 1   | 3-A   | 27  | LEU  |
| 1   | 3-A   | 41  | HIS  |
| 1   | 3-A   | 47  | GLU  |
| 1   | 3-A   | 48  | ASP  |
| 1   | 3-A   | 60  | ARG  |
| 1   | 3-A   | 69  | GLN  |
| 1   | 3-A   | 73  | VAL  |
| 1   | 3-A   | 74  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 3-A   | 75  | LEU  |
| 1   | 3-A   | 83  | GLN  |
| 1   | 3-A   | 87  | LEU  |
| 1   | 3-A   | 102 | LYS  |
| 1   | 3-A   | 125 | VAL  |
| 1   | 3-A   | 130 | MET  |
| 1   | 3-A   | 136 | ILE  |
| 1   | 3-A   | 141 | LEU  |
| 1   | 3-A   | 145 | CYS  |
| 1   | 3-A   | 154 | TYR  |
| 1   | 3-A   | 155 | ASP  |
| 1   | 3-A   | 162 | MET  |
| 1   | 3-A   | 167 | LEU  |
| 1   | 3-A   | 214 | ASN  |
| 1   | 3-A   | 232 | LEU  |
| 1   | 3-A   | 235 | MET  |
| 1   | 3-A   | 241 | PRO  |
| 1   | 3-A   | 267 | SER  |
| 1   | 3-A   | 276 | MET  |
| 1   | 3-A   | 279 | ARG  |
| 1   | 3-A   | 280 | THR  |
| 1   | 3-A   | 282 | LEU  |
| 1   | 3-A   | 286 | LEU  |
| 1   | 3-A   | 301 | SER  |
| 1   | 3-A   | 304 | THR  |
| 1   | 4-A   | 1   | SER  |
| 1   | 4-A   | 6   | MET  |
| 1   | 4-A   | 12  | LYS  |
| 1   | 4-A   | 24  | THR  |
| 1   | 4-A   | 25  | THR  |
| 1   | 4-A   | 27  | LEU  |
| 1   | 4-A   | 34  | ASP  |
| 1   | 4-A   | 55  | GLU  |
| 1   | 4-A   | 58  | LEU  |
| 1   | 4-A   | 60  | ARG  |
| 1   | 4-A   | 69  | GLN  |
| 1   | 4-A   | 73  | VAL  |
| 1   | 4-A   | 75  | LEU  |
| 1   | 4-A   | 93  | THR  |
| 1   | 4-A   | 108 | PRO  |
| 1   | 4-A   | 121 | SER  |
| 1   | 4-A   | 128 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 4-A   | 130 | MET  |
| 1   | 4-A   | 137 | LYS  |
| 1   | 4-A   | 139 | SER  |
| 1   | 4-A   | 141 | LEU  |
| 1   | 4-A   | 144 | SER  |
| 1   | 4-A   | 154 | TYR  |
| 1   | 4-A   | 155 | ASP  |
| 1   | 4-A   | 165 | MET  |
| 1   | 4-A   | 188 | ARG  |
| 1   | 4-A   | 216 | ASP  |
| 1   | 4-A   | 222 | ARG  |
| 1   | 4-A   | 225 | THR  |
| 1   | 4-A   | 227 | LEU  |
| 1   | 4-A   | 248 | ASP  |
| 1   | 4-A   | 256 | GLN  |
| 1   | 4-A   | 274 | ASN  |
| 1   | 4-A   | 276 | MET  |
| 1   | 4-A   | 277 | ASN  |
| 1   | 4-A   | 297 | VAL  |
| 1   | 4-A   | 301 | SER  |
| 1   | 4-A   | 304 | THR  |
| 1   | 5-A   | 27  | LEU  |
| 1   | 5-A   | 49  | MET  |
| 1   | 5-A   | 55  | GLU  |
| 1   | 5-A   | 58  | LEU  |
| 1   | 5-A   | 59  | ILE  |
| 1   | 5-A   | 72  | ASN  |
| 1   | 5-A   | 90  | LYS  |
| 1   | 5-A   | 99  | PRO  |
| 1   | 5-A   | 104 | VAL  |
| 1   | 5-A   | 117 | CYS  |
| 1   | 5-A   | 119 | ASN  |
| 1   | 5-A   | 137 | LYS  |
| 1   | 5-A   | 142 | ASN  |
| 1   | 5-A   | 156 | CYS  |
| 1   | 5-A   | 169 | THR  |
| 1   | 5-A   | 189 | GLN  |
| 1   | 5-A   | 216 | ASP  |
| 1   | 5-A   | 221 | ASN  |
| 1   | 5-A   | 222 | ARG  |
| 1   | 5-A   | 233 | VAL  |
| 1   | 5-A   | 235 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 5-A   | 236 | LYS  |
| 1   | 5-A   | 245 | ASP  |
| 1   | 5-A   | 256 | GLN  |
| 1   | 5-A   | 270 | GLU  |
| 1   | 5-A   | 276 | MET  |
| 1   | 5-A   | 277 | ASN  |
| 1   | 5-A   | 279 | ARG  |
| 1   | 5-A   | 297 | VAL  |
| 1   | 5-A   | 298 | ARG  |
| 1   | 5-A   | 299 | GLN  |
| 1   | 5-A   | 300 | CYS  |
| 1   | 6-A   | 24  | THR  |
| 1   | 6-A   | 27  | LEU  |
| 1   | 6-A   | 51  | ASN  |
| 1   | 6-A   | 59  | ILE  |
| 1   | 6-A   | 60  | ARG  |
| 1   | 6-A   | 61  | LYS  |
| 1   | 6-A   | 67  | LEU  |
| 1   | 6-A   | 72  | ASN  |
| 1   | 6-A   | 74  | GLN  |
| 1   | 6-A   | 75  | LEU  |
| 1   | 6-A   | 87  | LEU  |
| 1   | 6-A   | 97  | LYS  |
| 1   | 6-A   | 107 | GLN  |
| 1   | 6-A   | 123 | SER  |
| 1   | 6-A   | 128 | CYS  |
| 1   | 6-A   | 141 | LEU  |
| 1   | 6-A   | 144 | SER  |
| 1   | 6-A   | 151 | ASN  |
| 1   | 6-A   | 152 | ILE  |
| 1   | 6-A   | 155 | ASP  |
| 1   | 6-A   | 221 | ASN  |
| 1   | 6-A   | 222 | ARG  |
| 1   | 6-A   | 223 | PHE  |
| 1   | 6-A   | 233 | VAL  |
| 1   | 6-A   | 235 | MET  |
| 1   | 6-A   | 236 | LYS  |
| 1   | 6-A   | 244 | GLN  |
| 1   | 6-A   | 249 | ILE  |
| 1   | 6-A   | 270 | GLU  |
| 1   | 6-A   | 282 | LEU  |
| 1   | 6-A   | 294 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 7-A   | 1   | SER  |
| 1   | 7-A   | 5   | LYS  |
| 1   | 7-A   | 27  | LEU  |
| 1   | 7-A   | 46  | SER  |
| 1   | 7-A   | 47  | GLU  |
| 1   | 7-A   | 60  | ARG  |
| 1   | 7-A   | 72  | ASN  |
| 1   | 7-A   | 78  | ILE  |
| 1   | 7-A   | 81  | SER  |
| 1   | 7-A   | 87  | LEU  |
| 1   | 7-A   | 88  | LYS  |
| 1   | 7-A   | 90  | LYS  |
| 1   | 7-A   | 93  | THR  |
| 1   | 7-A   | 125 | VAL  |
| 1   | 7-A   | 126 | TYR  |
| 1   | 7-A   | 144 | SER  |
| 1   | 7-A   | 151 | ASN  |
| 1   | 7-A   | 155 | ASP  |
| 1   | 7-A   | 156 | CYS  |
| 1   | 7-A   | 192 | GLN  |
| 1   | 7-A   | 214 | ASN  |
| 1   | 7-A   | 216 | ASP  |
| 1   | 7-A   | 217 | ARG  |
| 1   | 7-A   | 221 | ASN  |
| 1   | 7-A   | 222 | ARG  |
| 1   | 7-A   | 232 | LEU  |
| 1   | 7-A   | 242 | LEU  |
| 1   | 7-A   | 249 | ILE  |
| 1   | 7-A   | 256 | GLN  |
| 1   | 7-A   | 270 | GLU  |
| 1   | 7-A   | 280 | THR  |
| 1   | 7-A   | 282 | LEU  |
| 1   | 7-A   | 298 | ARG  |
| 1   | 7-A   | 301 | SER  |
| 1   | 7-A   | 304 | THR  |
| 1   | 7-A   | 306 | GLN  |
| 1   | 8-A   | 5   | LYS  |
| 1   | 8-A   | 6   | MET  |
| 1   | 8-A   | 27  | LEU  |
| 1   | 8-A   | 47  | GLU  |
| 1   | 8-A   | 48  | ASP  |
| 1   | 8-A   | 58  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 8-A   | 60  | ARG  |
| 1   | 8-A   | 69  | GLN  |
| 1   | 8-A   | 74  | GLN  |
| 1   | 8-A   | 75  | LEU  |
| 1   | 8-A   | 88  | LYS  |
| 1   | 8-A   | 90  | LYS  |
| 1   | 8-A   | 104 | VAL  |
| 1   | 8-A   | 141 | LEU  |
| 1   | 8-A   | 142 | ASN  |
| 1   | 8-A   | 151 | ASN  |
| 1   | 8-A   | 153 | ASP  |
| 1   | 8-A   | 154 | TYR  |
| 1   | 8-A   | 155 | ASP  |
| 1   | 8-A   | 157 | VAL  |
| 1   | 8-A   | 158 | SER  |
| 1   | 8-A   | 177 | LEU  |
| 1   | 8-A   | 188 | ARG  |
| 1   | 8-A   | 217 | ARG  |
| 1   | 8-A   | 221 | ASN  |
| 1   | 8-A   | 227 | LEU  |
| 1   | 8-A   | 235 | MET  |
| 1   | 8-A   | 236 | LYS  |
| 1   | 8-A   | 276 | MET  |
| 1   | 8-A   | 279 | ARG  |
| 1   | 8-A   | 282 | LEU  |
| 1   | 8-A   | 299 | GLN  |
| 1   | 8-A   | 306 | GLN  |
| 1   | 9-A   | 5   | LYS  |
| 1   | 9-A   | 27  | LEU  |
| 1   | 9-A   | 47  | GLU  |
| 1   | 9-A   | 51  | ASN  |
| 1   | 9-A   | 59  | ILE  |
| 1   | 9-A   | 60  | ARG  |
| 1   | 9-A   | 72  | ASN  |
| 1   | 9-A   | 74  | GLN  |
| 1   | 9-A   | 75  | LEU  |
| 1   | 9-A   | 87  | LEU  |
| 1   | 9-A   | 90  | LYS  |
| 1   | 9-A   | 92  | ASP  |
| 1   | 9-A   | 102 | LYS  |
| 1   | 9-A   | 123 | SER  |
| 1   | 9-A   | 125 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 9-A   | 136 | ILE  |
| 1   | 9-A   | 141 | LEU  |
| 1   | 9-A   | 145 | CYS  |
| 1   | 9-A   | 154 | TYR  |
| 1   | 9-A   | 158 | SER  |
| 1   | 9-A   | 178 | GLU  |
| 1   | 9-A   | 190 | THR  |
| 1   | 9-A   | 217 | ARG  |
| 1   | 9-A   | 221 | ASN  |
