



## wwPDB EM Map/Model Validation Report ⓘ

Oct 25, 2016 – 02:04 PM EDT

PDB ID : 5LER  
EMDB ID: : EMD-4044  
Title : Structure of the bacterial sex F pilus (13.2 Angstrom rise)  
Authors : Costa, T.R.D.; Ilangovan, I.; Ukleja, M.; Redzej, A.; Santini, J.M.; Smith, T.K.; Egelman, E.H.; Waksman, G.  
Deposited on : 2016-06-30  
Resolution : 5.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

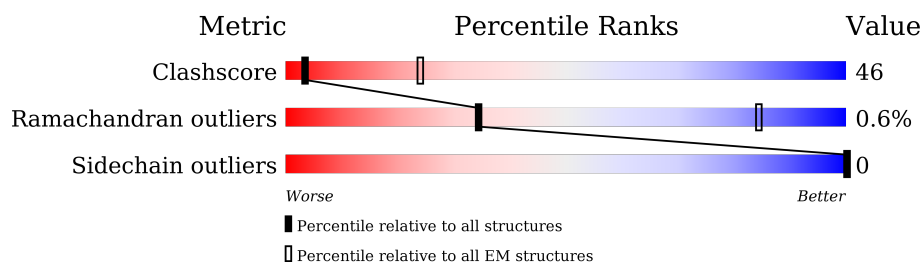
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.00 Å.

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






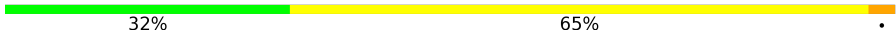
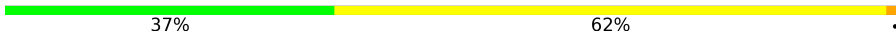
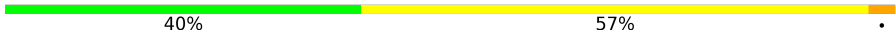
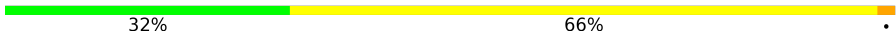
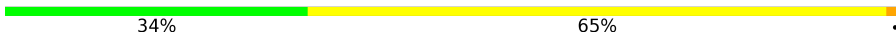
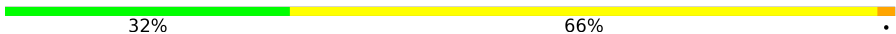
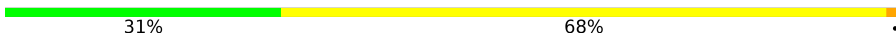
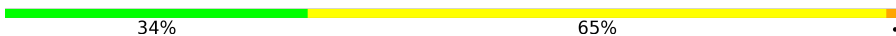
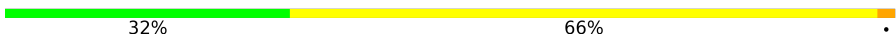
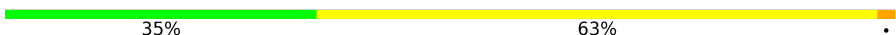
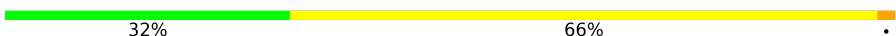











| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 114402                      | 924                         |
| Ramachandran outliers | 111179                      | 726                         |
| Sidechain outliers    | 111093                      | 686                         |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 1A    | 65     | 32% 66% .        |
| 1   | 1B    | 65     | 34% 65% .        |
| 1   | 1C    | 65     | 34% 65% .        |
| 1   | 1D    | 65     | 31% 66% .        |
| 1   | 1E    | 65     | 34% 65% .        |
| 1   | 1F    | 65     | 32% 65% .        |
| 1   | 1G    | 65     | 35% 62% .        |
| 1   | 1H    | 65     | 32% 66% .        |
| 1   | 1I    | 65     | 34% 65% .        |



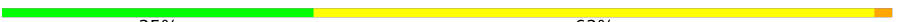
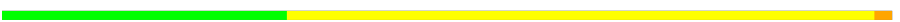





















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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | 1J    | 65     |  32% 65%   |
| 1   | 1K    | 65     |  34% 63%   |
| 1   | 1L    | 65     |  35% 63%   |
| 1   | 1M    | 65     |  32% 65%   |
| 1   | 1N    | 65     |  37% 62%   |
| 1   | 1O    | 65     |  40% 57%   |
| 1   | 2A    | 65     |  32% 66%   |
| 1   | 2B    | 65     |  34% 65%   |
| 1   | 2C    | 65     |  32% 66%   |
| 1   | 2D    | 65     |  31% 68%   |
| 1   | 2E    | 65     |  34% 65%   |
| 1   | 2F    | 65     |  32% 66%   |
| 1   | 2G    | 65     |  35% 63% |
| 1   | 2H    | 65     |  32% 66% |
| 1   | 2I    | 65     |  34% 65% |
| 1   | 2J    | 65     |  34% 65% |
| 1   | 2K    | 65     |  35% 63% |
| 1   | 2L    | 65     |  35% 63% |
| 1   | 2M    | 65     |  32% 66% |
| 1   | 2N    | 65     |  37% 60% |
| 1   | 2O    | 65     |  40% 58% |
| 1   | 3A    | 65     |  32% 66% |
| 1   | 3B    | 65     |  34% 65% |
| 1   | 3C    | 65     |  32% 66% |
| 1   | 3D    | 65     |  31% 68% |




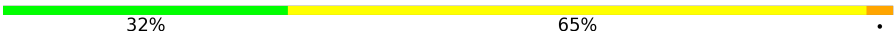
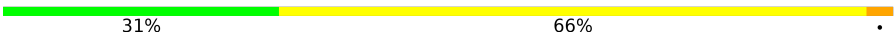
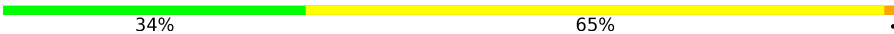
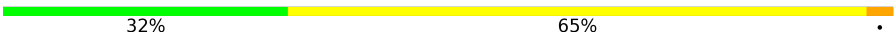
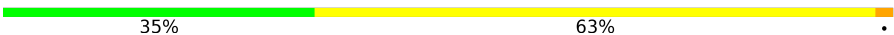
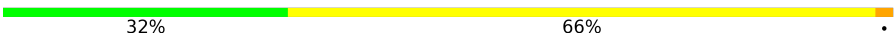
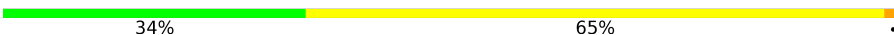
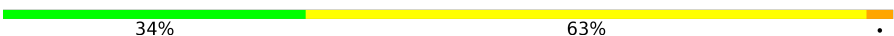
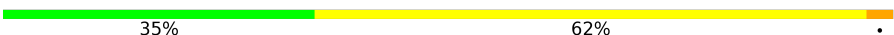




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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | 3E    | 65     |  34% 65% .   |
| 1   | 3F    | 65     |  32% 66% .   |
| 1   | 3G    | 65     |  35% 63% .   |
| 1   | 3H    | 65     |  32% 66% .   |
| 1   | 3I    | 65     |  34% 65% .   |
| 1   | 3J    | 65     |  34% 63% .   |
| 1   | 3K    | 65     |  35% 62% .   |
| 1   | 3L    | 65     |  35% 63% .   |
| 1   | 3M    | 65     |  32% 65% .   |
| 1   | 3N    | 65     |  37% 60% .   |
| 1   | 3O    | 65     |  40% 57% .   |
| 1   | 4A    | 65     |  32% 65% .   |
| 1   | 4B    | 65     |  34% 65% . |
| 1   | 4C    | 65     |  32% 66% . |
| 1   | 4D    | 65     |  32% 66% . |
| 1   | 4E    | 65     |  34% 65% . |
| 1   | 4F    | 65     |  32% 66% . |
| 1   | 4G    | 65     |  35% 63% . |
| 1   | 4H    | 65     |  32% 66% . |
| 1   | 4I    | 65     |  34% 65% . |
| 1   | 4J    | 65     |  34% 63% . |
| 1   | 4K    | 65     |  35% 62% . |
| 1   | 4L    | 65     |  35% 63% . |
| 1   | 4M    | 65     |  32% 66% . |
| 1   | 4N    | 65     |  37% 60% . |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | 4O    | 65     |  40%57%.   |
| 1   | 5A    | 65     |  32%66%.   |
| 1   | 5B    | 65     |  35%62%.   |
| 1   | 5C    | 65     |  32%65%.   |
| 1   | 5D    | 65     |  31%66%.   |
| 1   | 5E    | 65     |  34%65%.   |
| 1   | 5F    | 65     |  32%65%.   |
| 1   | 5G    | 65     |  35%63%.   |
| 1   | 5H    | 65     |  32%66%.   |
| 1   | 5I    | 65     |  34%65%.   |
| 1   | 5J    | 65     |  34%63%.   |
| 1   | 5K    | 65     |  35%62%.  |
| 1   | 5L    | 65     |  34%65%. |
| 1   | 5M    | 65     |  31%66%. |
| 1   | 5N    | 65     |  37%62%. |
| 1   | 5O    | 65     |  40%57%. |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 36539 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Pilin.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1   | 1A    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 475   | 314 | 73 | 83 | 5 |         |       |
| 1   | 1B    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 476   | 314 | 74 | 83 | 5 |         |       |
| 1   | 1C    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 476   | 314 | 74 | 83 | 5 |         |       |
| 1   | 1D    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 476   | 314 | 74 | 83 | 5 |         |       |
| 1   | 1E    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 476   | 314 | 74 | 83 | 5 |         |       |
| 1   | 1F    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 476   | 314 | 74 | 83 | 5 |         |       |
| 1   | 1G    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 476   | 314 | 74 | 83 | 5 |         |       |
| 1   | 1H    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 476   | 314 | 74 | 83 | 5 |         |       |
| 1   | 1I    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 476   | 314 | 74 | 83 | 5 |         |       |
| 1   | 1J    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 476   | 314 | 74 | 83 | 5 |         |       |
| 1   | 1K    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 476   | 314 | 74 | 83 | 5 |         |       |
| 1   | 1L    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 476   | 314 | 74 | 83 | 5 |         |       |
| 1   | 1M    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 476   | 314 | 74 | 83 | 5 |         |       |
| 1   | 1N    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 476   | 314 | 74 | 83 | 5 |         |       |
| 1   | 1O    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 476   | 314 | 74 | 83 | 5 |         |       |
| 1   | 2A    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 476   | 314 | 74 | 83 | 5 |         |       |
| 1   | 2B    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 476   | 314 | 74 | 83 | 5 |         |       |

