



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2020 – 01:18 pm BST

PDB ID : 5EJU  
Title : Ensemble refinement of the Crystal Structure of the Reversibly photoswitching chromoprotein Dathail, Ground State  
Authors : Close, D.W.; Langan, P.S.; Bradbury, A.R.M.  
Deposited on : 2015-11-02  
Resolution : 1.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

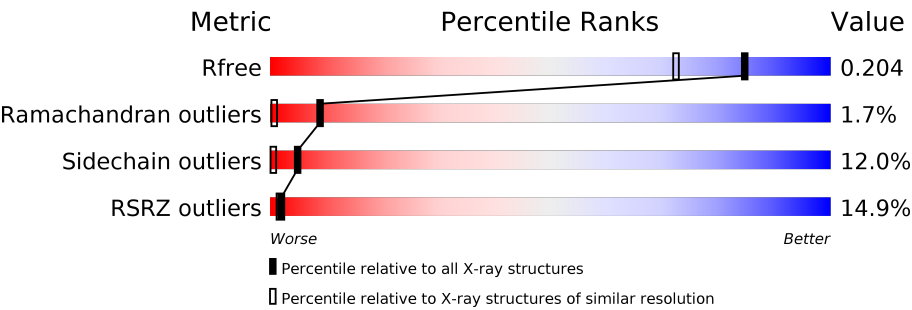
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1827 (1.66-1.66)                                      |
| Ramachandran outliers | 138981                      | 1891 (1.66-1.66)                                      |
| Sidechain outliers    | 138945                      | 1891 (1.66-1.66)                                      |
| RSRZ outliers         | 127900                      | 1791 (1.66-1.66)                                      |