| 1   | 9-A   | 222 | ARG  |
| 1   | 9-A   | 225 | THR  |
| 1   | 9-A   | 229 | ASP  |
| 1   | 9-A   | 240 | GLU  |
| 1   | 9-A   | 242 | LEU  |
| 1   | 9-A   | 249 | ILE  |
| 1   | 9-A   | 259 | ILE  |
| 1   | 9-A   | 274 | ASN  |
| 1   | 9-A   | 279 | ARG  |
| 1   | 9-A   | 286 | LEU  |
| 1   | 9-A   | 297 | VAL  |
| 1   | 9-A   | 301 | SER  |
| 1   | 9-A   | 303 | VAL  |
| 1   | 9-A   | 304 | THR  |
| 1   | 9-A   | 306 | GLN  |
| 1   | 10-A  | 3   | PHE  |
| 1   | 10-A  | 4   | ARG  |
| 1   | 10-A  | 5   | LYS  |
| 1   | 10-A  | 6   | MET  |
| 1   | 10-A  | 25  | THR  |
| 1   | 10-A  | 27  | LEU  |
| 1   | 10-A  | 46  | SER  |
| 1   | 10-A  | 47  | GLU  |
| 1   | 10-A  | 49  | MET  |
| 1   | 10-A  | 62  | SER  |
| 1   | 10-A  | 74  | GLN  |
| 1   | 10-A  | 100 | LYS  |
| 1   | 10-A  | 102 | LYS  |
| 1   | 10-A  | 141 | LEU  |
| 1   | 10-A  | 142 | ASN  |
| 1   | 10-A  | 152 | ILE  |
| 1   | 10-A  | 153 | ASP  |
| 1   | 10-A  | 155 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 10-A  | 156 | CYS  |
| 1   | 10-A  | 162 | MET  |
| 1   | 10-A  | 165 | MET  |
| 1   | 10-A  | 167 | LEU  |
| 1   | 10-A  | 168 | PRO  |
| 1   | 10-A  | 214 | ASN  |
| 1   | 10-A  | 216 | ASP  |
| 1   | 10-A  | 217 | ARG  |
| 1   | 10-A  | 221 | ASN  |
| 1   | 10-A  | 222 | ARG  |
| 1   | 10-A  | 249 | ILE  |
| 1   | 10-A  | 279 | ARG  |
| 1   | 10-A  | 286 | LEU  |
| 1   | 10-A  | 301 | SER  |
| 1   | 10-A  | 306 | GLN  |
| 1   | 11-A  | 3   | PHE  |
| 1   | 11-A  | 6   | MET  |
| 1   | 11-A  | 12  | LYS  |
| 1   | 11-A  | 24  | THR  |
| 1   | 11-A  | 27  | LEU  |
| 1   | 11-A  | 45  | THR  |
| 1   | 11-A  | 47  | GLU  |
| 1   | 11-A  | 50  | LEU  |
| 1   | 11-A  | 51  | ASN  |
| 1   | 11-A  | 58  | LEU  |
| 1   | 11-A  | 60  | ARG  |
| 1   | 11-A  | 67  | LEU  |
| 1   | 11-A  | 74  | GLN  |
| 1   | 11-A  | 75  | LEU  |
| 1   | 11-A  | 87  | LEU  |
| 1   | 11-A  | 90  | LYS  |
| 1   | 11-A  | 104 | VAL  |
| 1   | 11-A  | 110 | GLN  |
| 1   | 11-A  | 122 | PRO  |
| 1   | 11-A  | 141 | LEU  |
| 1   | 11-A  | 145 | CYS  |
| 1   | 11-A  | 152 | ILE  |
| 1   | 11-A  | 153 | ASP  |
| 1   | 11-A  | 158 | SER  |
| 1   | 11-A  | 167 | LEU  |
| 1   | 11-A  | 190 | THR  |
| 1   | 11-A  | 213 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 11-A  | 222 | ARG  |
| 1   | 11-A  | 242 | LEU  |
| 1   | 11-A  | 267 | SER  |
| 1   | 11-A  | 286 | LEU  |
| 1   | 11-A  | 298 | ARG  |
| 1   | 11-A  | 299 | GLN  |
| 1   | 11-A  | 300 | CYS  |
| 1   | 11-A  | 301 | SER  |
| 1   | 11-A  | 304 | THR  |
| 1   | 11-A  | 305 | PHE  |
| 1   | 11-A  | 306 | GLN  |
| 1   | 12-A  | 4   | ARG  |
| 1   | 12-A  | 27  | LEU  |
| 1   | 12-A  | 51  | ASN  |
| 1   | 12-A  | 58  | LEU  |
| 1   | 12-A  | 60  | ARG  |
| 1   | 12-A  | 74  | GLN  |
| 1   | 12-A  | 75  | LEU  |
| 1   | 12-A  | 81  | SER  |
| 1   | 12-A  | 92  | ASP  |
| 1   | 12-A  | 100 | LYS  |
| 1   | 12-A  | 102 | LYS  |
| 1   | 12-A  | 123 | SER  |
| 1   | 12-A  | 125 | VAL  |
| 1   | 12-A  | 128 | CYS  |
| 1   | 12-A  | 141 | LEU  |
| 1   | 12-A  | 142 | ASN  |
| 1   | 12-A  | 151 | ASN  |
| 1   | 12-A  | 165 | MET  |
| 1   | 12-A  | 188 | ARG  |
| 1   | 12-A  | 189 | GLN  |
| 1   | 12-A  | 190 | THR  |
| 1   | 12-A  | 192 | GLN  |
| 1   | 12-A  | 221 | ASN  |
| 1   | 12-A  | 222 | ARG  |
| 1   | 12-A  | 223 | PHE  |
| 1   | 12-A  | 225 | THR  |
| 1   | 12-A  | 232 | LEU  |
| 1   | 12-A  | 242 | LEU  |
| 1   | 12-A  | 249 | ILE  |
| 1   | 12-A  | 267 | SER  |
| 1   | 12-A  | 270 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 12-A  | 276 | MET  |
| 1   | 12-A  | 277 | ASN  |
| 1   | 12-A  | 286 | LEU  |
| 1   | 12-A  | 290 | GLU  |
| 1   | 12-A  | 297 | VAL  |
| 1   | 12-A  | 298 | ARG  |
| 1   | 13-A  | 5   | LYS  |
| 1   | 13-A  | 6   | MET  |
| 1   | 13-A  | 19  | GLN  |
| 1   | 13-A  | 27  | LEU  |
| 1   | 13-A  | 47  | GLU  |
| 1   | 13-A  | 50  | LEU  |
| 1   | 13-A  | 51  | ASN  |
| 1   | 13-A  | 55  | GLU  |
| 1   | 13-A  | 58  | LEU  |
| 1   | 13-A  | 60  | ARG  |
| 1   | 13-A  | 67  | LEU  |
| 1   | 13-A  | 72  | ASN  |
| 1   | 13-A  | 74  | GLN  |
| 1   | 13-A  | 83  | GLN  |
| 1   | 13-A  | 119 | ASN  |
| 1   | 13-A  | 125 | VAL  |
| 1   | 13-A  | 127 | GLN  |
| 1   | 13-A  | 128 | CYS  |
| 1   | 13-A  | 130 | MET  |
| 1   | 13-A  | 136 | ILE  |
| 1   | 13-A  | 139 | SER  |
| 1   | 13-A  | 141 | LEU  |
| 1   | 13-A  | 153 | ASP  |
| 1   | 13-A  | 155 | ASP  |
| 1   | 13-A  | 167 | LEU  |
| 1   | 13-A  | 188 | ARG  |
| 1   | 13-A  | 190 | THR  |
| 1   | 13-A  | 192 | GLN  |
| 1   | 13-A  | 198 | THR  |
| 1   | 13-A  | 216 | ASP  |
| 1   | 13-A  | 232 | LEU  |
| 1   | 13-A  | 233 | VAL  |
| 1   | 13-A  | 243 | THR  |
| 1   | 13-A  | 256 | GLN  |
| 1   | 13-A  | 276 | MET  |
| 1   | 13-A  | 277 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 13-A  | 298 | ARG  |
| 1   | 13-A  | 301 | SER  |
| 1   | 13-A  | 303 | VAL  |
| 1   | 13-A  | 304 | THR  |
| 1   | 13-A  | 305 | PHE  |
| 1   | 13-A  | 306 | GLN  |
| 1   | 14-A  | 3   | PHE  |
| 1   | 14-A  | 4   | ARG  |
| 1   | 14-A  | 27  | LEU  |
| 1   | 14-A  | 33  | ASP  |
| 1   | 14-A  | 47  | GLU  |
| 1   | 14-A  | 50  | LEU  |
| 1   | 14-A  | 58  | LEU  |
| 1   | 14-A  | 60  | ARG  |
| 1   | 14-A  | 69  | GLN  |
| 1   | 14-A  | 74  | GLN  |
| 1   | 14-A  | 87  | LEU  |
| 1   | 14-A  | 102 | LYS  |
| 1   | 14-A  | 104 | VAL  |
| 1   | 14-A  | 107 | GLN  |
| 1   | 14-A  | 125 | VAL  |
| 1   | 14-A  | 127 | GLN  |
| 1   | 14-A  | 137 | LYS  |
| 1   | 14-A  | 142 | ASN  |
| 1   | 14-A  | 151 | ASN  |
| 1   | 14-A  | 154 | TYR  |
| 1   | 14-A  | 155 | ASP  |
| 1   | 14-A  | 188 | ARG  |
| 1   | 14-A  | 189 | GLN  |
| 1   | 14-A  | 190 | THR  |
| 1   | 14-A  | 216 | ASP  |
| 1   | 14-A  | 217 | ARG  |
| 1   | 14-A  | 227 | LEU  |
| 1   | 14-A  | 232 | LEU  |
| 1   | 14-A  | 233 | VAL  |
| 1   | 14-A  | 242 | LEU  |
| 1   | 14-A  | 256 | GLN  |
| 1   | 14-A  | 298 | ARG  |
| 1   | 14-A  | 299 | GLN  |
| 1   | 14-A  | 301 | SER  |
| 1   | 14-A  | 303 | VAL  |
| 1   | 14-A  | 304 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 14-A  | 305 | PHE  |
| 1   | 14-A  | 306 | GLN  |
| 1   | 15-A  | 6   | MET  |
| 1   | 15-A  | 25  | THR  |
| 1   | 15-A  | 26  | THR  |
| 1   | 15-A  | 27  | LEU  |
| 1   | 15-A  | 45  | THR  |
| 1   | 15-A  | 46  | SER  |
| 1   | 15-A  | 50  | LEU  |
| 1   | 15-A  | 58  | LEU  |
| 1   | 15-A  | 59  | ILE  |
| 1   | 15-A  | 60  | ARG  |
| 1   | 15-A  | 61  | LYS  |
| 1   | 15-A  | 75  | LEU  |
| 1   | 15-A  | 90  | LYS  |
| 1   | 15-A  | 101 | TYR  |
| 1   | 15-A  | 102 | LYS  |
| 1   | 15-A  | 125 | VAL  |
| 1   | 15-A  | 136 | ILE  |
| 1   | 15-A  | 141 | LEU  |
| 1   | 15-A  | 142 | ASN  |
| 1   | 15-A  | 154 | TYR  |
| 1   | 15-A  | 178 | GLU  |
| 1   | 15-A  | 192 | GLN  |
| 1   | 15-A  | 217 | ARG  |
| 1   | 15-A  | 222 | ARG  |
| 1   | 15-A  | 225 | THR  |
| 1   | 15-A  | 229 | ASP  |