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| Mol | Chain | Residues | Atoms        |          |         |         |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|-------|
| 1   | 2C    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 2D    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 2E    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 2F    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 2G    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 2H    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 2I    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 2J    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 2K    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 2L    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 2M    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 2N    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 2O    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 3A    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 3B    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 3C    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 3D    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 3E    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 3F    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 3G    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 3H    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |

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| Mol | Chain | Residues | Atoms        |          |         |         |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|-------|
| 1   | 3I    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 3J    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 3K    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 3L    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 3M    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 3N    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 3O    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 4A    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 4B    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 4C    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 4D    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 4E    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 4F    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 4G    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 4H    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 4I    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 4J    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 4K    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 4L    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 4M    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 4N    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |

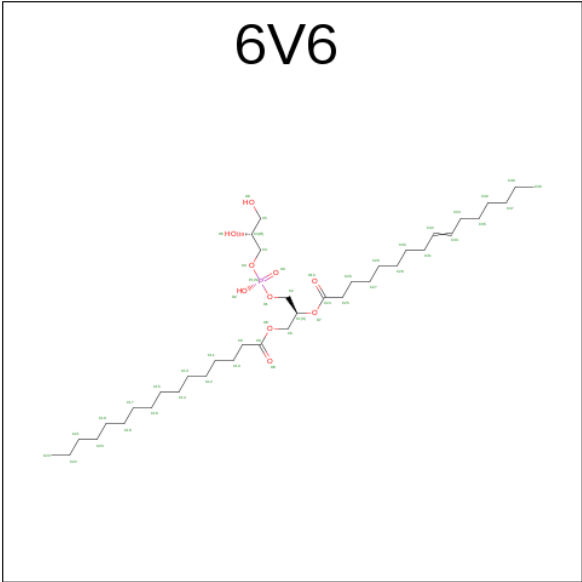
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| Mol | Chain | Residues | Atoms        |          |         |         |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|-------|
| 1   | 4O    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 5A    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 5B    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 5C    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 5D    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 5E    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 5F    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 5G    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 5H    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 5I    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 5J    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 5K    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 5L    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 5M    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 5N    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |
| 1   | 5O    | 65       | Total<br>476 | C<br>314 | N<br>74 | O<br>83 | S<br>5 | 0       | 0     |

- Molecule 2 is [(2 {S})-3-[(2 {R})-2,3-bis(oxidanyl)propoxy]-oxidanyl-phosphoryl]oxy-2-hexadec-9-enoyloxy-propyl] hexadecanoate (three-letter code: 6V6) (formula: C<sub>38</sub>H<sub>73</sub>O<sub>10</sub>P).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 2   | 1A    | 1        | Total | C | O | P | 0       |
|     |       |          | 12    | 5 | 6 | 1 |         |
| 2   | 1B    | 1        | Total | C | O | P | 0       |
|     |       |          | 12    | 5 | 6 | 1 |         |
| 2   | 1C    | 1        | Total | C | O | P | 0       |
|     |       |          | 12    | 5 | 6 | 1 |         |
| 2   | 1D    | 1        | Total | C | O | P | 0       |
|     |       |          | 12    | 5 | 6 | 1 |         |
| 2   | 1E    | 1        | Total | C | O | P | 0       |
|     |       |          | 12    | 5 | 6 | 1 |         |
| 2   | 1F    | 1        | Total | C | O | P | 0       |
|     |       |          | 12    | 5 | 6 | 1 |         |
| 2   | 1G    | 1        | Total | C | O | P | 0       |
|     |       |          | 12    | 5 | 6 | 1 |         |
| 2   | 1H    | 1        | Total | C | O | P | 0       |
|     |       |          | 12    | 5 | 6 | 1 |         |
| 2   | 1I    | 1        | Total | C | O | P | 0       |
|     |       |          | 12    | 5 | 6 | 1 |         |
| 2   | 1J    | 1        | Total | C | O | P | 0       |
|     |       |          | 12    | 5 | 6 | 1 |         |
| 2   | 1K    | 1        | Total | C | O | P | 0       |
|     |       |          | 12    | 5 | 6 | 1 |         |
| 2   | 1L    | 1        | Total | C | O | P | 0       |
|     |       |          | 12    | 5 | 6 | 1 |         |
| 2   | 1M    | 1        | Total | C | O | P | 0       |
|     |       |          | 12    | 5 | 6 | 1 |         |
| 2   | 1N    | 1        | Total | C | O | P | 0       |
|     |       |          | 12    | 5 | 6 | 1 |         |

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| Mol | Chain | Residues | Atoms       |        |        |        | AltConf |
|-----|-------|----------|-------------|--------|--------|--------|---------|
| 2   | 2A    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 2B    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 2C    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 2D    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 2E    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 2F    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 2G    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 2H    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 2I    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 2J    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 2K    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 2L    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 2M    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 2N    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 3A    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 3B    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 3C    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 3D    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 3E    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 3F    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 3G    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |

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| Mol | Chain | Residues | Atoms       |        |        |        | AltConf |
|-----|-------|----------|-------------|--------|--------|--------|---------|
| 2   | 3H    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 3I    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 3J    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 3K    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 3L    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 3M    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 3N    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 4A    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 4B    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 4C    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 4D    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 4E    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 4F    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 4G    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 4H    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 4I    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 4J    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 4K    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 4L    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 4M    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 4N    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |

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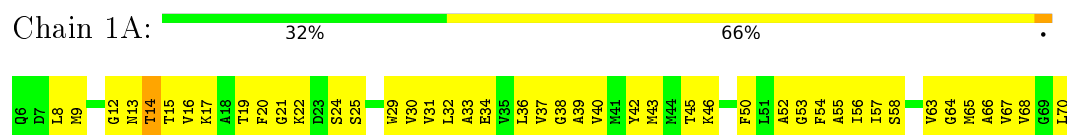
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| Mol | Chain | Residues | Atoms       |        |        |        | AltConf |
|-----|-------|----------|-------------|--------|--------|--------|---------|
| 2   | 5A    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 5B    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 5C    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 5D    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 5E    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 5F    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 5G    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 5H    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 5I    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 5J    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 5K    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 5L    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 5M    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |
| 2   | 5N    | 1        | Total<br>12 | C<br>5 | O<br>6 | P<br>1 | 0       |

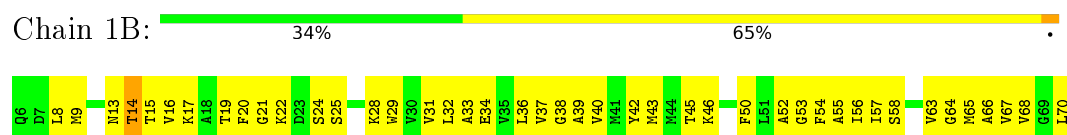
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