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

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | 1-A   | 229    | <div><div>14%</div><div><div></div><div>81%</div><div>10%</div><div>•</div><div>7%</div></div></div> |
| 1   | 10-A  | 229    | <div><div>14%</div><div><div></div><div>79%</div><div>14%</div><div></div><div>7%</div></div></div>  |
| 1   | 11-A  | 229    | <div><div>14%</div><div><div></div><div>79%</div><div>11%</div><div>•</div><div>7%</div></div></div> |
| 1   | 12-A  | 229    | <div><div>14%</div><div><div></div><div>82%</div><div>10%</div><div>•</div><div>7%</div></div></div> |
| 1   | 13-A  | 229    | <div><div>14%</div><div><div></div><div>76%</div><div>15%</div><div>•</div><div>7%</div></div></div> |
| 1   | 14-A  | 229    | <div><div>14%</div><div><div></div><div>82%</div><div>9%</div><div>•</div><div>7%</div></div></div>  |
| 1   | 15-A  | 229    | <div><div>14%</div><div><div></div><div>81%</div><div>11%</div><div>•</div><div>7%</div></div></div> |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 16-A  | 229    |                  |
| 1   | 17-A  | 229    |                  |
| 1   | 18-A  | 229    |                  |
| 1   | 19-A  | 229    |                  |
| 1   | 2-A   | 229    |                  |
| 1   | 20-A  | 229    |                  |
| 1   | 21-A  | 229    |                  |
| 1   | 22-A  | 229    |                  |
| 1   | 23-A  | 229    |                  |
| 1   | 24-A  | 229    |                  |
| 1   | 25-A  | 229    |                  |
| 1   | 26-A  | 229    |                  |
| 1   | 27-A  | 229    |                  |
| 1   | 28-A  | 229    |                  |
| 1   | 29-A  | 229    |                  |
| 1   | 3-A   | 229    |                  |
| 1   | 30-A  | 229    |                  |
| 1   | 31-A  | 229    |                  |
| 1   | 32-A  | 229    |                  |
| 1   | 33-A  | 229    |                  |
| 1   | 34-A  | 229    |                  |
| 1   | 35-A  | 229    |                  |
| 1   | 36-A  | 229    |                  |
| 1   | 37-A  | 229    |                  |
| 1   | 38-A  | 229    |                  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 39-A  | 229    |                  |
| 1   | 4-A   | 229    |                  |
| 1   | 40-A  | 229    |                  |
| 1   | 41-A  | 229    |                  |
| 1   | 42-A  | 229    |                  |
| 1   | 43-A  | 229    |                  |
| 1   | 44-A  | 229    |                  |
| 1   | 45-A  | 229    |                  |
| 1   | 46-A  | 229    |                  |
| 1   | 47-A  | 229    |                  |
| 1   | 5-A   | 229    |                  |
| 1   | 6-A   | 229    |                  |
| 1   | 7-A   | 229    |                  |
| 1   | 8-A   | 229    |                  |
| 1   | 9-A   | 229    |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 167541 atoms, of which 78255 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Reversibly photoswitching protein Dathail.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|---------|-------|
| 1   | 1-A   | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 2-A   | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 3-A   | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 4-A   | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 5-A   | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 6-A   | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 7-A   | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 8-A   | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 9-A   | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 10-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 11-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 12-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 13-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 14-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 15-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 16-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |      |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|---------|-------|
| 1   | 17-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 18-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 19-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 20-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 21-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 22-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 23-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 24-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 25-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 26-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 27-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 28-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 29-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 30-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 31-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 32-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 33-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 34-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 35-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 36-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 37-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |      |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|---------|-------|
| 1   | 38-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 39-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 40-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 41-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 42-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 43-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 44-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 45-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 46-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |
| 1   | 47-A  | 214      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3410  | 1118 | 1665 | 286 | 331 | 10 |         |         |       |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 2   | 1-A   | 165      | Total | O   | 0       | 0       |
|     |       |          | 165   | 165 |         |         |
| 2   | 2-A   | 173      | Total | O   | 0       | 0       |
|     |       |          | 173   | 173 |         |         |
| 2   | 3-A   | 140      | Total | O   | 0       | 0       |
|     |       |          | 140   | 140 |         |         |
| 2   | 4-A   | 153      | Total | O   | 0       | 0       |
|     |       |          | 153   | 153 |         |         |
| 2   | 5-A   | 167      | Total | O   | 0       | 0       |
|     |       |          | 167   | 167 |         |         |
| 2   | 6-A   | 150      | Total | O   | 0       | 0       |
|     |       |          | 150   | 150 |         |         |
| 2   | 7-A   | 150      | Total | O   | 0       | 0       |
|     |       |          | 150   | 150 |         |         |
| 2   | 8-A   | 160      | Total | O   | 0       | 0       |
|     |       |          | 160   | 160 |         |         |
| 2   | 9-A   | 160      | Total | O   | 0       | 0       |
|     |       |          | 160   | 160 |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 2   | 10-A  | 152      | Total<br>152 | O<br>152 | 0       | 0       |
| 2   | 11-A  | 173      | Total<br>173 | O<br>173 | 0       | 0       |
| 2   | 12-A  | 160      | Total<br>160 | O<br>160 | 0       | 0       |
| 2   | 13-A  | 152      | Total<br>152 | O<br>152 | 0       | 0       |
| 2   | 14-A  | 157      | Total<br>157 | O<br>157 | 0       | 0       |
| 2   | 15-A  | 148      | Total<br>148 | O<br>148 | 0       | 0       |
| 2   | 16-A  | 152      | Total<br>152 | O<br>152 | 0       | 0       |
| 2   | 17-A  | 147      | Total<br>147 | O<br>147 | 0       | 0       |
| 2   | 18-A  | 156      | Total<br>156 | O<br>156 | 0       | 0       |
| 2   | 19-A  | 151      | Total<br>151 | O<br>151 | 0       | 0       |
| 2   | 20-A  | 147      | Total<br>147 | O<br>147 | 0       | 0       |
| 2   | 21-A  | 148      | Total<br>148 | O<br>148 | 0       | 0       |
| 2   | 22-A  | 169      | Total<br>169 | O<br>169 | 0       | 0       |
| 2   | 23-A  | 144      | Total<br>144 | O<br>144 | 0       | 0       |
| 2   | 24-A  | 138      | Total<br>138 | O<br>138 | 0       | 0       |
| 2   | 25-A  | 149      | Total<br>149 | O<br>149 | 0       | 0       |
| 2   | 26-A  | 143      | Total<br>143 | O<br>143 | 0       | 0       |
| 2   | 27-A  | 148      | Total<br>148 | O<br>148 | 0       | 0       |
| 2   | 28-A  | 165      | Total<br>165 | O<br>165 | 0       | 0       |
| 2   | 29-A  | 146      | Total<br>146 | O<br>146 | 0       | 0       |
| 2   | 30-A  | 165      | Total<br>165 | O<br>165 | 0       | 0       |