| 1   | 15-A  | 235 | MET  |
| 1   | 15-A  | 236 | LYS  |
| 1   | 15-A  | 256 | GLN  |
| 1   | 15-A  | 267 | SER  |
| 1   | 15-A  | 270 | GLU  |
| 1   | 15-A  | 277 | ASN  |
| 1   | 15-A  | 279 | ARG  |
| 1   | 15-A  | 284 | SER  |
| 1   | 15-A  | 298 | ARG  |
| 1   | 15-A  | 300 | CYS  |
| 1   | 15-A  | 303 | VAL  |
| 1   | 15-A  | 304 | THR  |
| 1   | 15-A  | 306 | GLN  |
| 1   | 16-A  | 5   | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 16-A  | 6   | MET  |
| 1   | 16-A  | 19  | GLN  |
| 1   | 16-A  | 25  | THR  |
| 1   | 16-A  | 27  | LEU  |
| 1   | 16-A  | 50  | LEU  |
| 1   | 16-A  | 51  | ASN  |
| 1   | 16-A  | 72  | ASN  |
| 1   | 16-A  | 75  | LEU  |
| 1   | 16-A  | 102 | LYS  |
| 1   | 16-A  | 119 | ASN  |
| 1   | 16-A  | 130 | MET  |
| 1   | 16-A  | 137 | LYS  |
| 1   | 16-A  | 141 | LEU  |
| 1   | 16-A  | 156 | CYS  |
| 1   | 16-A  | 165 | MET  |
| 1   | 16-A  | 178 | GLU  |
| 1   | 16-A  | 188 | ARG  |
| 1   | 16-A  | 216 | ASP  |
| 1   | 16-A  | 217 | ARG  |
| 1   | 16-A  | 221 | ASN  |
| 1   | 16-A  | 222 | ARG  |
| 1   | 16-A  | 223 | PHE  |
| 1   | 16-A  | 236 | LYS  |
| 1   | 16-A  | 257 | THR  |
| 1   | 16-A  | 276 | MET  |
| 1   | 16-A  | 286 | LEU  |
| 1   | 16-A  | 298 | ARG  |
| 1   | 16-A  | 304 | THR  |
| 1   | 16-A  | 306 | GLN  |
| 1   | 17-A  | 1   | SER  |
| 1   | 17-A  | 5   | LYS  |
| 1   | 17-A  | 6   | MET  |
| 1   | 17-A  | 27  | LEU  |
| 1   | 17-A  | 47  | GLU  |
| 1   | 17-A  | 48  | ASP  |
| 1   | 17-A  | 55  | GLU  |
| 1   | 17-A  | 59  | ILE  |
| 1   | 17-A  | 60  | ARG  |
| 1   | 17-A  | 74  | GLN  |
| 1   | 17-A  | 107 | GLN  |
| 1   | 17-A  | 110 | GLN  |
| 1   | 17-A  | 119 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 17-A  | 154 | TYR  |
| 1   | 17-A  | 188 | ARG  |
| 1   | 17-A  | 213 | ILE  |
| 1   | 17-A  | 216 | ASP  |
| 1   | 17-A  | 217 | ARG  |
| 1   | 17-A  | 221 | ASN  |
| 1   | 17-A  | 227 | LEU  |
| 1   | 17-A  | 232 | LEU  |
| 1   | 17-A  | 233 | VAL  |
| 1   | 17-A  | 235 | MET  |
| 1   | 17-A  | 236 | LYS  |
| 1   | 17-A  | 240 | GLU  |
| 1   | 17-A  | 249 | ILE  |
| 1   | 17-A  | 256 | GLN  |
| 1   | 17-A  | 270 | GLU  |
| 1   | 17-A  | 286 | LEU  |
| 1   | 17-A  | 288 | GLU  |
| 1   | 17-A  | 300 | CYS  |
| 1   | 17-A  | 306 | GLN  |
| 1   | 18-A  | 5   | LYS  |
| 1   | 18-A  | 6   | MET  |
| 1   | 18-A  | 24  | THR  |
| 1   | 18-A  | 27  | LEU  |
| 1   | 18-A  | 47  | GLU  |
| 1   | 18-A  | 48  | ASP  |
| 1   | 18-A  | 58  | LEU  |
| 1   | 18-A  | 60  | ARG  |
| 1   | 18-A  | 67  | LEU  |
| 1   | 18-A  | 69  | GLN  |
| 1   | 18-A  | 72  | ASN  |
| 1   | 18-A  | 73  | VAL  |
| 1   | 18-A  | 74  | GLN  |
| 1   | 18-A  | 87  | LEU  |
| 1   | 18-A  | 90  | LYS  |
| 1   | 18-A  | 102 | LYS  |
| 1   | 18-A  | 107 | GLN  |
| 1   | 18-A  | 141 | LEU  |
| 1   | 18-A  | 165 | MET  |
| 1   | 18-A  | 167 | LEU  |
| 1   | 18-A  | 190 | THR  |
| 1   | 18-A  | 217 | ARG  |
| 1   | 18-A  | 221 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 18-A  | 227 | LEU  |
| 1   | 18-A  | 232 | LEU  |
| 1   | 18-A  | 236 | LYS  |
| 1   | 18-A  | 249 | ILE  |
| 1   | 18-A  | 270 | GLU  |
| 1   | 18-A  | 276 | MET  |
| 1   | 18-A  | 286 | LEU  |
| 1   | 18-A  | 297 | VAL  |
| 1   | 18-A  | 305 | PHE  |
| 1   | 18-A  | 306 | GLN  |
| 1   | 19-A  | 5   | LYS  |
| 1   | 19-A  | 6   | MET  |
| 1   | 19-A  | 24  | THR  |
| 1   | 19-A  | 27  | LEU  |
| 1   | 19-A  | 47  | GLU  |
| 1   | 19-A  | 50  | LEU  |
| 1   | 19-A  | 55  | GLU  |
| 1   | 19-A  | 58  | LEU  |
| 1   | 19-A  | 60  | ARG  |
| 1   | 19-A  | 73  | VAL  |
| 1   | 19-A  | 87  | LEU  |
| 1   | 19-A  | 100 | LYS  |
| 1   | 19-A  | 102 | LYS  |
| 1   | 19-A  | 104 | VAL  |
| 1   | 19-A  | 141 | LEU  |
| 1   | 19-A  | 188 | ARG  |
| 1   | 19-A  | 213 | ILE  |
| 1   | 19-A  | 216 | ASP  |
| 1   | 19-A  | 217 | ARG  |
| 1   | 19-A  | 222 | ARG  |
| 1   | 19-A  | 232 | LEU  |
| 1   | 19-A  | 235 | MET  |
| 1   | 19-A  | 244 | GLN  |
| 1   | 19-A  | 249 | ILE  |
| 1   | 19-A  | 276 | MET  |
| 1   | 19-A  | 277 | ASN  |
| 1   | 19-A  | 286 | LEU  |
| 1   | 19-A  | 301 | SER  |
| 1   | 19-A  | 304 | THR  |
| 1   | 20-A  | 12  | LYS  |
| 1   | 20-A  | 24  | THR  |
| 1   | 20-A  | 27  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 20-A  | 33  | ASP  |
| 1   | 20-A  | 45  | THR  |
| 1   | 20-A  | 47  | GLU  |
| 1   | 20-A  | 59  | ILE  |
| 1   | 20-A  | 62  | SER  |
| 1   | 20-A  | 69  | GLN  |
| 1   | 20-A  | 73  | VAL  |
| 1   | 20-A  | 75  | LEU  |
| 1   | 20-A  | 107 | GLN  |
| 1   | 20-A  | 110 | GLN  |
| 1   | 20-A  | 125 | VAL  |
| 1   | 20-A  | 130 | MET  |
| 1   | 20-A  | 136 | ILE  |
| 1   | 20-A  | 165 | MET  |
| 1   | 20-A  | 213 | ILE  |
| 1   | 20-A  | 221 | ASN  |
| 1   | 20-A  | 222 | ARG  |
| 1   | 20-A  | 225 | THR  |
| 1   | 20-A  | 227 | LEU  |
| 1   | 20-A  | 235 | MET  |
| 1   | 20-A  | 236 | LYS  |
| 1   | 20-A  | 244 | GLN  |
| 1   | 20-A  | 256 | GLN  |
| 1   | 20-A  | 267 | SER  |
| 1   | 20-A  | 276 | MET  |
| 1   | 20-A  | 277 | ASN  |
| 1   | 20-A  | 286 | LEU  |
| 1   | 20-A  | 298 | ARG  |
| 1   | 20-A  | 306 | GLN  |
| 1   | 21-A  | 1   | SER  |
| 1   | 21-A  | 25  | THR  |
| 1   | 21-A  | 27  | LEU  |
| 1   | 21-A  | 46  | SER  |
| 1   | 21-A  | 47  | GLU  |
| 1   | 21-A  | 55  | GLU  |
| 1   | 21-A  | 61  | LYS  |
| 1   | 21-A  | 74  | GLN  |
| 1   | 21-A  | 100 | LYS  |
| 1   | 21-A  | 123 | SER  |
| 1   | 21-A  | 130 | MET  |
| 1   | 21-A  | 141 | LEU  |
| 1   | 21-A  | 154 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 21-A  | 155 | ASP  |
| 1   | 21-A  | 216 | ASP  |
| 1   | 21-A  | 222 | ARG  |
| 1   | 21-A  | 223 | PHE  |
| 1   | 21-A  | 227 | LEU  |
| 1   | 21-A  | 232 | LEU  |
| 1   | 21-A  | 249 | ILE  |
| 1   | 21-A  | 267 | SER  |
| 1   | 21-A  | 286 | LEU  |
| 1   | 21-A  | 298 | ARG  |
| 1   | 21-A  | 304 | THR  |
| 1   | 21-A  | 305 | PHE  |
| 1   | 21-A  | 306 | GLN  |
| 1   | 22-A  | 46  | SER  |
| 1   | 22-A  | 47  | GLU  |
| 1   | 22-A  | 53  | ASN  |
| 1   | 22-A  | 59  | ILE  |
| 1   | 22-A  | 60  | ARG  |
| 1   | 22-A  | 72  | ASN  |
| 1   | 22-A  | 119 | ASN  |
| 1   | 22-A  | 137 | LYS  |
| 1   | 22-A  | 141 | LEU  |
| 1   | 22-A  | 154 | TYR  |
| 1   | 22-A  | 188 | ARG  |
| 1   | 22-A  | 190 | THR  |
| 1   | 22-A  | 213 | ILE  |
| 1   | 22-A  | 216 | ASP  |
| 1   | 22-A  | 222 | ARG  |
| 1   | 22-A  | 240 | GLU  |
| 1   | 22-A  | 298 | ARG  |
| 1   | 22-A  | 301 | SER  |
| 1   | 22-A  | 306 | GLN  |
| 1   | 23-A  | 1   | SER  |
| 1   | 23-A  | 12  | LYS  |
| 1   | 23-A  | 24  | THR  |
| 1   | 23-A  | 25  | THR  |
| 1   | 23-A  | 27  | LEU  |
| 1   | 23-A  | 45  | THR  |
| 1   | 23-A  | 46  | SER  |
| 1   | 23-A  | 47  | GLU  |
| 1   | 23-A  | 53  | ASN  |
| 1   | 23-A  | 59  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 23-A  | 67  | LEU  |
| 1   | 23-A  | 72  | ASN  |
| 1   | 23-A  | 87  | LEU  |