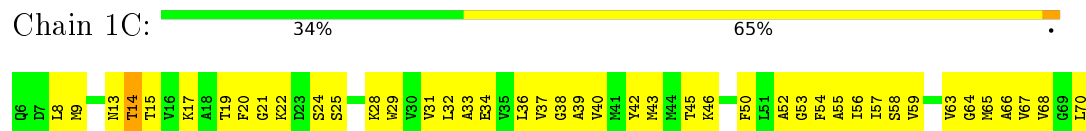
- Molecule 1: Pilin



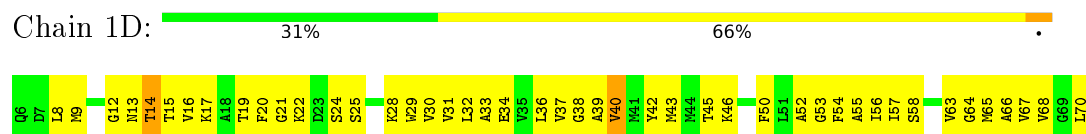
- Molecule 1: Pilin



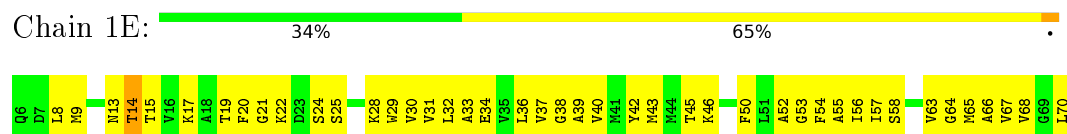
- Molecule 1: Pilin



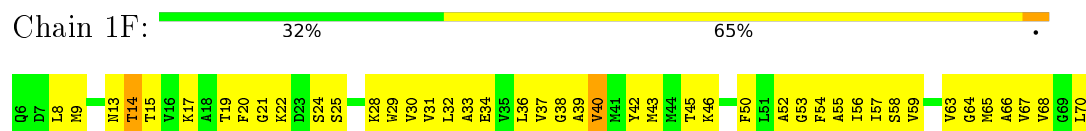
- Molecule 1: Pilin



- Molecule 1: Pilin



- Molecule 1: Pilin

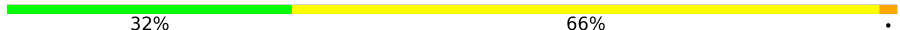


- Molecule 1: Pilin

Chain 1G:  35% 62%



- Molecule 1: Pilin

Chain 1H:  32% 66%



- Molecule 1: Pilin

Chain 1I:  34% 65%

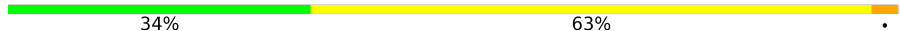


- Molecule 1: Pilin

Chain 1J:  32% 65%



- Molecule 1: Pilin

Chain 1K:  34% 63%



- Molecule 1: Pilin

Chain 1L:  35% 63%



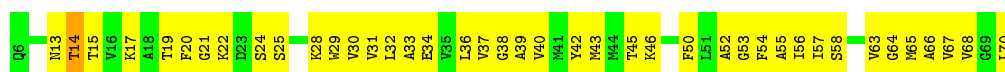
- Molecule 1: Pilin

Chain 1M:  32% 65%



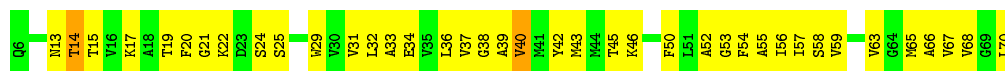
- Molecule 1: Pilin

Chain 1N:  37% 62%



- Molecule 1: Pilin

Chain 1O: 40% 57%



- Molecule 1: Pilin

Chain 2A: 32% 66%



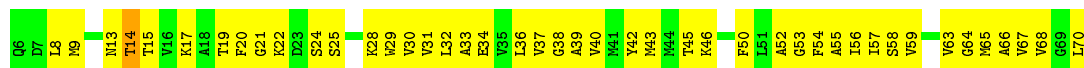
- Molecule 1: Pilin

Chain 2B: 34% 65%



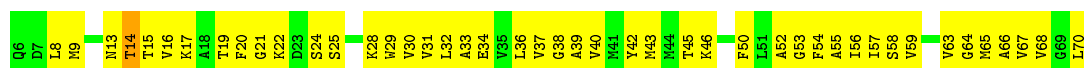
- Molecule 1: Pilin

Chain 2C: 32% 66%



- Molecule 1: Pilin

Chain 2D: 31% 68%



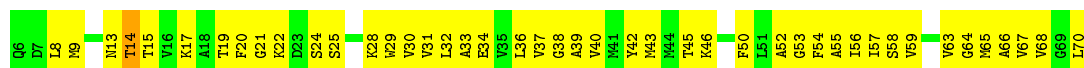
- Molecule 1: Pilin

Chain 2E: 34% 65%



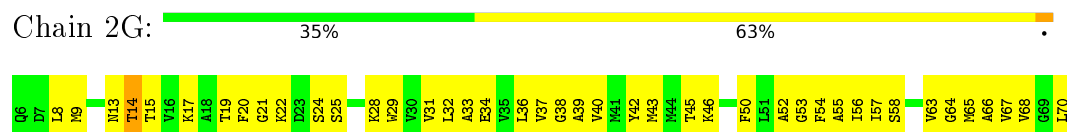
- Molecule 1: Pilin

Chain 2F: 32% 66%

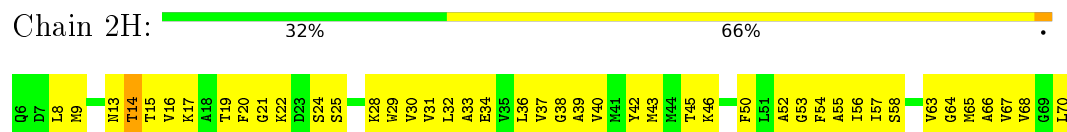


- Molecule 1: Pilin

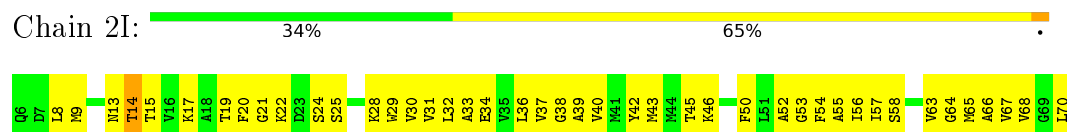




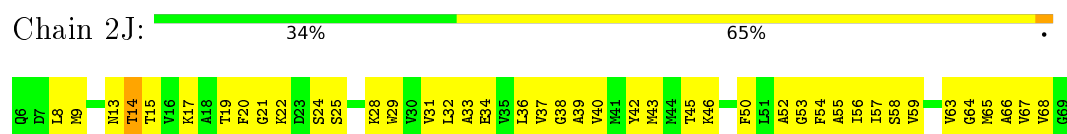
- Molecule 1: Pilin



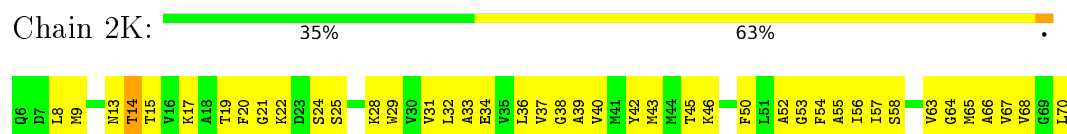
- Molecule 1: Pilin



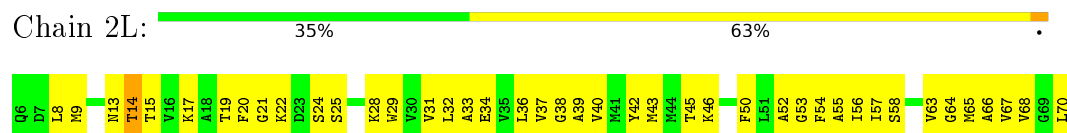
- Molecule 1: Pilin



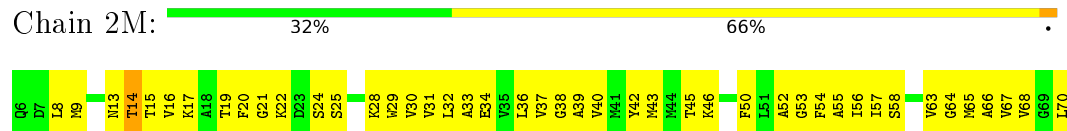
- Molecule 1: Pilin



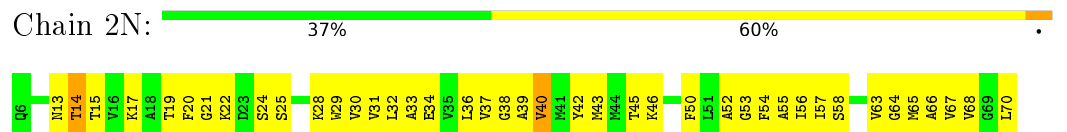
- Molecule 1: Pilin



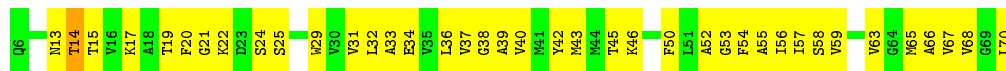
- Molecule 1: Pilin



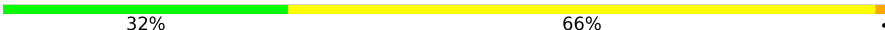
- Molecule 1: Pilin



## • Molecule 1: Pilin

Chain 2O:  40% 58%

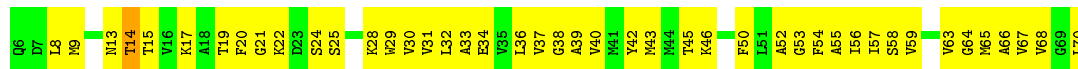
## • Molecule 1: Pilin

Chain 3A:  32% 66%

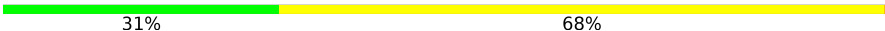
## • Molecule 1: Pilin

Chain 3B:  34% 65%

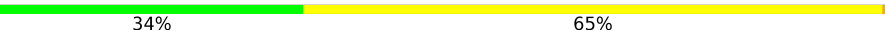
## • Molecule 1: Pilin

Chain 3C:  32% 66%

## • Molecule 1: Pilin

Chain 3D:  31% 68%

## • Molecule 1: Pilin

Chain 3E:  34% 65%

## • Molecule 1: Pilin

Chain 3F:  32% 66%

## • Molecule 1: Pilin

Chain 3G:  35% 63%



- Molecule 1: Pilin

Chain 3H: 32% 66%



- Molecule 1: Pilin

Chain 3I: 34% 65%



- Molecule 1: Pilin

Chain 3J: 34% 63%



- Molecule 1: Pilin

Chain 3K: 35% 62%



- Molecule 1: Pilin

Chain 3L: 35% 63%



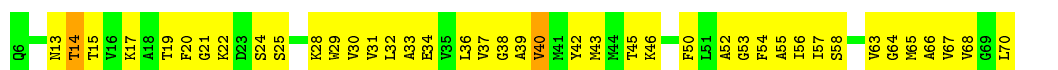
- Molecule 1: Pilin

Chain 3M: 32% 65%

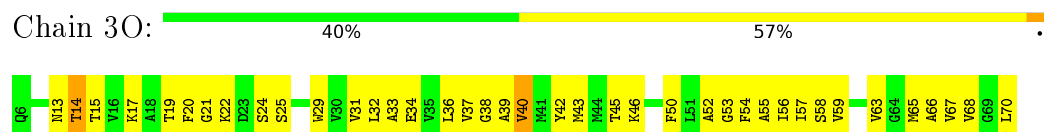


- Molecule 1: Pilin

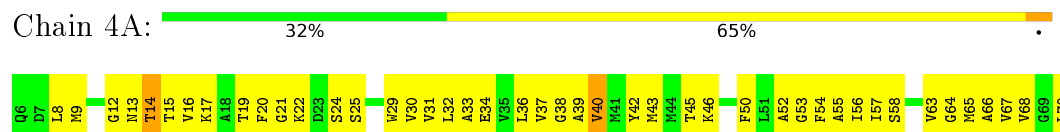
Chain 3N: 37% 60%



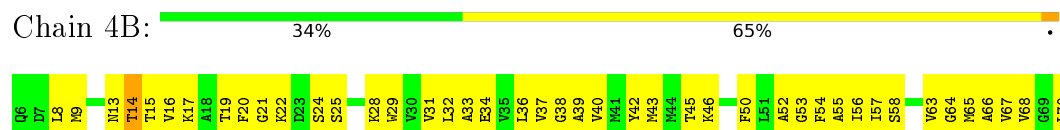
- Molecule 1: Pilin



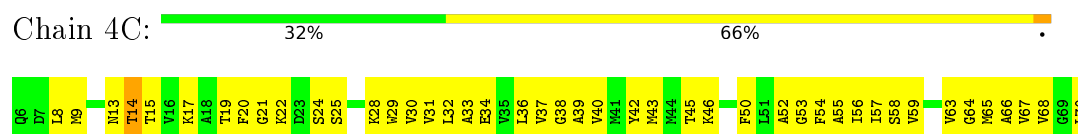
- Molecule 1: Pilin



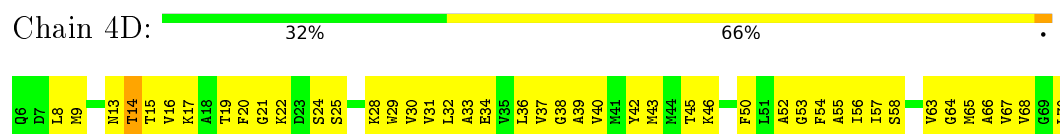
- Molecule 1: Pilin



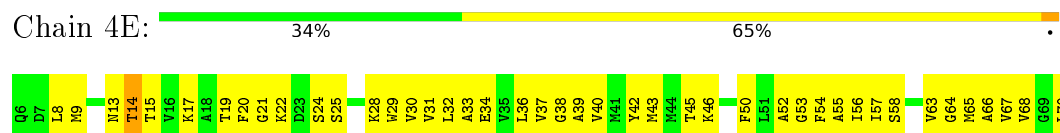
- Molecule 1: Pilin



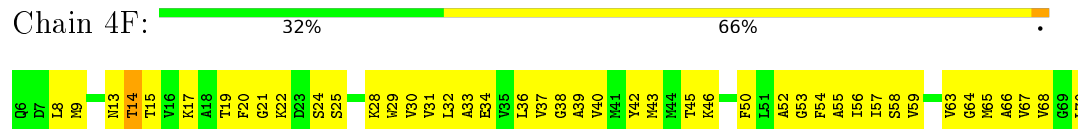
- Molecule 1: Pilin



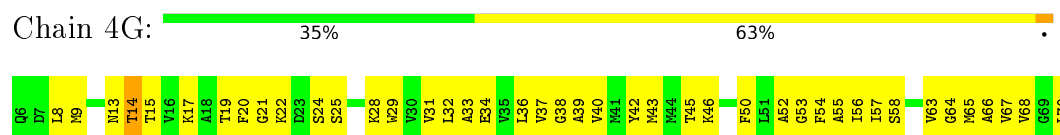
- Molecule 1: Pilin



- Molecule 1: Pilin



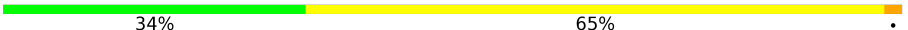
- Molecule 1: Pilin



## • Molecule 1: Pilin

Chain 4H:  32% 66%

## • Molecule 1: Pilin

Chain 4I:  34% 65%

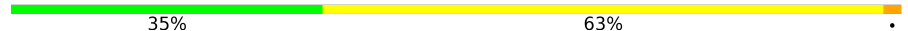
## • Molecule 1: Pilin

Chain 4J:  34% 63%

## • Molecule 1: Pilin

Chain 4K:  35% 62%

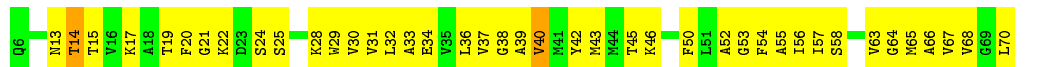
## • Molecule 1: Pilin

Chain 4L:  35% 63%

## • Molecule 1: Pilin

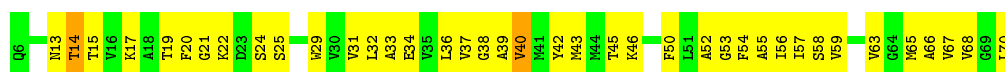
Chain 4M:  32% 66%

## • Molecule 1: Pilin

Chain 4N:  37% 60%

## • Molecule 1: Pilin

Chain 4O:  40% 57%



- Molecule 1: Pilin

Chain 5A: 32% 66%



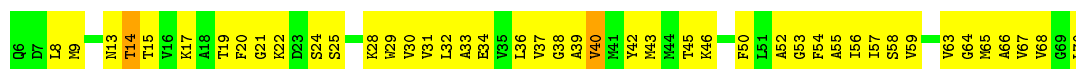
- Molecule 1: Pilin

Chain 5B: 35% 62%



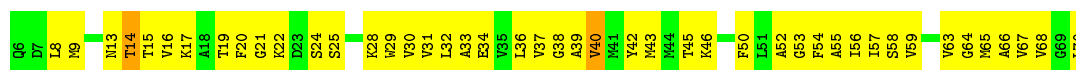
- Molecule 1: Pilin

Chain 5C: 32% 65%



- Molecule 1: Pilin

Chain 5D: 31% 66%



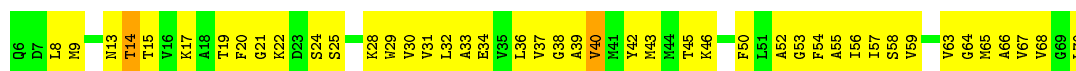
- Molecule 1: Pilin

Chain 5E: 34% 65%



- Molecule 1: Pilin

Chain 5F: 32% 65%

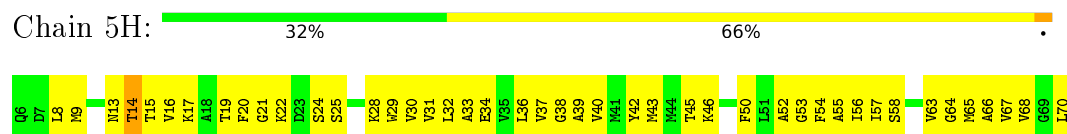


- Molecule 1: Pilin

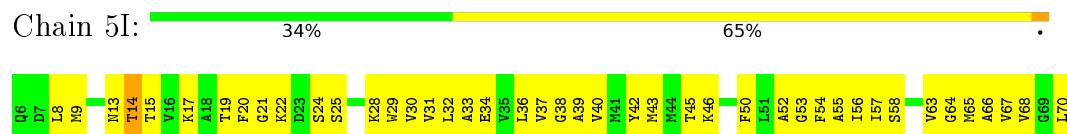
Chain 5G: 35% 63%



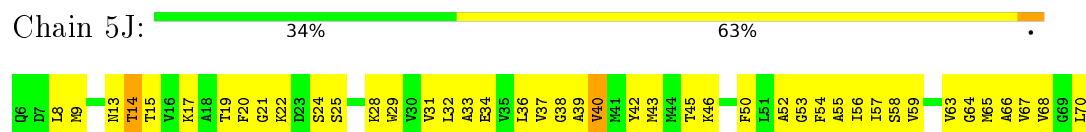
- Molecule 1: Pilin



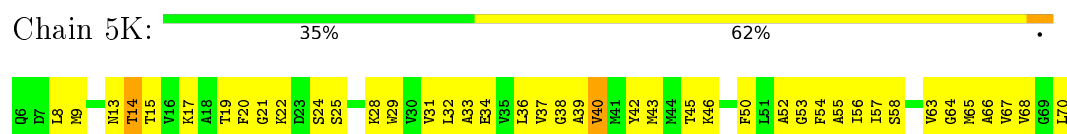
• Molecule 1: Pilin



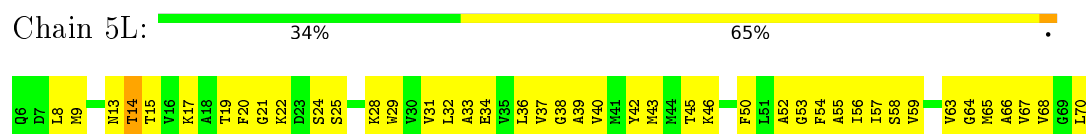
• Molecule 1: Pilin



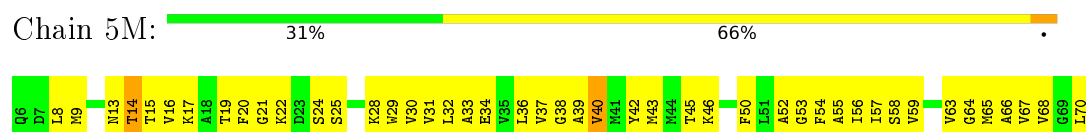
• Molecule 1: Pilin



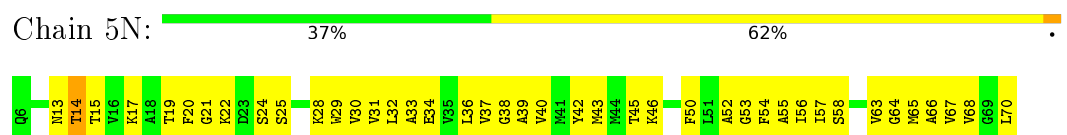
• Molecule 1: Pilin



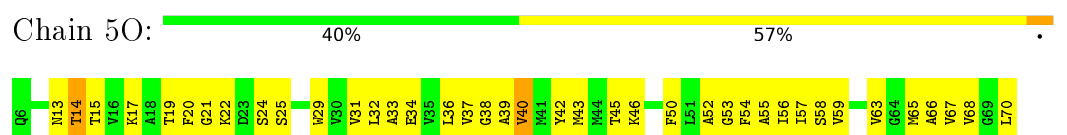
• Molecule 1: Pilin



• Molecule 1: Pilin



• Molecule 1: Pilin



## 4 Experimental information

| Property                             | Value               | Source    |
|--------------------------------------|---------------------|-----------|
| Reconstruction method                | HELICAL             | Depositor |
| Imposed symmetry                     | POINT, Not provided | Depositor |
| Number of segments used              | 11969               | Depositor |
| Resolution determination method      | OTHER               | Depositor |
| CTF correction method                | Not provided        | Depositor |
| Microscope                           | FEI POLARA 300      | Depositor |
| Voltage (kV)                         | 300                 | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | Not provided        | Depositor |