*Continued on next page...*



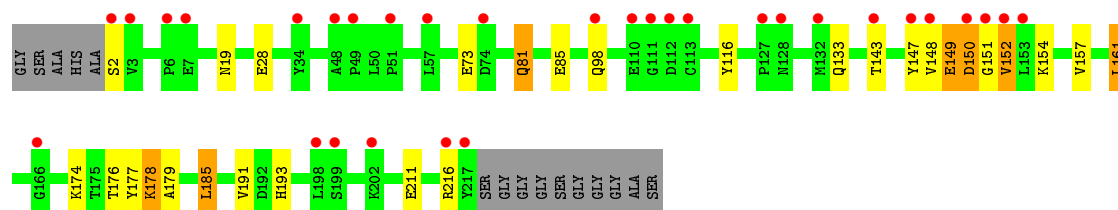
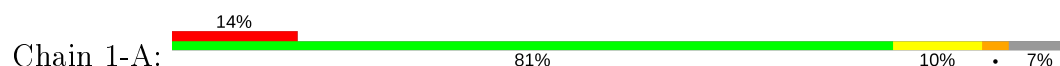
*Continued from previous page...*

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 2   | 31-A  | 163      | Total<br>163 | O<br>163 | 0       | 0       |
| 2   | 32-A  | 163      | Total<br>163 | O<br>163 | 0       | 0       |
| 2   | 33-A  | 154      | Total<br>154 | O<br>154 | 0       | 0       |
| 2   | 34-A  | 147      | Total<br>147 | O<br>147 | 0       | 0       |
| 2   | 35-A  | 135      | Total<br>135 | O<br>135 | 0       | 0       |
| 2   | 36-A  | 160      | Total<br>160 | O<br>160 | 0       | 0       |
| 2   | 37-A  | 156      | Total<br>156 | O<br>156 | 0       | 0       |
| 2   | 38-A  | 149      | Total<br>149 | O<br>149 | 0       | 0       |
| 2   | 39-A  | 154      | Total<br>154 | O<br>154 | 0       | 0       |
| 2   | 40-A  | 164      | Total<br>164 | O<br>164 | 0       | 0       |
| 2   | 41-A  | 156      | Total<br>156 | O<br>156 | 0       | 0       |
| 2   | 42-A  | 142      | Total<br>142 | O<br>142 | 0       | 0       |
| 2   | 43-A  | 162      | Total<br>162 | O<br>162 | 0       | 0       |
| 2   | 44-A  | 159      | Total<br>159 | O<br>159 | 0       | 0       |
| 2   | 45-A  | 143      | Total<br>143 | O<br>143 | 0       | 0       |
| 2   | 46-A  | 174      | Total<br>174 | O<br>174 | 0       | 0       |
| 2   | 47-A  | 162      | Total<br>162 | O<br>162 | 0       | 0       |

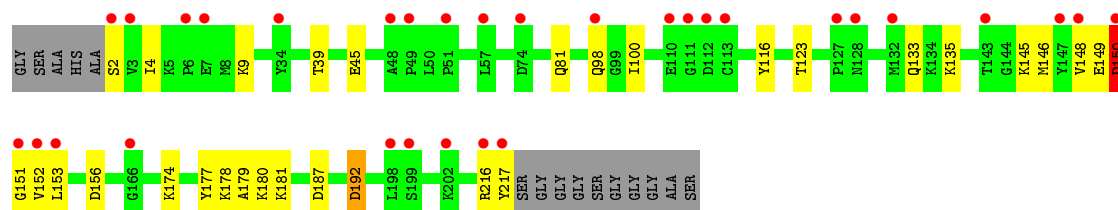
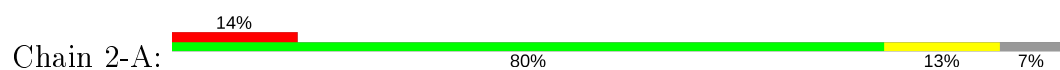
### 3 Residue-property plots [i](#)