| 1   | 23-A  | 100 | LYS  |
| 1   | 23-A  | 102 | LYS  |
| 1   | 23-A  | 107 | GLN  |
| 1   | 23-A  | 119 | ASN  |
| 1   | 23-A  | 125 | VAL  |
| 1   | 23-A  | 136 | ILE  |
| 1   | 23-A  | 141 | LEU  |
| 1   | 23-A  | 145 | CYS  |
| 1   | 23-A  | 152 | ILE  |
| 1   | 23-A  | 153 | ASP  |
| 1   | 23-A  | 154 | TYR  |
| 1   | 23-A  | 166 | GLU  |
| 1   | 23-A  | 188 | ARG  |
| 1   | 23-A  | 190 | THR  |
| 1   | 23-A  | 192 | GLN  |
| 1   | 23-A  | 216 | ASP  |
| 1   | 23-A  | 222 | ARG  |
| 1   | 23-A  | 225 | THR  |
| 1   | 23-A  | 232 | LEU  |
| 1   | 23-A  | 235 | MET  |
| 1   | 23-A  | 256 | GLN  |
| 1   | 23-A  | 271 | LEU  |
| 1   | 23-A  | 276 | MET  |
| 1   | 23-A  | 279 | ARG  |
| 1   | 23-A  | 298 | ARG  |
| 1   | 23-A  | 304 | THR  |
| 1   | 23-A  | 306 | GLN  |
| 1   | 24-A  | 1   | SER  |
| 1   | 24-A  | 4   | ARG  |
| 1   | 24-A  | 6   | MET  |
| 1   | 24-A  | 24  | THR  |
| 1   | 24-A  | 27  | LEU  |
| 1   | 24-A  | 34  | ASP  |
| 1   | 24-A  | 41  | HIS  |
| 1   | 24-A  | 46  | SER  |
| 1   | 24-A  | 49  | MET  |
| 1   | 24-A  | 50  | LEU  |
| 1   | 24-A  | 53  | ASN  |
| 1   | 24-A  | 59  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 24-A  | 60  | ARG  |
| 1   | 24-A  | 100 | LYS  |
| 1   | 24-A  | 106 | ILE  |
| 1   | 24-A  | 107 | GLN  |
| 1   | 24-A  | 137 | LYS  |
| 1   | 24-A  | 145 | CYS  |
| 1   | 24-A  | 154 | TYR  |
| 1   | 24-A  | 188 | ARG  |
| 1   | 24-A  | 213 | ILE  |
| 1   | 24-A  | 217 | ARG  |
| 1   | 24-A  | 221 | ASN  |
| 1   | 24-A  | 222 | ARG  |
| 1   | 24-A  | 227 | LEU  |
| 1   | 24-A  | 232 | LEU  |
| 1   | 24-A  | 244 | GLN  |
| 1   | 24-A  | 256 | GLN  |
| 1   | 24-A  | 267 | SER  |
| 1   | 24-A  | 271 | LEU  |
| 1   | 24-A  | 276 | MET  |
| 1   | 24-A  | 290 | GLU  |
| 1   | 24-A  | 298 | ARG  |
| 1   | 24-A  | 303 | VAL  |
| 1   | 24-A  | 305 | PHE  |
| 1   | 25-A  | 1   | SER  |
| 1   | 25-A  | 6   | MET  |
| 1   | 25-A  | 27  | LEU  |
| 1   | 25-A  | 33  | ASP  |
| 1   | 25-A  | 45  | THR  |
| 1   | 25-A  | 47  | GLU  |
| 1   | 25-A  | 48  | ASP  |
| 1   | 25-A  | 49  | MET  |
| 1   | 25-A  | 50  | LEU  |
| 1   | 25-A  | 51  | ASN  |
| 1   | 25-A  | 61  | LYS  |
| 1   | 25-A  | 67  | LEU  |
| 1   | 25-A  | 72  | ASN  |
| 1   | 25-A  | 74  | GLN  |
| 1   | 25-A  | 87  | LEU  |
| 1   | 25-A  | 100 | LYS  |
| 1   | 25-A  | 107 | GLN  |
| 1   | 25-A  | 126 | TYR  |
| 1   | 25-A  | 141 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 25-A  | 154 | TYR  |
| 1   | 25-A  | 165 | MET  |
| 1   | 25-A  | 221 | ASN  |
| 1   | 25-A  | 222 | ARG  |
| 1   | 25-A  | 223 | PHE  |
| 1   | 25-A  | 227 | LEU  |
| 1   | 25-A  | 245 | ASP  |
| 1   | 25-A  | 267 | SER  |
| 1   | 25-A  | 271 | LEU  |
| 1   | 25-A  | 274 | ASN  |
| 1   | 25-A  | 276 | MET  |
| 1   | 25-A  | 298 | ARG  |
| 1   | 25-A  | 299 | GLN  |
| 1   | 25-A  | 303 | VAL  |
| 1   | 25-A  | 304 | THR  |
| 1   | 25-A  | 306 | GLN  |
| 1   | 26-A  | 1   | SER  |
| 1   | 26-A  | 6   | MET  |
| 1   | 26-A  | 27  | LEU  |
| 1   | 26-A  | 45  | THR  |
| 1   | 26-A  | 50  | LEU  |
| 1   | 26-A  | 60  | ARG  |
| 1   | 26-A  | 67  | LEU  |
| 1   | 26-A  | 69  | GLN  |
| 1   | 26-A  | 73  | VAL  |
| 1   | 26-A  | 90  | LYS  |
| 1   | 26-A  | 102 | LYS  |
| 1   | 26-A  | 104 | VAL  |
| 1   | 26-A  | 107 | GLN  |
| 1   | 26-A  | 119 | ASN  |
| 1   | 26-A  | 130 | MET  |
| 1   | 26-A  | 142 | ASN  |
| 1   | 26-A  | 165 | MET  |
| 1   | 26-A  | 177 | LEU  |
| 1   | 26-A  | 189 | GLN  |
| 1   | 26-A  | 190 | THR  |
| 1   | 26-A  | 216 | ASP  |
| 1   | 26-A  | 227 | LEU  |
| 1   | 26-A  | 236 | LYS  |
| 1   | 26-A  | 271 | LEU  |
| 1   | 26-A  | 276 | MET  |
| 1   | 26-A  | 279 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 26-A  | 286 | LEU  |
| 1   | 26-A  | 298 | ARG  |
| 1   | 26-A  | 303 | VAL  |
| 1   | 26-A  | 305 | PHE  |
| 1   | 27-A  | 5   | LYS  |
| 1   | 27-A  | 6   | MET  |
| 1   | 27-A  | 27  | LEU  |
| 1   | 27-A  | 41  | HIS  |
| 1   | 27-A  | 47  | GLU  |
| 1   | 27-A  | 49  | MET  |
| 1   | 27-A  | 51  | ASN  |
| 1   | 27-A  | 59  | ILE  |
| 1   | 27-A  | 62  | SER  |
| 1   | 27-A  | 67  | LEU  |
| 1   | 27-A  | 74  | GLN  |
| 1   | 27-A  | 87  | LEU  |
| 1   | 27-A  | 100 | LYS  |
| 1   | 27-A  | 123 | SER  |
| 1   | 27-A  | 130 | MET  |
| 1   | 27-A  | 136 | ILE  |
| 1   | 27-A  | 156 | CYS  |
| 1   | 27-A  | 165 | MET  |
| 1   | 27-A  | 169 | THR  |
| 1   | 27-A  | 189 | GLN  |
| 1   | 27-A  | 213 | ILE  |
| 1   | 27-A  | 216 | ASP  |
| 1   | 27-A  | 217 | ARG  |
| 1   | 27-A  | 225 | THR  |
| 1   | 27-A  | 227 | LEU  |
| 1   | 27-A  | 235 | MET  |
| 1   | 27-A  | 242 | LEU  |
| 1   | 27-A  | 274 | ASN  |
| 1   | 27-A  | 276 | MET  |
| 1   | 27-A  | 298 | ARG  |
| 1   | 27-A  | 303 | VAL  |
| 1   | 27-A  | 305 | PHE  |
| 1   | 27-A  | 306 | GLN  |
| 1   | 28-A  | 5   | LYS  |
| 1   | 28-A  | 25  | THR  |
| 1   | 28-A  | 27  | LEU  |
| 1   | 28-A  | 49  | MET  |
| 1   | 28-A  | 50  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 28-A  | 58  | LEU  |
| 1   | 28-A  | 73  | VAL  |
| 1   | 28-A  | 78  | ILE  |
| 1   | 28-A  | 100 | LYS  |
| 1   | 28-A  | 102 | LYS  |
| 1   | 28-A  | 104 | VAL  |
| 1   | 28-A  | 107 | GLN  |
| 1   | 28-A  | 130 | MET  |
| 1   | 28-A  | 155 | ASP  |
| 1   | 28-A  | 213 | ILE  |
| 1   | 28-A  | 216 | ASP  |
| 1   | 28-A  | 221 | ASN  |
| 1   | 28-A  | 222 | ARG  |
| 1   | 28-A  | 223 | PHE  |
| 1   | 28-A  | 228 | ASN  |
| 1   | 28-A  | 232 | LEU  |
| 1   | 28-A  | 235 | MET  |
| 1   | 28-A  | 236 | LYS  |
| 1   | 28-A  | 242 | LEU  |
| 1   | 28-A  | 245 | ASP  |
| 1   | 28-A  | 249 | ILE  |
| 1   | 28-A  | 256 | GLN  |
| 1   | 28-A  | 286 | LEU  |
| 1   | 28-A  | 298 | ARG  |
| 1   | 28-A  | 303 | VAL  |
| 1   | 28-A  | 304 | THR  |
| 1   | 28-A  | 305 | PHE  |
| 1   | 28-A  | 306 | GLN  |
| 1   | 29-A  | 1   | SER  |
| 1   | 29-A  | 22  | CYS  |
| 1   | 29-A  | 24  | THR  |
| 1   | 29-A  | 25  | THR  |
| 1   | 29-A  | 45  | THR  |
| 1   | 29-A  | 47  | GLU  |
| 1   | 29-A  | 48  | ASP  |
| 1   | 29-A  | 49  | MET  |
| 1   | 29-A  | 50  | LEU  |
| 1   | 29-A  | 58  | LEU  |
| 1   | 29-A  | 69  | GLN  |
| 1   | 29-A  | 72  | ASN  |
| 1   | 29-A  | 73  | VAL  |
| 1   | 29-A  | 97  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 29-A  | 100 | LYS  |
| 1   | 29-A  | 106 | ILE  |
| 1   | 29-A  | 121 | SER  |
| 1   | 29-A  | 123 | SER  |
| 1   | 29-A  | 125 | VAL  |
| 1   | 29-A  | 128 | CYS  |
| 1   | 29-A  | 141 | LEU  |
| 1   | 29-A  | 142 | ASN  |
| 1   | 29-A  | 144 | SER  |
| 1   | 29-A  | 152 | ILE  |
| 1   | 29-A  | 153 | ASP  |
| 1   | 29-A  | 155 | ASP  |
| 1   | 29-A  | 165 | MET  |
| 1   | 29-A  | 177 | LEU  |
| 1   | 29-A  | 188 | ARG  |
| 1   | 29-A  | 189 | GLN  |
| 1   | 29-A  | 214 | ASN  |
| 1   | 29-A  | 217 | ARG  |
| 1   | 29-A  | 222 | ARG  |
| 1   | 29-A  | 242 | LEU  |
| 1   | 29-A  | 248 | ASP  |
| 1   | 29-A  | 249 | ILE  |