| Minimum defocus (nm)                 | Not provided        | Depositor |
| Maximum defocus (nm)                 | Not provided        | Depositor |
| Magnification                        | Not provided        | Depositor |
| Image detector                       | Not provided        | Depositor |



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6V6

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         | $\# Z  > 2$ | RMSZ        | $\# Z  > 2$ |
| 1   | 1A    | 0.52         | 0/481       | 0.61        | 0/649       |
| 1   | 1B    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 1C    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 1D    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 1E    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 1F    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 1G    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 1H    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 1I    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 1J    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 1K    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 1L    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 1M    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 1N    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 1O    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 2A    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 2B    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 2C    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 2D    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 2E    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 2F    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 2G    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 2H    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 2I    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 2J    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 2K    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 2L    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 2M    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 2N    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 2O    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 3A    | 0.52         | 0/482       | 0.61        | 0/651       |
| 1   | 3B    | 0.52         | 0/482       | 0.61        | 0/651       |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >2 | RMSZ        | # Z  >2 |
| 1   | 3C    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 3D    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 3E    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 3F    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 3G    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 3H    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 3I    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 3J    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 3K    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 3L    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 3M    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 3N    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 3O    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 4A    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 4B    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 4C    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 4D    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 4E    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 4F    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 4G    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 4H    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 4I    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 4J    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 4K    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 4L    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 4M    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 4N    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 4O    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 5A    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 5B    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 5C    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 5D    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 5E    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 5F    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 5G    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 5H    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 5I    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 5J    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 5K    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 5L    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 5M    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 5N    | 0.52         | 0/482   | 0.61        | 0/651   |
| 1   | 5O    | 0.52         | 0/482   | 0.61        | 0/651   |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >2 | RMSZ        | # Z  >2 |
| All | All   | 0.52         | 0/36149 | 0.61        | 0/48823 |