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

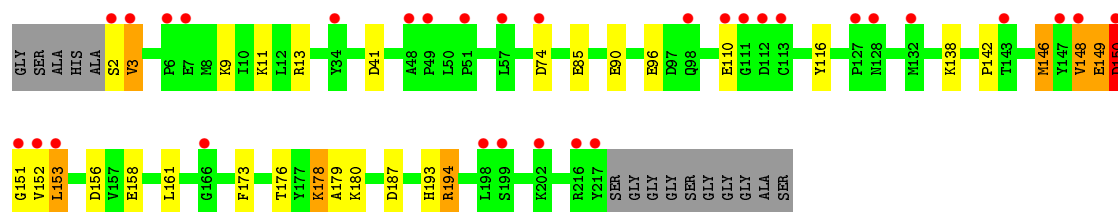
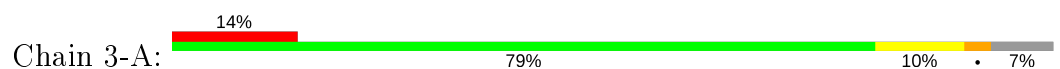
- Molecule 1: Reversibly photoswitching protein Dathail



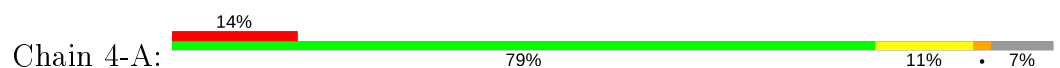
- Molecule 1: Reversibly photoswitching protein Dathail

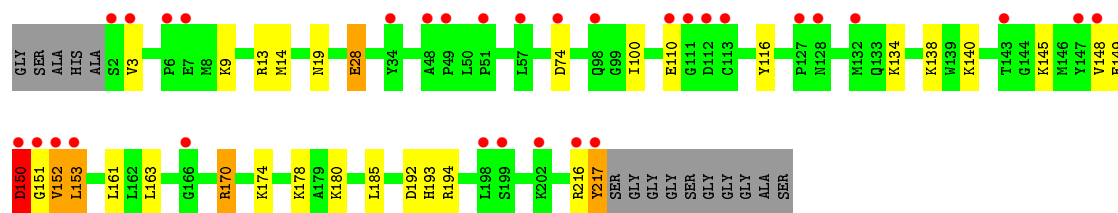


- Molecule 1: Reversibly photoswitching protein Dathail

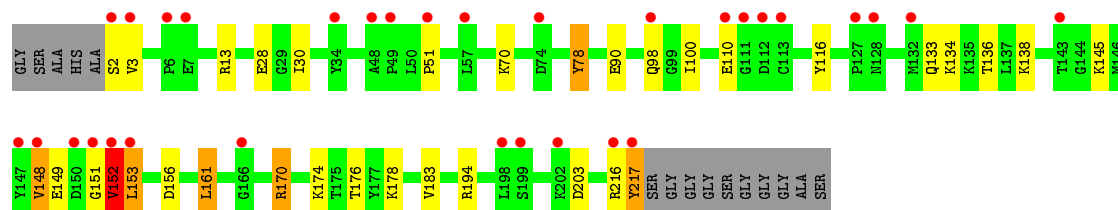
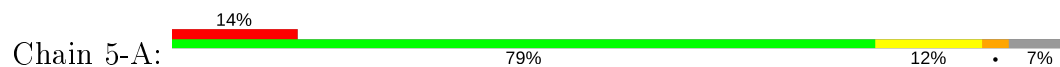


- Molecule 1: Reversibly photoswitching protein Dathail

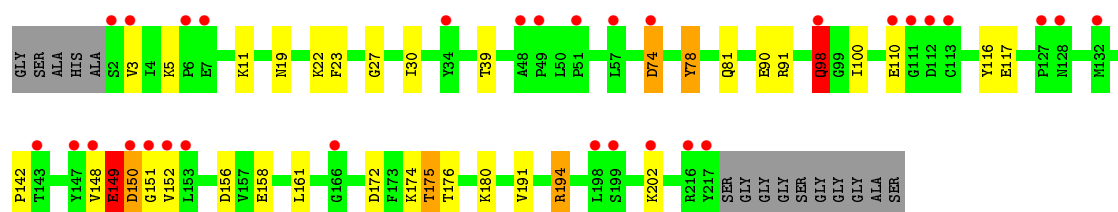
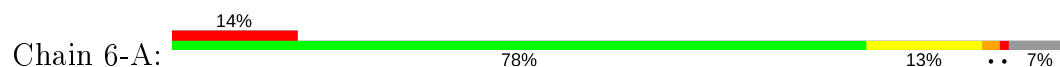