| 1   | 29-A  | 256 | GLN  |
| 1   | 29-A  | 276 | MET  |
| 1   | 29-A  | 286 | LEU  |
| 1   | 29-A  | 287 | LEU  |
| 1   | 29-A  | 288 | GLU  |
| 1   | 29-A  | 290 | GLU  |
| 1   | 29-A  | 299 | GLN  |
| 1   | 29-A  | 304 | THR  |
| 1   | 30-A  | 6   | MET  |
| 1   | 30-A  | 24  | THR  |
| 1   | 30-A  | 27  | LEU  |
| 1   | 30-A  | 41  | HIS  |
| 1   | 30-A  | 45  | THR  |
| 1   | 30-A  | 46  | SER  |
| 1   | 30-A  | 47  | GLU  |
| 1   | 30-A  | 58  | LEU  |
| 1   | 30-A  | 60  | ARG  |
| 1   | 30-A  | 66  | PHE  |
| 1   | 30-A  | 72  | ASN  |
| 1   | 30-A  | 73  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 30-A  | 90  | LYS  |
| 1   | 30-A  | 100 | LYS  |
| 1   | 30-A  | 104 | VAL  |
| 1   | 30-A  | 107 | GLN  |
| 1   | 30-A  | 119 | ASN  |
| 1   | 30-A  | 141 | LEU  |
| 1   | 30-A  | 154 | TYR  |
| 1   | 30-A  | 155 | ASP  |
| 1   | 30-A  | 156 | CYS  |
| 1   | 30-A  | 167 | LEU  |
| 1   | 30-A  | 222 | ARG  |
| 1   | 30-A  | 227 | LEU  |
| 1   | 30-A  | 267 | SER  |
| 1   | 30-A  | 272 | LEU  |
| 1   | 30-A  | 279 | ARG  |
| 1   | 30-A  | 299 | GLN  |
| 1   | 30-A  | 306 | GLN  |
| 1   | 31-A  | 6   | MET  |
| 1   | 31-A  | 24  | THR  |
| 1   | 31-A  | 25  | THR  |
| 1   | 31-A  | 26  | THR  |
| 1   | 31-A  | 27  | LEU  |
| 1   | 31-A  | 33  | ASP  |
| 1   | 31-A  | 47  | GLU  |
| 1   | 31-A  | 49  | MET  |
| 1   | 31-A  | 50  | LEU  |
| 1   | 31-A  | 58  | LEU  |
| 1   | 31-A  | 87  | LEU  |
| 1   | 31-A  | 97  | LYS  |
| 1   | 31-A  | 102 | LYS  |
| 1   | 31-A  | 107 | GLN  |
| 1   | 31-A  | 110 | GLN  |
| 1   | 31-A  | 128 | CYS  |
| 1   | 31-A  | 139 | SER  |
| 1   | 31-A  | 141 | LEU  |
| 1   | 31-A  | 142 | ASN  |
| 1   | 31-A  | 152 | ILE  |
| 1   | 31-A  | 154 | TYR  |
| 1   | 31-A  | 155 | ASP  |
| 1   | 31-A  | 156 | CYS  |
| 1   | 31-A  | 165 | MET  |
| 1   | 31-A  | 166 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 31-A  | 188 | ARG  |
| 1   | 31-A  | 213 | ILE  |
| 1   | 31-A  | 217 | ARG  |
| 1   | 31-A  | 221 | ASN  |
| 1   | 31-A  | 222 | ARG  |
| 1   | 31-A  | 223 | PHE  |
| 1   | 31-A  | 225 | THR  |
| 1   | 31-A  | 227 | LEU  |
| 1   | 31-A  | 232 | LEU  |
| 1   | 31-A  | 242 | LEU  |
| 1   | 31-A  | 245 | ASP  |
| 1   | 31-A  | 271 | LEU  |
| 1   | 31-A  | 276 | MET  |
| 1   | 31-A  | 298 | ARG  |
| 1   | 31-A  | 305 | PHE  |
| 1   | 31-A  | 306 | GLN  |
| 1   | 32-A  | 1   | SER  |
| 1   | 32-A  | 6   | MET  |
| 1   | 32-A  | 12  | LYS  |
| 1   | 32-A  | 27  | LEU  |
| 1   | 32-A  | 39  | PRO  |
| 1   | 32-A  | 41  | HIS  |
| 1   | 32-A  | 46  | SER  |
| 1   | 32-A  | 58  | LEU  |
| 1   | 32-A  | 60  | ARG  |
| 1   | 32-A  | 65  | ASN  |
| 1   | 32-A  | 67  | LEU  |
| 1   | 32-A  | 72  | ASN  |
| 1   | 32-A  | 83  | GLN  |
| 1   | 32-A  | 90  | LYS  |
| 1   | 32-A  | 102 | LYS  |
| 1   | 32-A  | 107 | GLN  |
| 1   | 32-A  | 114 | VAL  |
| 1   | 32-A  | 122 | PRO  |
| 1   | 32-A  | 123 | SER  |
| 1   | 32-A  | 125 | VAL  |
| 1   | 32-A  | 141 | LEU  |
| 1   | 32-A  | 142 | ASN  |
| 1   | 32-A  | 155 | ASP  |
| 1   | 32-A  | 162 | MET  |
| 1   | 32-A  | 165 | MET  |
| 1   | 32-A  | 166 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 32-A  | 177 | LEU  |
| 1   | 32-A  | 188 | ARG  |
| 1   | 32-A  | 216 | ASP  |
| 1   | 32-A  | 217 | ARG  |
| 1   | 32-A  | 221 | ASN  |
| 1   | 32-A  | 227 | LEU  |
| 1   | 32-A  | 232 | LEU  |
| 1   | 32-A  | 235 | MET  |
| 1   | 32-A  | 249 | ILE  |
| 1   | 32-A  | 298 | ARG  |
| 1   | 32-A  | 305 | PHE  |
| 1   | 33-A  | 3   | PHE  |
| 1   | 33-A  | 5   | LYS  |
| 1   | 33-A  | 6   | MET  |
| 1   | 33-A  | 24  | THR  |
| 1   | 33-A  | 27  | LEU  |
| 1   | 33-A  | 49  | MET  |
| 1   | 33-A  | 50  | LEU  |
| 1   | 33-A  | 58  | LEU  |
| 1   | 33-A  | 60  | ARG  |
| 1   | 33-A  | 74  | GLN  |
| 1   | 33-A  | 90  | LYS  |
| 1   | 33-A  | 97  | LYS  |
| 1   | 33-A  | 107 | GLN  |
| 1   | 33-A  | 119 | ASN  |
| 1   | 33-A  | 123 | SER  |
| 1   | 33-A  | 136 | ILE  |
| 1   | 33-A  | 140 | PHE  |
| 1   | 33-A  | 141 | LEU  |
| 1   | 33-A  | 144 | SER  |
| 1   | 33-A  | 167 | LEU  |
| 1   | 33-A  | 216 | ASP  |
| 1   | 33-A  | 221 | ASN  |
| 1   | 33-A  | 235 | MET  |
| 1   | 33-A  | 242 | LEU  |
| 1   | 33-A  | 244 | GLN  |
| 1   | 33-A  | 249 | ILE  |
| 1   | 33-A  | 271 | LEU  |
| 1   | 33-A  | 279 | ARG  |
| 1   | 33-A  | 286 | LEU  |
| 1   | 33-A  | 287 | LEU  |
| 1   | 33-A  | 294 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 33-A  | 300 | CYS  |
| 1   | 33-A  | 301 | SER  |
| 1   | 34-A  | 6   | MET  |
| 1   | 34-A  | 25  | THR  |
| 1   | 34-A  | 27  | LEU  |
| 1   | 34-A  | 45  | THR  |
| 1   | 34-A  | 47  | GLU  |
| 1   | 34-A  | 48  | ASP  |
| 1   | 34-A  | 49  | MET  |
| 1   | 34-A  | 58  | LEU  |
| 1   | 34-A  | 60  | ARG  |
| 1   | 34-A  | 61  | LYS  |
| 1   | 34-A  | 74  | GLN  |
| 1   | 34-A  | 102 | LYS  |
| 1   | 34-A  | 128 | CYS  |
| 1   | 34-A  | 130 | MET  |
| 1   | 34-A  | 141 | LEU  |
| 1   | 34-A  | 153 | ASP  |
| 1   | 34-A  | 156 | CYS  |
| 1   | 34-A  | 162 | MET  |
| 1   | 34-A  | 165 | MET  |
| 1   | 34-A  | 217 | ARG  |
| 1   | 34-A  | 221 | ASN  |
| 1   | 34-A  | 224 | THR  |
| 1   | 34-A  | 225 | THR  |
| 1   | 34-A  | 232 | LEU  |
| 1   | 34-A  | 235 | MET  |
| 1   | 34-A  | 244 | GLN  |
| 1   | 34-A  | 249 | ILE  |
| 1   | 34-A  | 254 | SER  |
| 1   | 34-A  | 256 | GLN  |
| 1   | 34-A  | 267 | SER  |
| 1   | 34-A  | 270 | GLU  |
| 1   | 34-A  | 276 | MET  |
| 1   | 34-A  | 279 | ARG  |
| 1   | 34-A  | 287 | LEU  |
| 1   | 34-A  | 298 | ARG  |
| 1   | 34-A  | 305 | PHE  |
| 1   | 34-A  | 306 | GLN  |
| 1   | 35-A  | 4   | ARG  |
| 1   | 35-A  | 5   | LYS  |
| 1   | 35-A  | 6   | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 35-A  | 27  | LEU  |
| 1   | 35-A  | 47  | GLU  |
| 1   | 35-A  | 58  | LEU  |
| 1   | 35-A  | 59  | ILE  |
| 1   | 35-A  | 60  | ARG  |
| 1   | 35-A  | 61  | LYS  |
| 1   | 35-A  | 73  | VAL  |
| 1   | 35-A  | 97  | LYS  |
| 1   | 35-A  | 102 | LYS  |
| 1   | 35-A  | 104 | VAL  |
| 1   | 35-A  | 110 | GLN  |
| 1   | 35-A  | 122 | PRO  |
| 1   | 35-A  | 123 | SER  |
| 1   | 35-A  | 125 | VAL  |
| 1   | 35-A  | 139 | SER  |
| 1   | 35-A  | 142 | ASN  |
| 1   | 35-A  | 153 | ASP  |
| 1   | 35-A  | 154 | TYR  |
| 1   | 35-A  | 155 | ASP  |
| 1   | 35-A  | 165 | MET  |
| 1   | 35-A  | 188 | ARG  |
| 1   | 35-A  | 216 | ASP  |
| 1   | 35-A  | 217 | ARG  |
| 1   | 35-A  | 222 | ARG  |
| 1   | 35-A  | 223 | PHE  |
| 1   | 35-A  | 227 | LEU  |
| 1   | 35-A  | 233 | VAL  |
| 1   | 35-A  | 235 | MET  |
| 1   | 35-A  | 236 | LYS  |
| 1   | 35-A  | 267 | SER  |
| 1   | 35-A  | 270 | GLU  |
| 1   | 35-A  | 271 | LEU  |
| 1   | 35-A  | 272 | LEU  |
| 1   | 35-A  | 274 | ASN  |
| 1   | 35-A  | 279 | ARG  |
| 1   | 35-A  | 286 | LEU  |
| 1   | 35-A  | 287 | LEU  |
| 1   | 35-A  | 300 | CYS  |
| 1   | 35-A  | 304 | THR  |
| 1   | 36-A  | 5   | LYS  |