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   | 1A    | 0                   | 1                   |
| 1   | 1B    | 0                   | 1                   |
| 1   | 1C    | 0                   | 1                   |
| 1   | 1D    | 0                   | 1                   |
| 1   | 1E    | 0                   | 1                   |
| 1   | 1F    | 0                   | 1                   |
| 1   | 1G    | 0                   | 1                   |
| 1   | 1H    | 0                   | 1                   |
| 1   | 1I    | 0                   | 1                   |
| 1   | 1J    | 0                   | 1                   |
| 1   | 1K    | 0                   | 1                   |
| 1   | 1L    | 0                   | 1                   |
| 1   | 1M    | 0                   | 1                   |
| 1   | 1N    | 0                   | 1                   |
| 1   | 1O    | 0                   | 1                   |
| 1   | 2A    | 0                   | 1                   |
| 1   | 2B    | 0                   | 1                   |
| 1   | 2C    | 0                   | 1                   |
| 1   | 2D    | 0                   | 1                   |
| 1   | 2E    | 0                   | 1                   |
| 1   | 2F    | 0                   | 1                   |
| 1   | 2G    | 0                   | 1                   |
| 1   | 2H    | 0                   | 1                   |
| 1   | 2I    | 0                   | 1                   |
| 1   | 2J    | 0                   | 1                   |
| 1   | 2K    | 0                   | 1                   |
| 1   | 2L    | 0                   | 1                   |
| 1   | 2M    | 0                   | 1                   |
| 1   | 2N    | 0                   | 1                   |
| 1   | 2O    | 0                   | 1                   |
| 1   | 3A    | 0                   | 1                   |
| 1   | 3B    | 0                   | 1                   |
| 1   | 3C    | 0                   | 1                   |
| 1   | 3D    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | 3E    | 0                   | 1                   |
| 1   | 3F    | 0                   | 1                   |
| 1   | 3G    | 0                   | 1                   |
| 1   | 3H    | 0                   | 1                   |
| 1   | 3I    | 0                   | 1                   |
| 1   | 3J    | 0                   | 1                   |
| 1   | 3K    | 0                   | 1                   |
| 1   | 3L    | 0                   | 1                   |
| 1   | 3M    | 0                   | 1                   |
| 1   | 3N    | 0                   | 1                   |
| 1   | 3O    | 0                   | 1                   |
| 1   | 4A    | 0                   | 1                   |
| 1   | 4B    | 0                   | 1                   |
| 1   | 4C    | 0                   | 1                   |
| 1   | 4D    | 0                   | 1                   |
| 1   | 4E    | 0                   | 1                   |
| 1   | 4F    | 0                   | 1                   |
| 1   | 4G    | 0                   | 1                   |
| 1   | 4H    | 0                   | 1                   |
| 1   | 4I    | 0                   | 1                   |
| 1   | 4J    | 0                   | 1                   |
| 1   | 4K    | 0                   | 1                   |
| 1   | 4L    | 0                   | 1                   |
| 1   | 4M    | 0                   | 1                   |
| 1   | 4N    | 0                   | 1                   |
| 1   | 4O    | 0                   | 1                   |
| 1   | 5A    | 0                   | 1                   |
| 1   | 5B    | 0                   | 1                   |
| 1   | 5C    | 0                   | 1                   |
| 1   | 5D    | 0                   | 1                   |
| 1   | 5E    | 0                   | 1                   |
| 1   | 5F    | 0                   | 1                   |
| 1   | 5G    | 0                   | 1                   |
| 1   | 5H    | 0                   | 1                   |
| 1   | 5I    | 0                   | 1                   |
| 1   | 5J    | 0                   | 1                   |
| 1   | 5K    | 0                   | 1                   |
| 1   | 5L    | 0                   | 1                   |
| 1   | 5M    | 0                   | 1                   |
| 1   | 5N    | 0                   | 1                   |
| 1   | 5O    | 0                   | 1                   |
| All | All   | 0                   | 75                  |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 75 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | 1A    | 14  | THR  | Peptide |
| 1   | 1B    | 14  | THR  | Peptide |
| 1   | 1C    | 14  | THR  | Peptide |
| 1   | 1D    | 14  | THR  | Peptide |
| 1   | 1E    | 14  | THR  | 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   | 1A    | 475   | 0        | 508      | 55      | 0            |
| 1   | 1B    | 476   | 0        | 509      | 56      | 0            |
| 1   | 1C    | 476   | 0        | 509      | 65      | 0            |
| 1   | 1D    | 476   | 0        | 509      | 64      | 0            |
| 1   | 1E    | 476   | 0        | 509      | 60      | 0            |
| 1   | 1F    | 476   | 0        | 509      | 61      | 0            |
| 1   | 1G    | 476   | 0        | 509      | 58      | 0            |
| 1   | 1H    | 476   | 0        | 509      | 59      | 0            |
| 1   | 1I    | 476   | 0        | 509      | 59      | 0            |
| 1   | 1J    | 476   | 0        | 509      | 62      | 0            |
| 1   | 1K    | 476   | 0        | 509      | 57      | 0            |
| 1   | 1L    | 476   | 0        | 509      | 56      | 0            |
| 1   | 1M    | 476   | 0        | 509      | 65      | 0            |
| 1   | 1N    | 476   | 0        | 509      | 51      | 0            |
| 1   | 1O    | 476   | 0        | 509      | 52      | 0            |
| 1   | 2A    | 476   | 0        | 509      | 52      | 0            |
| 1   | 2B    | 476   | 0        | 509      | 53      | 0            |
| 1   | 2C    | 476   | 0        | 509      | 65      | 0            |
| 1   | 2D    | 476   | 0        | 509      | 61      | 0            |
| 1   | 2E    | 476   | 0        | 509      | 58      | 0            |
| 1   | 2F    | 476   | 0        | 509      | 61      | 0            |
| 1   | 2G    | 476   | 0        | 509      | 56      | 0            |
| 1   | 2H    | 476   | 0        | 509      | 60      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 2I    | 476   | 0        | 509      | 57      | 0            |
| 1   | 2J    | 476   | 0        | 509      | 61      | 0            |
| 1   | 2K    | 476   | 0        | 509      | 56      | 0            |
| 1   | 2L    | 476   | 0        | 509      | 56      | 0            |
| 1   | 2M    | 476   | 0        | 509      | 66      | 0            |
| 1   | 2N    | 476   | 0        | 509      | 52      | 0            |
| 1   | 2O    | 476   | 0        | 509      | 51      | 0            |
| 1   | 3A    | 476   | 0        | 509      | 52      | 0            |
| 1   | 3B    | 476   | 0        | 509      | 56      | 0            |
| 1   | 3C    | 476   | 0        | 509      | 65      | 0            |
| 1   | 3D    | 476   | 0        | 509      | 64      | 0            |
| 1   | 3E    | 476   | 0        | 509      | 58      | 0            |
| 1   | 3F    | 476   | 0        | 509      | 61      | 0            |
| 1   | 3G    | 476   | 0        | 509      | 57      | 0            |
| 1   | 3H    | 476   | 0        | 509      | 59      | 0            |