| 1   | 36-A  | 6   | MET  |
| 1   | 36-A  | 25  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 36-A  | 27  | LEU  |
| 1   | 36-A  | 45  | THR  |
| 1   | 36-A  | 47  | GLU  |
| 1   | 36-A  | 75  | LEU  |
| 1   | 36-A  | 107 | GLN  |
| 1   | 36-A  | 122 | PRO  |
| 1   | 36-A  | 136 | ILE  |
| 1   | 36-A  | 141 | LEU  |
| 1   | 36-A  | 142 | ASN  |
| 1   | 36-A  | 165 | MET  |
| 1   | 36-A  | 188 | ARG  |
| 1   | 36-A  | 222 | ARG  |
| 1   | 36-A  | 227 | LEU  |
| 1   | 36-A  | 232 | LEU  |
| 1   | 36-A  | 242 | LEU  |
| 1   | 36-A  | 249 | ILE  |
| 1   | 36-A  | 256 | GLN  |
| 1   | 36-A  | 277 | ASN  |
| 1   | 36-A  | 279 | ARG  |
| 1   | 36-A  | 286 | LEU  |
| 1   | 36-A  | 288 | GLU  |
| 1   | 36-A  | 294 | PHE  |
| 1   | 36-A  | 299 | GLN  |
| 1   | 36-A  | 305 | PHE  |
| 1   | 37-A  | 1   | SER  |
| 1   | 37-A  | 5   | LYS  |
| 1   | 37-A  | 25  | THR  |
| 1   | 37-A  | 27  | LEU  |
| 1   | 37-A  | 47  | GLU  |
| 1   | 37-A  | 50  | LEU  |
| 1   | 37-A  | 62  | SER  |
| 1   | 37-A  | 72  | ASN  |
| 1   | 37-A  | 75  | LEU  |
| 1   | 37-A  | 97  | LYS  |
| 1   | 37-A  | 102 | LYS  |
| 1   | 37-A  | 106 | ILE  |
| 1   | 37-A  | 125 | VAL  |
| 1   | 37-A  | 128 | CYS  |
| 1   | 37-A  | 136 | ILE  |
| 1   | 37-A  | 141 | LEU  |
| 1   | 37-A  | 155 | ASP  |
| 1   | 37-A  | 167 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 37-A  | 189 | GLN  |
| 1   | 37-A  | 190 | THR  |
| 1   | 37-A  | 217 | ARG  |
| 1   | 37-A  | 222 | ARG  |
| 1   | 37-A  | 223 | PHE  |
| 1   | 37-A  | 232 | LEU  |
| 1   | 37-A  | 235 | MET  |
| 1   | 37-A  | 236 | LYS  |
| 1   | 37-A  | 240 | GLU  |
| 1   | 37-A  | 241 | PRO  |
| 1   | 37-A  | 242 | LEU  |
| 1   | 37-A  | 244 | GLN  |
| 1   | 37-A  | 249 | ILE  |
| 1   | 37-A  | 256 | GLN  |
| 1   | 37-A  | 271 | LEU  |
| 1   | 37-A  | 272 | LEU  |
| 1   | 37-A  | 276 | MET  |
| 1   | 37-A  | 286 | LEU  |
| 1   | 37-A  | 300 | CYS  |
| 1   | 37-A  | 301 | SER  |
| 1   | 37-A  | 303 | VAL  |
| 1   | 37-A  | 305 | PHE  |
| 1   | 38-A  | 25  | THR  |
| 1   | 38-A  | 27  | LEU  |
| 1   | 38-A  | 47  | GLU  |
| 1   | 38-A  | 48  | ASP  |
| 1   | 38-A  | 49  | MET  |
| 1   | 38-A  | 58  | LEU  |
| 1   | 38-A  | 59  | ILE  |
| 1   | 38-A  | 60  | ARG  |
| 1   | 38-A  | 61  | LYS  |
| 1   | 38-A  | 67  | LEU  |
| 1   | 38-A  | 69  | GLN  |
| 1   | 38-A  | 75  | LEU  |
| 1   | 38-A  | 90  | LYS  |
| 1   | 38-A  | 97  | LYS  |
| 1   | 38-A  | 102 | LYS  |
| 1   | 38-A  | 104 | VAL  |
| 1   | 38-A  | 119 | ASN  |
| 1   | 38-A  | 121 | SER  |
| 1   | 38-A  | 125 | VAL  |
| 1   | 38-A  | 136 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 38-A  | 137 | LYS  |
| 1   | 38-A  | 142 | ASN  |
| 1   | 38-A  | 153 | ASP  |
| 1   | 38-A  | 154 | TYR  |
| 1   | 38-A  | 156 | CYS  |
| 1   | 38-A  | 167 | LEU  |
| 1   | 38-A  | 169 | THR  |
| 1   | 38-A  | 178 | GLU  |
| 1   | 38-A  | 216 | ASP  |
| 1   | 38-A  | 217 | ARG  |
| 1   | 38-A  | 221 | ASN  |
| 1   | 38-A  | 222 | ARG  |
| 1   | 38-A  | 224 | THR  |
| 1   | 38-A  | 227 | LEU  |
| 1   | 38-A  | 232 | LEU  |
| 1   | 38-A  | 233 | VAL  |
| 1   | 38-A  | 236 | LYS  |
| 1   | 38-A  | 240 | GLU  |
| 1   | 38-A  | 241 | PRO  |
| 1   | 38-A  | 244 | GLN  |
| 1   | 38-A  | 256 | GLN  |
| 1   | 38-A  | 271 | LEU  |
| 1   | 38-A  | 273 | GLN  |
| 1   | 38-A  | 279 | ARG  |
| 1   | 38-A  | 297 | VAL  |
| 1   | 38-A  | 299 | GLN  |
| 1   | 38-A  | 300 | CYS  |
| 1   | 38-A  | 301 | SER  |
| 1   | 38-A  | 305 | PHE  |
| 1   | 39-A  | 1   | SER  |
| 1   | 39-A  | 5   | LYS  |
| 1   | 39-A  | 24  | THR  |
| 1   | 39-A  | 27  | LEU  |
| 1   | 39-A  | 50  | LEU  |
| 1   | 39-A  | 59  | ILE  |
| 1   | 39-A  | 60  | ARG  |
| 1   | 39-A  | 61  | LYS  |
| 1   | 39-A  | 69  | GLN  |
| 1   | 39-A  | 75  | LEU  |
| 1   | 39-A  | 97  | LYS  |
| 1   | 39-A  | 102 | LYS  |
| 1   | 39-A  | 107 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 39-A  | 130 | MET  |
| 1   | 39-A  | 137 | LYS  |
| 1   | 39-A  | 141 | LEU  |
| 1   | 39-A  | 152 | ILE  |
| 1   | 39-A  | 154 | TYR  |
| 1   | 39-A  | 155 | ASP  |
| 1   | 39-A  | 157 | VAL  |
| 1   | 39-A  | 158 | SER  |
| 1   | 39-A  | 180 | ASN  |
| 1   | 39-A  | 189 | GLN  |
| 1   | 39-A  | 216 | ASP  |
| 1   | 39-A  | 222 | ARG  |
| 1   | 39-A  | 223 | PHE  |
| 1   | 39-A  | 224 | THR  |
| 1   | 39-A  | 235 | MET  |
| 1   | 39-A  | 244 | GLN  |
| 1   | 39-A  | 256 | GLN  |
| 1   | 39-A  | 271 | LEU  |
| 1   | 39-A  | 273 | GLN  |
| 1   | 39-A  | 276 | MET  |
| 1   | 39-A  | 287 | LEU  |
| 1   | 39-A  | 298 | ARG  |
| 1   | 39-A  | 299 | GLN  |
| 1   | 39-A  | 301 | SER  |
| 1   | 39-A  | 304 | THR  |
| 1   | 39-A  | 306 | GLN  |
| 1   | 40-A  | 5   | LYS  |
| 1   | 40-A  | 24  | THR  |
| 1   | 40-A  | 27  | LEU  |
| 1   | 40-A  | 41  | HIS  |
| 1   | 40-A  | 46  | SER  |
| 1   | 40-A  | 49  | MET  |
| 1   | 40-A  | 50  | LEU  |
| 1   | 40-A  | 58  | LEU  |
| 1   | 40-A  | 60  | ARG  |
| 1   | 40-A  | 69  | GLN  |
| 1   | 40-A  | 72  | ASN  |
| 1   | 40-A  | 81  | SER  |
| 1   | 40-A  | 82  | MET  |
| 1   | 40-A  | 86  | VAL  |
| 1   | 40-A  | 90  | LYS  |
| 1   | 40-A  | 104 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 40-A  | 107 | GLN  |
| 1   | 40-A  | 110 | GLN  |
| 1   | 40-A  | 142 | ASN  |
| 1   | 40-A  | 145 | CYS  |
| 1   | 40-A  | 153 | ASP  |
| 1   | 40-A  | 154 | TYR  |
| 1   | 40-A  | 167 | LEU  |
| 1   | 40-A  | 217 | ARG  |
| 1   | 40-A  | 222 | ARG  |
| 1   | 40-A  | 223 | PHE  |
| 1   | 40-A  | 227 | LEU  |
| 1   | 40-A  | 244 | GLN  |
| 1   | 40-A  | 271 | LEU  |
| 1   | 40-A  | 274 | ASN  |
| 1   | 40-A  | 277 | ASN  |
| 1   | 40-A  | 287 | LEU  |
| 1   | 40-A  | 294 | PHE  |
| 1   | 40-A  | 298 | ARG  |
| 1   | 40-A  | 304 | THR  |
| 1   | 40-A  | 306 | GLN  |
| 1   | 41-A  | 1   | SER  |
| 1   | 41-A  | 4   | ARG  |
| 1   | 41-A  | 12  | LYS  |
| 1   | 41-A  | 19  | GLN  |
| 1   | 41-A  | 27  | LEU  |
| 1   | 41-A  | 47  | GLU  |
| 1   | 41-A  | 48  | ASP  |
| 1   | 41-A  | 55  | GLU  |
| 1   | 41-A  | 58  | LEU  |
| 1   | 41-A  | 72  | ASN  |
| 1   | 41-A  | 75  | LEU  |
| 1   | 41-A  | 87  | LEU  |
| 1   | 41-A  | 90  | LYS  |
| 1   | 41-A  | 102 | LYS  |
| 1   | 41-A  | 122 | PRO  |
| 1   | 41-A  | 123 | SER  |
| 1   | 41-A  | 128 | CYS  |
| 1   | 41-A  | 137 | LYS  |
| 1   | 41-A  | 141 | LEU  |
| 1   | 41-A  | 167 | LEU  |
| 1   | 41-A  | 216 | ASP  |
| 1   | 41-A  | 217 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 41-A  | 222 | ARG  |
| 1   | 41-A  | 223 | PHE  |
| 1   | 41-A  | 225 | THR  |
| 1   | 41-A  | 229 | ASP  |
| 1   | 41-A  | 235 | MET  |
| 1   | 41-A  | 244 | GLN  |
| 1   | 41-A  | 245 | ASP  |
| 1   | 41-A  | 249 | ILE  |
| 1   | 41-A  | 272 | LEU  |
| 1   | 41-A  | 276 | MET  |
| 1   | 41-A  | 298 | ARG  |
| 1   | 41-A  | 299 | GLN  |
| 1   | 41-A  | 306 | GLN  |
| 1   | 42-A  | 8   | PHE  |
| 1   | 42-A  | 19  | GLN  |
| 1   | 42-A  | 24  | THR  |
| 1   | 42-A  | 26  | THR  |
| 1   | 42-A  | 51  | ASN  |
| 1   | 42-A  | 58  | LEU  |
| 1   | 42-A  | 59  | ILE  |
| 1   | 42-A  | 60  | ARG  |
| 1   | 42-A  | 69  | GLN  |
| 1   | 42-A  | 72  | ASN  |
| 1   | 42-A  | 87  | LEU  |
| 1   | 42-A  | 102 | LYS  |
| 1   | 42-A  | 104 | VAL  |
| 1   | 42-A  | 139 | SER  |
| 1   | 42-A  | 154 | TYR  |
| 1   | 42-A  | 156 | CYS  |
| 1   | 42-A  | 162 | MET  |
| 1   | 42-A  | 166 | GLU  |
| 1   | 42-A  | 180 | ASN  |
| 1   | 42-A  | 216 | ASP  |
| 1   | 42-A  | 217 | ARG  |
| 1   | 42-A  | 223 | PHE  |
| 1   | 42-A  | 227 | LEU  |
| 1   | 42-A  | 228 | ASN  |
| 1   | 42-A  | 232 | LEU  |
| 1   | 42-A  | 235 | MET  |
| 1   | 42-A  | 244 | GLN  |
| 1   | 42-A  | 256 | GLN  |
| 1   | 42-A  | 267 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 42-A  | 271 | LEU  |
| 1   | 42-A  | 277 | ASN  |
| 1   | 42-A  | 287 | LEU  |
| 1   | 42-A  | 298 | ARG  |
| 1   | 42-A  | 299 | GLN  |
| 1   | 42-A  | 300 | CYS  |
| 1   | 42-A  | 304 | THR  |
| 1   | 43-A  | 6   | MET  |
| 1   | 43-A  | 12  | LYS  |
| 1   | 43-A  | 24  | THR  |
| 1   | 43-A  | 25  | THR  |
| 1   | 43-A  | 26  | THR  |
| 1   | 43-A  | 27  | LEU  |
| 1   | 43-A  | 41  | HIS  |
| 1   | 43-A  | 47  | GLU  |
| 1   | 43-A  | 49  | MET  |
| 1   | 43-A  | 51  | ASN  |
| 1   | 43-A  | 58  | LEU  |
| 1   | 43-A  | 60  | ARG  |
| 1   | 43-A  | 61  | LYS  |
| 1   | 43-A  | 67  | LEU  |
| 1   | 43-A  | 73  | VAL  |
| 1   | 43-A  | 75  | LEU  |
| 1   | 43-A  | 86  | VAL  |
| 1   | 43-A  | 88  | LYS  |
| 1   | 43-A  | 97  | LYS  |
| 1   | 43-A  | 102 | LYS  |
| 1   | 43-A  | 123 | SER  |
| 1   | 43-A  | 137 | LYS  |
| 1   | 43-A  | 141 | LEU  |
| 1   | 43-A  | 155 | ASP  |
| 1   | 43-A  | 165 | MET  |
| 1   | 43-A  | 166 | GLU  |
| 1   | 43-A  | 222 | ARG  |
| 1   | 43-A  | 225 | THR  |
| 1   | 43-A  | 232 | LEU  |
| 1   | 43-A  | 233 | VAL  |
| 1   | 43-A  | 235 | MET  |
| 1   | 43-A  | 236 | LYS  |
| 1   | 43-A  | 242 | LEU  |
| 1   | 43-A  | 249 | ILE  |
| 1   | 43-A  | 256 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 43-A  | 273 | GLN  |
| 1   | 43-A  | 276 | MET  |
| 1   | 43-A  | 286 | LEU  |
| 1   | 43-A  | 298 | ARG  |
| 1   | 43-A  | 301 | SER  |
| 1   | 43-A  | 303 | VAL  |
| 1   | 43-A  | 305 | PHE  |
| 1   | 43-A  | 306 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (329) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-A   | 19  | GLN  |
| 1   | 1-A   | 69  | GLN  |
| 1   | 1-A   | 83  | GLN  |
| 1   | 1-A   | 214 | ASN  |
| 1   | 1-A   | 256 | GLN  |
| 1   | 2-A   | 41  | HIS  |
| 1   | 2-A   | 51  | ASN  |
| 1   | 2-A   | 64  | HIS  |
| 1   | 2-A   | 74  | GLN  |
| 1   | 2-A   | 107 | GLN  |
| 1   | 2-A   | 110 | GLN  |
| 1   | 2-A   | 238 | ASN  |
| 1   | 2-A   | 244 | GLN  |
| 1   | 3-A   | 28  | ASN  |
| 1   | 3-A   | 64  | HIS  |
| 1   | 3-A   | 74  | GLN  |
| 1   | 3-A   | 84  | ASN  |
| 1   | 3-A   | 192 | GLN  |
| 1   | 3-A   | 238 | ASN  |
| 1   | 3-A   | 273 | GLN  |
| 1   | 3-A   | 274 | ASN  |
| 1   | 3-A   | 277 | ASN  |
| 1   | 4-A   | 28  | ASN  |
| 1   | 4-A   | 41  | HIS  |
| 1   | 4-A   | 83  | GLN  |
| 1   | 4-A   | 110 | GLN  |
| 1   | 4-A   | 119 | ASN  |
| 1   | 4-A   | 238 | ASN  |
| 1   | 4-A   | 244 | GLN  |
| 1   | 4-A   | 273 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 4-A   | 274 | ASN  |
| 1   | 5-A   | 28  | ASN  |
| 1   | 5-A   | 41  | HIS  |
| 1   | 5-A   | 69  | GLN  |
| 1   | 5-A   | 74  | GLN  |
| 1   | 5-A   | 83  | GLN  |
| 1   | 5-A   | 110 | GLN  |
| 1   | 5-A   | 119 | ASN  |
| 1   | 5-A   | 221 | ASN  |
| 1   | 5-A   | 244 | GLN  |
| 1   | 5-A   | 256 | GLN  |
| 1   | 6-A   | 28  | ASN  |
| 1   | 6-A   | 83  | GLN  |
| 1   | 6-A   | 107 | GLN  |
| 1   | 6-A   | 151 | ASN  |
| 1   | 6-A   | 180 | ASN  |
| 1   | 6-A   | 221 | ASN  |
| 1   | 6-A   | 244 | GLN  |
| 1   | 7-A   | 28  | ASN  |
| 1   | 7-A   | 41  | HIS  |
| 1   | 7-A   | 72  | ASN  |
| 1   | 7-A   | 110 | GLN  |
| 1   | 7-A   | 119 | ASN  |
| 1   | 7-A   | 151 | ASN  |
| 1   | 7-A   | 180 | ASN  |
| 1   | 7-A   | 192 | GLN  |
| 1   | 7-A   | 306 | GLN  |
| 1   | 8-A   | 19  | GLN  |
| 1   | 8-A   | 28  | ASN  |
| 1   | 8-A   | 192 | GLN  |
| 1   | 8-A   | 221 | ASN  |
| 1   | 8-A   | 238 | ASN  |
| 1   | 9-A   | 28  | ASN  |
| 1   | 9-A   | 41  | HIS  |
| 1   | 9-A   | 74  | GLN  |
| 1   | 9-A   | 83  | GLN  |
| 1   | 9-A   | 110 | GLN  |
| 1   | 9-A   | 151 | ASN  |
| 1   | 9-A   | 180 | ASN  |
| 1   | 9-A   | 192 | GLN  |
| 1   | 9-A   | 221 | ASN  |
| 1   | 10-A  | 19  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 10-A  | 28  | ASN  |
| 1   | 10-A  | 74  | GLN  |
| 1   | 10-A  | 192 | GLN  |
| 1   | 10-A  | 214 | ASN  |
| 1   | 10-A  | 221 | ASN  |
| 1   | 10-A  | 256 | GLN  |
| 1   | 11-A  | 19  | GLN  |
| 1   | 11-A  | 28  | ASN  |
| 1   | 11-A  | 69  | GLN  |
| 1   | 11-A  | 180 | ASN  |
| 1   | 11-A  | 238 | ASN  |
| 1   | 11-A  | 244 | GLN  |
| 1   | 11-A  | 299 | GLN  |
| 1   | 11-A  | 306 | GLN  |
| 1   | 12-A  | 19  | GLN  |
| 1   | 12-A  | 28  | ASN  |
| 1   | 12-A  | 51  | ASN  |
| 1   | 12-A  | 64  | HIS  |
| 1   | 12-A  | 142 | ASN  |
| 1   | 12-A  | 151 | ASN  |
| 1   | 12-A  | 189 | GLN  |
| 1   | 12-A  | 192 | GLN  |
| 1   | 12-A  | 221 | ASN  |
| 1   | 12-A  | 238 | ASN  |
| 1   | 12-A  | 244 | GLN  |
| 1   | 13-A  | 28  | ASN  |
| 1   | 13-A  | 65  | ASN  |
| 1   | 13-A  | 142 | ASN  |
| 1   | 13-A  | 180 | ASN  |
| 1   | 13-A  | 192 | GLN  |
| 1   | 13-A  | 306 | GLN  |
| 1   | 14-A  | 28  | ASN  |
| 1   | 14-A  | 65  | ASN  |
| 1   | 14-A  | 69  | GLN  |
| 1   | 14-A  | 151 | ASN  |
| 1   | 14-A  | 189 | GLN  |
| 1   | 14-A  | 192 | GLN  |
| 1   | 14-A  | 238 | ASN  |
| 1   | 14-A  | 244 | GLN  |
| 1   | 14-A  | 306 | GLN  |
| 1   | 15-A  | 28  | ASN  |
| 1   | 15-A  | 41  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 15-A  | 65  | ASN  |
| 1   | 15-A  | 107 | GLN  |
| 1   | 15-A  | 110 | GLN  |
| 1   | 15-A  | 180 | ASN  |
| 1   | 15-A  | 192 | GLN  |
| 1   | 15-A  | 214 | ASN  |
| 1   | 15-A  | 238 | ASN  |
| 1   | 15-A  | 244 | GLN  |
| 1   | 16-A  | 19  | GLN  |
| 1   | 16-A  | 28  | ASN  |
| 1   | 16-A  | 65  | ASN  |
| 1   | 16-A  | 83  | GLN  |
| 1   | 16-A  | 107 | GLN  |
| 1   | 16-A  | 192 | GLN  |
| 1   | 16-A  | 221 | ASN  |
| 1   | 16-A  | 244 | GLN  |
| 1   | 17-A  | 28  | ASN  |
| 1   | 17-A  | 65  | ASN  |
| 1   | 17-A  | 189 | GLN  |
| 1   | 17-A  | 221 | ASN  |
| 1   | 17-A  | 244 | GLN  |
| 1   | 17-A  | 306 | GLN  |
| 1   | 18-A  | 28  | ASN  |
| 1   | 18-A  | 65  | ASN  |
| 1   | 18-A  | 107 | GLN  |
| 1   | 18-A  | 189 | GLN  |
| 1   | 18-A  | 274 | ASN  |
| 1   | 19-A  | 28  | ASN  |
| 1   | 19-A  | 41  | HIS  |
| 1   | 19-A  | 65  | ASN  |
| 1   | 19-A  | 107 | GLN  |
| 1   | 19-A  | 180 | ASN  |
| 1   | 19-A  | 238 | ASN  |
| 1   | 19-A  | 244 | GLN  |
| 1   | 19-A  | 277 | ASN  |