| 1   | 3I    | 476   | 0        | 509      | 57      | 0            |
| 1   | 3J    | 476   | 0        | 509      | 61      | 0            |
| 1   | 3K    | 476   | 0        | 509      | 58      | 0            |
| 1   | 3L    | 476   | 0        | 509      | 56      | 0            |
| 1   | 3M    | 476   | 0        | 509      | 63      | 0            |
| 1   | 3N    | 476   | 0        | 509      | 53      | 0            |
| 1   | 3O    | 476   | 0        | 509      | 50      | 0            |
| 1   | 4A    | 476   | 0        | 509      | 53      | 0            |
| 1   | 4B    | 476   | 0        | 509      | 55      | 0            |
| 1   | 4C    | 476   | 0        | 509      | 63      | 0            |
| 1   | 4D    | 476   | 0        | 509      | 65      | 0            |
| 1   | 4E    | 476   | 0        | 509      | 59      | 0            |
| 1   | 4F    | 476   | 0        | 509      | 62      | 0            |
| 1   | 4G    | 476   | 0        | 509      | 59      | 0            |
| 1   | 4H    | 476   | 0        | 509      | 62      | 0            |
| 1   | 4I    | 476   | 0        | 509      | 60      | 0            |
| 1   | 4J    | 476   | 0        | 509      | 58      | 0            |
| 1   | 4K    | 476   | 0        | 509      | 55      | 0            |
| 1   | 4L    | 476   | 0        | 509      | 55      | 0            |
| 1   | 4M    | 476   | 0        | 509      | 63      | 0            |
| 1   | 4N    | 476   | 0        | 509      | 48      | 0            |
| 1   | 4O    | 476   | 0        | 509      | 51      | 0            |
| 1   | 5A    | 476   | 0        | 509      | 50      | 0            |
| 1   | 5B    | 476   | 0        | 509      | 53      | 0            |
| 1   | 5C    | 476   | 0        | 509      | 67      | 0            |
| 1   | 5D    | 476   | 0        | 509      | 66      | 0            |
| 1   | 5E    | 476   | 0        | 509      | 60      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 5F    | 476   | 0        | 509      | 65      | 0            |
| 1   | 5G    | 476   | 0        | 509      | 59      | 0            |
| 1   | 5H    | 476   | 0        | 509      | 61      | 0            |
| 1   | 5I    | 476   | 0        | 509      | 58      | 0            |
| 1   | 5J    | 476   | 0        | 509      | 59      | 0            |
| 1   | 5K    | 476   | 0        | 509      | 57      | 0            |
| 1   | 5L    | 476   | 0        | 509      | 60      | 0            |
| 1   | 5M    | 476   | 0        | 509      | 67      | 0            |
| 1   | 5N    | 476   | 0        | 509      | 53      | 0            |
| 1   | 5O    | 476   | 0        | 509      | 50      | 0            |
| 2   | 1A    | 12    | 0        | 0        | 0       | 0            |
| 2   | 1B    | 12    | 0        | 0        | 1       | 0            |
| 2   | 1C    | 12    | 0        | 0        | 1       | 0            |
| 2   | 1D    | 12    | 0        | 0        | 1       | 0            |
| 2   | 1E    | 12    | 0        | 0        | 1       | 0            |
| 2   | 1F    | 12    | 0        | 0        | 1       | 0            |
| 2   | 1G    | 12    | 0        | 0        | 2       | 0            |
| 2   | 1H    | 12    | 0        | 0        | 1       | 0            |
| 2   | 1I    | 12    | 0        | 0        | 2       | 0            |
| 2   | 1J    | 12    | 0        | 0        | 1       | 0            |
| 2   | 1K    | 12    | 0        | 0        | 1       | 0            |
| 2   | 1L    | 12    | 0        | 0        | 1       | 0            |
| 2   | 1M    | 12    | 0        | 0        | 1       | 0            |
| 2   | 1N    | 12    | 0        | 0        | 1       | 0            |
| 2   | 2A    | 12    | 0        | 0        | 0       | 0            |
| 2   | 2B    | 12    | 0        | 0        | 1       | 0            |
| 2   | 2C    | 12    | 0        | 0        | 1       | 0            |
| 2   | 2D    | 12    | 0        | 0        | 1       | 0            |
| 2   | 2E    | 12    | 0        | 0        | 1       | 0            |
| 2   | 2F    | 12    | 0        | 0        | 1       | 0            |
| 2   | 2G    | 12    | 0        | 0        | 1       | 0            |
| 2   | 2H    | 12    | 0        | 0        | 1       | 0            |
| 2   | 2I    | 12    | 0        | 0        | 2       | 0            |
| 2   | 2J    | 12    | 0        | 0        | 1       | 0            |
| 2   | 2K    | 12    | 0        | 0        | 1       | 0            |
| 2   | 2L    | 12    | 0        | 0        | 1       | 0            |
| 2   | 2M    | 12    | 0        | 0        | 1       | 0            |
| 2   | 2N    | 12    | 0        | 0        | 1       | 0            |
| 2   | 3A    | 12    | 0        | 0        | 0       | 0            |
| 2   | 3B    | 12    | 0        | 0        | 1       | 0            |
| 2   | 3C    | 12    | 0        | 0        | 1       | 0            |
| 2   | 3D    | 12    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | 3E    | 12    | 0        | 0        | 1       | 0            |
| 2   | 3F    | 12    | 0        | 0        | 1       | 0            |
| 2   | 3G    | 12    | 0        | 0        | 1       | 0            |
| 2   | 3H    | 12    | 0        | 0        | 1       | 0            |
| 2   | 3I    | 12    | 0        | 0        | 2       | 0            |
| 2   | 3J    | 12    | 0        | 0        | 1       | 0            |
| 2   | 3K    | 12    | 0        | 0        | 1       | 0            |
| 2   | 3L    | 12    | 0        | 0        | 1       | 0            |
| 2   | 3M    | 12    | 0        | 0        | 1       | 0            |
| 2   | 3N    | 12    | 0        | 0        | 1       | 0            |
| 2   | 4A    | 12    | 0        | 0        | 0       | 0            |
| 2   | 4B    | 12    | 0        | 0        | 1       | 0            |
| 2   | 4C    | 12    | 0        | 0        | 1       | 0            |
| 2   | 4D    | 12    | 0        | 0        | 1       | 0            |
| 2   | 4E    | 12    | 0        | 0        | 1       | 0            |
| 2   | 4F    | 12    | 0        | 0        | 1       | 0            |
| 2   | 4G    | 12    | 0        | 0        | 1       | 0            |
| 2   | 4H    | 12    | 0        | 0        | 1       | 0            |
| 2   | 4I    | 12    | 0        | 0        | 2       | 0            |
| 2   | 4J    | 12    | 0        | 0        | 1       | 0            |
| 2   | 4K    | 12    | 0        | 0        | 1       | 0            |
| 2   | 4L    | 12    | 0        | 0        | 1       | 0            |
| 2   | 4M    | 12    | 0        | 0        | 1       | 0            |
| 2   | 4N    | 12    | 0        | 0        | 1       | 0            |
| 2   | 5A    | 12    | 0        | 0        | 0       | 0            |
| 2   | 5B    | 12    | 0        | 0        | 1       | 0            |
| 2   | 5C    | 12    | 0        | 0        | 1       | 0            |
| 2   | 5D    | 12    | 0        | 0        | 1       | 0            |
| 2   | 5E    | 12    | 0        | 0        | 1       | 0            |
| 2   | 5F    | 12    | 0        | 0        | 1       | 0            |
| 2   | 5G    | 12    | 0        | 0        | 1       | 0            |
| 2   | 5H    | 12    | 0        | 0        | 1       | 0            |
| 2   | 5I    | 12    | 0        | 0        | 1       | 0            |
| 2   | 5J    | 12    | 0        | 0        | 1       | 0            |
| 2   | 5K    | 12    | 0        | 0        | 1       | 0            |
| 2   | 5L    | 12    | 0        | 0        | 1       | 0            |
| 2   | 5M    | 12    | 0        | 0        | 1       | 0            |
| 2   | 5N    | 12    | 0        | 0        | 1       | 0            |
| All | All   | 36539 | 0        | 38174    | 3428    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.



The worst 5 of 3428 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:3C:67:VAL:HG13 | 1:4A:9:MET:CE    | 1.15                     | 1.63              |
| 1:2C:67:VAL:HG13 | 1:3A:9:MET:CE    | 1.15                     | 1.61              |
| 1:4C:67:VAL:HG13 | 1:5A:9:MET:CE    | 1.17                     | 1.60              |
| 1:1A:9:MET:CE    | 1:5C:67:VAL:HG13 | 1.15                     | 1.60              |
| 1:3D:67:VAL:HG13 | 1:4B:9:MET:CE    | 1.39                     | 1.53              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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   | 1A    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 1B    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 1C    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 1D    | 63/65 (97%) | 52 (82%) | 10 (16%) | 1 (2%)   | 12          | 57  |
| 1   | 1E    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 1F    | 63/65 (97%) | 52 (82%) | 10 (16%) | 1 (2%)   | 12          | 57  |
| 1   | 1G    | 63/65 (97%) | 52 (82%) | 10 (16%) | 1 (2%)   | 12          | 57  |
| 1   | 1H    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 1I    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 1J    | 63/65 (97%) | 52 (82%) | 10 (16%) | 1 (2%)   | 12          | 57  |
| 1   | 1K    | 63/65 (97%) | 52 (82%) | 10 (16%) | 1 (2%)   | 12          | 57  |
| 1   | 1L    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 1M    | 63/65 (97%) | 52 (82%) | 10 (16%) | 1 (2%)   | 12          | 57  |
| 1   | 1N    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed    | Favoured | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------|----------|----------|----------|-------------|-----|
| 1   | 1O    | 63/65 (97%) | 52 (82%) | 10 (16%) | 1 (2%)   | 12          | 57  |
| 1   | 2A    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 2B    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 2C    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 2D    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 2E    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 2F    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 2G    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 2H    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 2I    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 2J    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 2K    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 2L    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 2M    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 2N    | 63/65 (97%) | 52 (82%) | 10 (16%) | 1 (2%)   | 12          | 57  |
| 1   | 2O    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 3A    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 3B    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 3C    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 3D    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 3E    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 3F    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 3G    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 3H    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 3I    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 3J    | 63/65 (97%) | 52 (82%) | 10 (16%) | 1 (2%)   | 12          | 57  |
| 1   | 3K    | 63/65 (97%) | 52 (82%) | 10 (16%) | 1 (2%)   | 12          | 57  |
| 1   | 3L    | 63/65 (97%) | 52 (82%) | 11 (18%) | 0        | 100         | 100 |
| 1   | 3M    | 63/65 (97%) | 52 (82%) | 10 (16%) | 1 (2%)   | 12          | 57  |
| 1   | 3N    | 63/65 (97%) | 52 (82%) | 10 (16%) | 1 (2%)   | 12          | 57  |
| 1   | 3O    | 63/65 (97%) | 52 (82%) | 10 (16%) | 1 (2%)   | 12          | 57  |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | 4A    | 63/65 (97%)     | 52 (82%)   | 10 (16%)  | 1 (2%)   | 12          | 57  |
| 1   | 4B    | 63/65 (97%)     | 52 (82%)   | 11 (18%)  | 0        | 100         | 100 |
| 1   | 4C    | 63/65 (97%)     | 52 (82%)   | 11 (18%)  | 0        | 100         | 100 |
| 1   | 4D    | 63/65 (97%)     | 52 (82%)   | 11 (18%)  | 0        | 100         | 100 |
| 1   | 4E    | 63/65 (97%)     | 52 (82%)   | 11 (18%)  | 0        | 100         | 100 |
| 1   | 4F    | 63/65 (97%)     | 52 (82%)   | 11 (18%)  | 0        | 100         | 100 |
| 1   | 4G    | 63/65 (97%)     | 52 (82%)   | 11 (18%)  | 0        | 100         | 100 |
| 1   | 4H    | 63/65 (97%)     | 52 (82%)   | 11 (18%)  | 0        | 100         | 100 |
| 1   | 4I    | 63/65 (97%)     | 52 (82%)   | 11 (18%)  | 0        | 100         | 100 |
| 1   | 4J    | 63/65 (97%)     | 52 (82%)   | 10 (16%)  | 1 (2%)   | 12          | 57  |
| 1   | 4K    | 63/65 (97%)     | 52 (82%)   | 10 (16%)  | 1 (2%)   | 12          | 57  |
| 1   | 4L    | 63/65 (97%)     | 52 (82%)   | 11 (18%)  | 0        | 100         | 100 |
| 1   | 4M    | 63/65 (97%)     | 52 (82%)   | 11 (18%)  | 0        | 100         | 100 |
| 1   | 4N    | 63/65 (97%)     | 52 (82%)   | 10 (16%)  | 1 (2%)   | 12          | 57  |
| 1   | 4O    | 63/65 (97%)     | 52 (82%)   | 10 (16%)  | 1 (2%)   | 12          | 57  |
| 1   | 5A    | 63/65 (97%)     | 52 (82%)   | 11 (18%)  | 0        | 100         | 100 |
| 1   | 5B    | 63/65 (97%)     | 52 (82%)   | 10 (16%)  | 1 (2%)   | 12          | 57  |
| 1   | 5C    | 63/65 (97%)     | 52 (82%)   | 10 (16%)  | 1 (2%)   | 12          | 57  |
| 1   | 5D    | 63/65 (97%)     | 52 (82%)   | 10 (16%)  | 1 (2%)   | 12          | 57  |
| 1   | 5E    | 63/65 (97%)     | 52 (82%)   | 11 (18%)  | 0        | 100         | 100 |
| 1   | 5F    | 63/65 (97%)     | 52 (82%)   | 10 (16%)  | 1 (2%)   | 12          | 57  |
| 1   | 5G    | 63/65 (97%)     | 52 (82%)   | 11 (18%)  | 0        | 100         | 100 |
| 1   | 5H    | 63/65 (97%)     | 52 (82%)   | 11 (18%)  | 0        | 100         | 100 |
| 1   | 5I    | 63/65 (97%)     | 52 (82%)   | 11 (18%)  | 0        | 100         | 100 |
| 1   | 5J    | 63/65 (97%)     | 52 (82%)   | 10 (16%)  | 1 (2%)   | 12          | 57  |
| 1   | 5K    | 63/65 (97%)     | 52 (82%)   | 10 (16%)  | 1 (2%)   | 12          | 57  |
| 1   | 5L    | 63/65 (97%)     | 52 (82%)   | 11 (18%)  | 0        | 100         | 100 |
| 1   | 5M    | 63/65 (97%)     | 52 (82%)   | 10 (16%)  | 1 (2%)   | 12          | 57  |
| 1   | 5N    | 63/65 (97%)     | 52 (82%)   | 11 (18%)  | 0        | 100         | 100 |
| 1   | 5O    | 63/65 (97%)     | 52 (82%)   | 10 (16%)  | 1 (2%)   | 12          | 57  |
| All | All   | 4725/4875 (97%) | 3900 (82%) | 799 (17%) | 26 (1%)  | 34          | 74  |

5 of 26 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1D    | 40  | VAL  |
| 1   | 1F    | 40  | VAL  |
| 1   | 1G    | 40  | VAL  |
| 1   | 1J    | 40  | VAL  |
| 1   | 1K    | 40  | VAL  |

### 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 PDB entries followed by that with respect to all EM entries.

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   | 1A    | 50/51 (98%)  | 50 (100%) | 0        | 100         | 100 |
| 1   | 1B    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 1C    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 1D    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 1E    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 1F    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 1G    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 1H    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 1I    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 1J    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 1K    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 1L    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 1M    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 1N    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 1O    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 2A    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 2B    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 2C    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 2D    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 1   | 2E    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 2F    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 2G    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 2H    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 2I    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 2J    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 2K    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 2L    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 2M    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 2N    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 2O    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 3A    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 3B    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 3C    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 3D    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 3E    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 3F    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 3G    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 3H    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 3I    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 3J    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 3K    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 3L    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 3M    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 3N    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 3O    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 4A    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 4B    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 4C    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 4D    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |
| 1   | 4E    | 51/51 (100%) | 51 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 1   | 4F    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 4G    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 4H    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 4I    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 4J    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 4K    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 4L    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 4M    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 4N    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 4O    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 5A    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 5B    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 5C    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 5D    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 5E    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 5F    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 5G    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 5H    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 5I    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 5J    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 5K    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 5L    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 5M    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 5N    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| 1   | 5O    | 51/51 (100%)     | 51 (100%)   | 0        | 100         | 100 |
| All | All   | 3824/3825 (100%) | 3824 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