| 1   | 19-A  | 306 | GLN  |
| 1   | 20-A  | 28  | ASN  |
| 1   | 20-A  | 107 | GLN  |
| 1   | 20-A  | 110 | GLN  |
| 1   | 20-A  | 180 | ASN  |
| 1   | 20-A  | 221 | ASN  |
| 1   | 20-A  | 244 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 21-A  | 28  | ASN  |
| 1   | 21-A  | 142 | ASN  |
| 1   | 21-A  | 274 | ASN  |
| 1   | 22-A  | 28  | ASN  |
| 1   | 22-A  | 41  | HIS  |
| 1   | 22-A  | 53  | ASN  |
| 1   | 22-A  | 72  | ASN  |
| 1   | 22-A  | 110 | GLN  |
| 1   | 22-A  | 273 | GLN  |
| 1   | 23-A  | 28  | ASN  |
| 1   | 23-A  | 53  | ASN  |
| 1   | 23-A  | 69  | GLN  |
| 1   | 23-A  | 72  | ASN  |
| 1   | 23-A  | 74  | GLN  |
| 1   | 23-A  | 214 | ASN  |
| 1   | 23-A  | 238 | ASN  |
| 1   | 23-A  | 273 | GLN  |
| 1   | 24-A  | 28  | ASN  |
| 1   | 24-A  | 53  | ASN  |
| 1   | 24-A  | 84  | ASN  |
| 1   | 24-A  | 107 | GLN  |
| 1   | 24-A  | 110 | GLN  |
| 1   | 24-A  | 238 | ASN  |
| 1   | 25-A  | 28  | ASN  |
| 1   | 25-A  | 83  | GLN  |
| 1   | 25-A  | 107 | GLN  |
| 1   | 25-A  | 189 | GLN  |
| 1   | 25-A  | 221 | ASN  |
| 1   | 26-A  | 19  | GLN  |
| 1   | 26-A  | 28  | ASN  |
| 1   | 26-A  | 51  | ASN  |
| 1   | 26-A  | 83  | GLN  |
| 1   | 26-A  | 110 | GLN  |
| 1   | 26-A  | 180 | ASN  |
| 1   | 26-A  | 238 | ASN  |
| 1   | 26-A  | 244 | GLN  |
| 1   | 27-A  | 19  | GLN  |
| 1   | 27-A  | 28  | ASN  |
| 1   | 27-A  | 51  | ASN  |
| 1   | 27-A  | 69  | GLN  |
| 1   | 27-A  | 110 | GLN  |
| 1   | 27-A  | 189 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 28-A  | 19  | GLN  |
| 1   | 28-A  | 28  | ASN  |
| 1   | 28-A  | 72  | ASN  |
| 1   | 28-A  | 83  | GLN  |
| 1   | 28-A  | 110 | GLN  |
| 1   | 28-A  | 142 | ASN  |
| 1   | 28-A  | 189 | GLN  |
| 1   | 28-A  | 214 | ASN  |
| 1   | 28-A  | 221 | ASN  |
| 1   | 28-A  | 244 | GLN  |
| 1   | 28-A  | 273 | GLN  |
| 1   | 29-A  | 28  | ASN  |
| 1   | 29-A  | 69  | GLN  |
| 1   | 29-A  | 72  | ASN  |
| 1   | 29-A  | 83  | GLN  |
| 1   | 29-A  | 107 | GLN  |
| 1   | 29-A  | 214 | ASN  |
| 1   | 29-A  | 228 | ASN  |
| 1   | 29-A  | 299 | GLN  |
| 1   | 30-A  | 19  | GLN  |
| 1   | 30-A  | 28  | ASN  |
| 1   | 30-A  | 107 | GLN  |
| 1   | 30-A  | 214 | ASN  |
| 1   | 30-A  | 221 | ASN  |
| 1   | 30-A  | 228 | ASN  |
| 1   | 30-A  | 299 | GLN  |
| 1   | 30-A  | 306 | GLN  |
| 1   | 31-A  | 28  | ASN  |
| 1   | 31-A  | 74  | GLN  |
| 1   | 31-A  | 110 | GLN  |
| 1   | 31-A  | 180 | ASN  |
| 1   | 31-A  | 214 | ASN  |
| 1   | 31-A  | 221 | ASN  |
| 1   | 31-A  | 228 | ASN  |
| 1   | 31-A  | 256 | GLN  |
| 1   | 32-A  | 28  | ASN  |
| 1   | 32-A  | 83  | GLN  |
| 1   | 32-A  | 151 | ASN  |
| 1   | 32-A  | 228 | ASN  |
| 1   | 32-A  | 256 | GLN  |
| 1   | 33-A  | 28  | ASN  |
| 1   | 33-A  | 64  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 33-A  | 65  | ASN  |
| 1   | 33-A  | 69  | GLN  |
| 1   | 33-A  | 74  | GLN  |
| 1   | 33-A  | 107 | GLN  |
| 1   | 33-A  | 119 | ASN  |
| 1   | 33-A  | 151 | ASN  |
| 1   | 33-A  | 214 | ASN  |
| 1   | 33-A  | 228 | ASN  |
| 1   | 33-A  | 244 | GLN  |
| 1   | 33-A  | 273 | GLN  |
| 1   | 33-A  | 274 | ASN  |
| 1   | 34-A  | 28  | ASN  |
| 1   | 34-A  | 41  | HIS  |
| 1   | 34-A  | 110 | GLN  |
| 1   | 34-A  | 119 | ASN  |
| 1   | 34-A  | 151 | ASN  |
| 1   | 34-A  | 228 | ASN  |
| 1   | 34-A  | 277 | ASN  |
| 1   | 35-A  | 28  | ASN  |
| 1   | 35-A  | 119 | ASN  |
| 1   | 35-A  | 214 | ASN  |
| 1   | 35-A  | 228 | ASN  |
| 1   | 35-A  | 244 | GLN  |
| 1   | 36-A  | 28  | ASN  |
| 1   | 36-A  | 72  | ASN  |
| 1   | 36-A  | 110 | GLN  |
| 1   | 36-A  | 142 | ASN  |
| 1   | 36-A  | 214 | ASN  |
| 1   | 36-A  | 228 | ASN  |
| 1   | 37-A  | 28  | ASN  |
| 1   | 37-A  | 41  | HIS  |
| 1   | 37-A  | 64  | HIS  |
| 1   | 37-A  | 74  | GLN  |
| 1   | 37-A  | 142 | ASN  |
| 1   | 37-A  | 151 | ASN  |
| 1   | 37-A  | 180 | ASN  |
| 1   | 37-A  | 189 | GLN  |
| 1   | 37-A  | 214 | ASN  |
| 1   | 37-A  | 228 | ASN  |
| 1   | 38-A  | 28  | ASN  |
| 1   | 38-A  | 41  | HIS  |
| 1   | 38-A  | 214 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 38-A  | 221 | ASN  |
| 1   | 38-A  | 228 | ASN  |
| 1   | 38-A  | 244 | GLN  |
| 1   | 39-A  | 28  | ASN  |
| 1   | 39-A  | 69  | GLN  |
| 1   | 39-A  | 72  | ASN  |
| 1   | 39-A  | 107 | GLN  |
| 1   | 39-A  | 110 | GLN  |
| 1   | 39-A  | 119 | ASN  |
| 1   | 39-A  | 151 | ASN  |
| 1   | 39-A  | 214 | ASN  |
| 1   | 39-A  | 228 | ASN  |
| 1   | 39-A  | 244 | GLN  |
| 1   | 40-A  | 19  | GLN  |
| 1   | 40-A  | 28  | ASN  |
| 1   | 40-A  | 72  | ASN  |
| 1   | 40-A  | 83  | GLN  |
| 1   | 40-A  | 107 | GLN  |
| 1   | 40-A  | 119 | ASN  |
| 1   | 40-A  | 142 | ASN  |
| 1   | 40-A  | 151 | ASN  |
| 1   | 40-A  | 180 | ASN  |
| 1   | 40-A  | 214 | ASN  |
| 1   | 40-A  | 221 | ASN  |
| 1   | 40-A  | 228 | ASN  |
| 1   | 40-A  | 244 | GLN  |
| 1   | 40-A  | 306 | GLN  |
| 1   | 41-A  | 28  | ASN  |
| 1   | 41-A  | 51  | ASN  |
| 1   | 41-A  | 151 | ASN  |
| 1   | 41-A  | 214 | ASN  |
| 1   | 41-A  | 221 | ASN  |
| 1   | 41-A  | 228 | ASN  |
| 1   | 41-A  | 244 | GLN  |
| 1   | 41-A  | 306 | GLN  |
| 1   | 42-A  | 19  | GLN  |
| 1   | 42-A  | 28  | ASN  |
| 1   | 42-A  | 119 | ASN  |
| 1   | 42-A  | 142 | ASN  |
| 1   | 42-A  | 180 | ASN  |
| 1   | 42-A  | 274 | ASN  |
| 1   | 43-A  | 28  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 43-A  | 51  | ASN  |
| 1   | 43-A  | 214 | ASN  |
| 1   | 43-A  | 228 | ASN  |
| 1   | 43-A  | 244 | GLN  |
| 1   | 43-A  | 306 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 344 ligands modelled in this entry, 43 are monoatomic - leaving 301 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 | $\# Z  > 2$ |
| 2   | DMS  | 1-A   | 404 | -    | 3,3,3        | 0.61 | 0           | 3,3,3       | 0.95 | 0           |
| 2   | DMS  | 1-A   | 403 | -    | 3,3,3        | 0.73 | 0           | 3,3,3       | 1.16 | 0           |
| 2   | DMS  | 1-A   | 401 | -    | 3,3,3        | 0.64 | 0           | 3,3,3       | 1.35 | 1 (33%)     |
| 2   | DMS  | 1-A   | 402 | -    | 3,3,3        | 0.82 | 0           | 3,3,3       | 0.48 | 0           |
| 2   | DMS  | 1-A   | 405 | -    | 3,3,3        | 0.63 | 0           | 3,3,3       | 1.63 | 1 (33%)     |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|--------|------|------------------------|---------------------|
| 2   | 1-A   | 405 | DMS  | O-S-C2 | 2.57 | 119.66                 | 106.54              |
| 2   | 1-A   | 401 | DMS  | O-S-C2 | 2.28 | 118.19                 | 106.54              |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

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

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

### 6.3 Carbohydrates

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

### 6.4 Ligands

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

### 6.5 Other polymers

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