70 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | 6V6  | 1A    | 101 | -    | 11,11,48     | 0.57 | 0           | 11,14,54    | 0.53 | 0           |
| 2   | 6V6  | 1B    | 101 | -    | 11,11,48     | 0.57 | 0           | 11,14,54    | 0.53 | 0           |
| 2   | 6V6  | 1C    | 101 | -    | 11,11,48     | 0.57 | 0           | 11,14,54    | 0.53 | 0           |
| 2   | 6V6  | 1D    | 101 | -    | 11,11,48     | 0.57 | 0           | 11,14,54    | 0.52 | 0           |
| 2   | 6V6  | 1E    | 101 | -    | 11,11,48     | 0.57 | 0           | 11,14,54    | 0.52 | 0           |
| 2   | 6V6  | 1F    | 101 | -    | 11,11,48     | 0.57 | 0           | 11,14,54    | 0.54 | 0           |
| 2   | 6V6  | 1G    | 101 | -    | 11,11,48     | 0.57 | 0           | 11,14,54    | 0.52 | 0           |
| 2   | 6V6  | 1H    | 101 | -    | 11,11,48     | 0.57 | 0           | 11,14,54    | 0.52 | 0           |
| 2   | 6V6  | 1I    | 101 | -    | 11,11,48     | 0.56 | 0           | 11,14,54    | 0.52 | 0           |
| 2   | 6V6  | 1J    | 101 | -    | 11,11,48     | 0.57 | 0           | 11,14,54    | 0.52 | 0           |
| 2   | 6V6  | 1K    | 101 | -    | 11,11,48     | 0.57 | 0           | 11,14,54    | 0.51 | 0           |
| 2   | 6V6  | 1L    | 101 | -    | 11,11,48     | 0.57 | 0           | 11,14,54    | 0.52 | 0           |
| 2   | 6V6  | 1M    | 101 | -    | 11,11,48     | 0.57 | 0           | 11,14,54    | 0.51 | 0           |
| 2   | 6V6  | 1N    | 101 | -    | 11,11,48     | 0.57 | 0           | 11,14,54    | 0.53 | 0           |
| 2   | 6V6  | 2A    | 101 | -    | 11,11,48     | 0.57 | 0           | 11,14,54    | 0.53 | 0           |
| 2   | 6V6  | 2B    | 101 | -    | 11,11,48     | 0.57 | 0           | 11,14,54    | 0.53 | 0           |
| 2   | 6V6  | 2C    | 101 | -    | 11,11,48     | 0.57 | 0           | 11,14,54    | 0.53 | 0           |
| 2   | 6V6  | 2D    | 101 | -    | 11,11,48     | 0.58 | 0           | 11,14,54    | 0.52 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | 6V6  | 2E    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 2F    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.53 | 0        |
| 2   | 6V6  | 2G    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 2H    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 2I    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 2J    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 2K    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.51 | 0        |
| 2   | 6V6  | 2L    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 2M    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.51 | 0        |
| 2   | 6V6  | 2N    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.53 | 0        |
| 2   | 6V6  | 3A    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.53 | 0        |
| 2   | 6V6  | 3B    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.53 | 0        |
| 2   | 6V6  | 3C    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.53 | 0        |
| 2   | 6V6  | 3D    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 3E    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 3F    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.54 | 0        |
| 2   | 6V6  | 3G    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 3H    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 3I    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 3J    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 3K    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.51 | 0        |
| 2   | 6V6  | 3L    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 3M    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.51 | 0        |
| 2   | 6V6  | 3N    | 101 | -    | 11,11,48     | 0.58 | 0        | 11,14,54    | 0.53 | 0        |
| 2   | 6V6  | 4A    | 101 | -    | 11,11,48     | 0.56 | 0        | 11,14,54    | 0.53 | 0        |
| 2   | 6V6  | 4B    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.53 | 0        |
| 2   | 6V6  | 4C    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.53 | 0        |
| 2   | 6V6  | 4D    | 101 | -    | 11,11,48     | 0.58 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 4E    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 4F    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.54 | 0        |
| 2   | 6V6  | 4G    | 101 | -    | 11,11,48     | 0.58 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 4H    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 4I    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 4J    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 4K    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.51 | 0        |
| 2   | 6V6  | 4L    | 101 | -    | 11,11,48     | 0.56 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 4M    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.51 | 0        |
| 2   | 6V6  | 4N    | 101 | -    | 11,11,48     | 0.58 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 5A    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.53 | 0        |
| 2   | 6V6  | 5B    | 101 | -    | 11,11,48     | 0.58 | 0        | 11,14,54    | 0.53 | 0        |
| 2   | 6V6  | 5C    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.53 | 0        |
| 2   | 6V6  | 5D    | 101 | -    | 11,11,48     | 0.58 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 5E    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | 6V6  | 5F    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.53 | 0        |
| 2   | 6V6  | 5G    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 5H    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 5I    | 101 | -    | 11,11,48     | 0.56 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 5J    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 5K    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.51 | 0        |
| 2   | 6V6  | 5L    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.52 | 0        |
| 2   | 6V6  | 5M    | 101 | -    | 11,11,48     | 0.57 | 0        | 11,14,54    | 0.51 | 0        |
| 2   | 6V6  | 5N    | 101 | -    | 11,11,48     | 0.58 | 0        | 11,14,54    | 0.53 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | 6V6  | 1A    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 1B    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 1C    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 1D    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 1E    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 1F    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 1G    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 1H    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 1I    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 1J    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 1K    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 1L    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 1M    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 1N    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 2A    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 2B    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 2C    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 2D    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 2E    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 2F    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 2G    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 2H    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 2I    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 2J    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 2K    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 2L    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 2M    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | 6V6  | 2N    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 3A    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 3B    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 3C    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 3D    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 3E    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 3F    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 3G    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 3H    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 3I    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 3J    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 3K    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 3L    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 3M    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 3N    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 4A    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 4B    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 4C    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 4D    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 4E    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 4F    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 4G    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 4H    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 4I    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 4J    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 4K    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 4L    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 4M    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 4N    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 5A    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 5B    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 5C    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 5D    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 5E    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 5F    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 5G    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 5H    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 5I    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 5J    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 5K    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 5L    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |
| 2   | 6V6  | 5M    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | 6V6  | 5N    | 101 | -    | -       | 0/12/12/53 | 0/0/0/0 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

65 monomers are involved in 70 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | 1B    | 101 | 6V6  | 1       | 0            |
| 2   | 1C    | 101 | 6V6  | 1       | 0            |
| 2   | 1D    | 101 | 6V6  | 1       | 0            |
| 2   | 1E    | 101 | 6V6  | 1       | 0            |
| 2   | 1F    | 101 | 6V6  | 1       | 0            |
| 2   | 1G    | 101 | 6V6  | 2       | 0            |
| 2   | 1H    | 101 | 6V6  | 1       | 0            |
| 2   | 1I    | 101 | 6V6  | 2       | 0            |
| 2   | 1J    | 101 | 6V6  | 1       | 0            |
| 2   | 1K    | 101 | 6V6  | 1       | 0            |
| 2   | 1L    | 101 | 6V6  | 1       | 0            |
| 2   | 1M    | 101 | 6V6  | 1       | 0            |
| 2   | 1N    | 101 | 6V6  | 1       | 0            |
| 2   | 2B    | 101 | 6V6  | 1       | 0            |
| 2   | 2C    | 101 | 6V6  | 1       | 0            |
| 2   | 2D    | 101 | 6V6  | 1       | 0            |
| 2   | 2E    | 101 | 6V6  | 1       | 0            |
| 2   | 2F    | 101 | 6V6  | 1       | 0            |
| 2   | 2G    | 101 | 6V6  | 1       | 0            |
| 2   | 2H    | 101 | 6V6  | 1       | 0            |
| 2   | 2I    | 101 | 6V6  | 2       | 0            |
| 2   | 2J    | 101 | 6V6  | 1       | 0            |
| 2   | 2K    | 101 | 6V6  | 1       | 0            |
| 2   | 2L    | 101 | 6V6  | 1       | 0            |
| 2   | 2M    | 101 | 6V6  | 1       | 0            |
| 2   | 2N    | 101 | 6V6  | 1       | 0            |
| 2   | 3B    | 101 | 6V6  | 1       | 0            |
| 2   | 3C    | 101 | 6V6  | 1       | 0            |
| 2   | 3D    | 101 | 6V6  | 1       | 0            |
| 2   | 3E    | 101 | 6V6  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | 3F    | 101 | 6V6  | 1       | 0            |
| 2   | 3G    | 101 | 6V6  | 1       | 0            |
| 2   | 3H    | 101 | 6V6  | 1       | 0            |
| 2   | 3I    | 101 | 6V6  | 2       | 0            |
| 2   | 3J    | 101 | 6V6  | 1       | 0            |
| 2   | 3K    | 101 | 6V6  | 1       | 0            |
| 2   | 3L    | 101 | 6V6  | 1       | 0            |
| 2   | 3M    | 101 | 6V6  | 1       | 0            |
| 2   | 3N    | 101 | 6V6  | 1       | 0            |
| 2   | 4B    | 101 | 6V6  | 1       | 0            |
| 2   | 4C    | 101 | 6V6  | 1       | 0            |
| 2   | 4D    | 101 | 6V6  | 1       | 0            |
| 2   | 4E    | 101 | 6V6  | 1       | 0            |
| 2   | 4F    | 101 | 6V6  | 1       | 0            |
| 2   | 4G    | 101 | 6V6  | 1       | 0            |
| 2   | 4H    | 101 | 6V6  | 1       | 0            |
| 2   | 4I    | 101 | 6V6  | 2       | 0            |
| 2   | 4J    | 101 | 6V6  | 1       | 0            |
| 2   | 4K    | 101 | 6V6  | 1       | 0            |
| 2   | 4L    | 101 | 6V6  | 1       | 0            |
| 2   | 4M    | 101 | 6V6  | 1       | 0            |
| 2   | 4N    | 101 | 6V6  | 1       | 0            |
| 2   | 5B    | 101 | 6V6  | 1       | 0            |
| 2   | 5C    | 101 | 6V6  | 1       | 0            |
| 2   | 5D    | 101 | 6V6  | 1       | 0            |
| 2   | 5E    | 101 | 6V6  | 1       | 0            |
| 2   | 5F    | 101 | 6V6  | 1       | 0            |
| 2   | 5G    | 101 | 6V6  | 1       | 0            |
| 2   | 5H    | 101 | 6V6  | 1       | 0            |
| 2   | 5I    | 101 | 6V6  | 1       | 0            |
| 2   | 5J    | 101 | 6V6  | 1       | 0            |
| 2   | 5K    | 101 | 6V6  | 1       | 0            |
| 2   | 5L    | 101 | 6V6  | 1       | 0            |
| 2   | 5M    | 101 | 6V6  | 1       | 0            |
| 2   | 5N    | 101 | 6V6  | 1       | 0            |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.