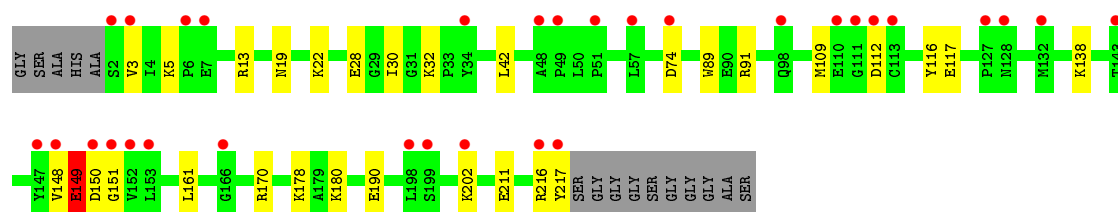
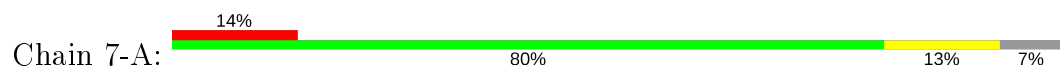
- Molecule 1: Reversibly photoswitching protein Dathail



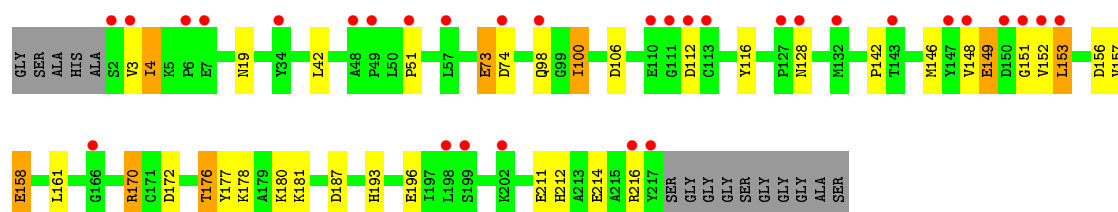
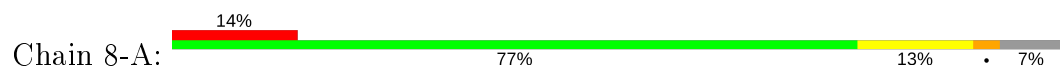
- Molecule 1: Reversibly photoswitching protein Dathail



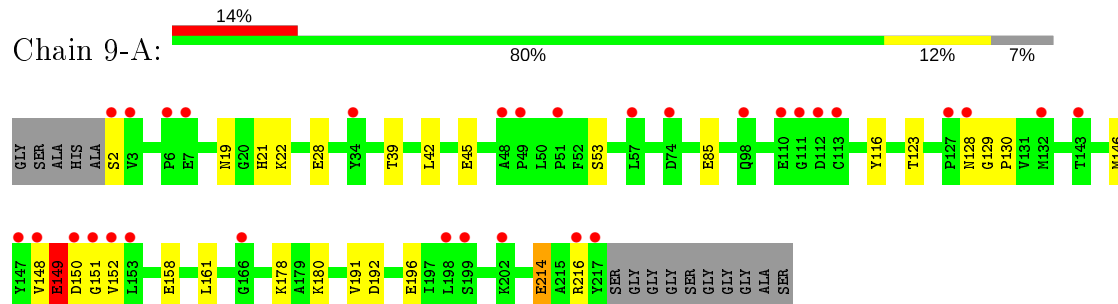
- Molecule 1: Reversibly photoswitching protein Dathail



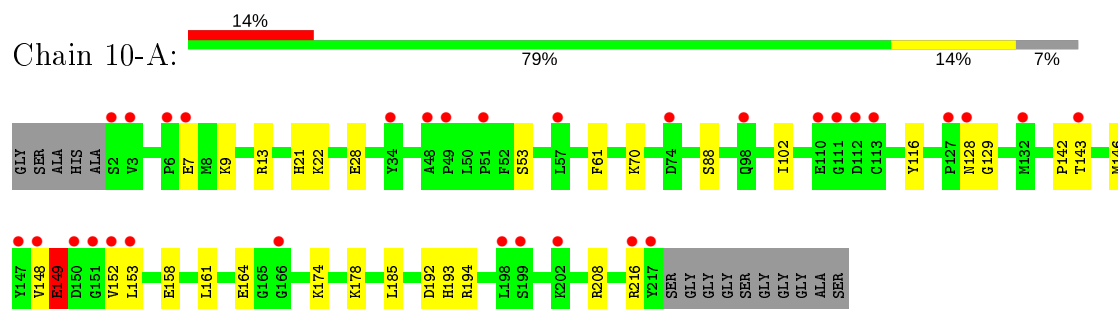
- Molecule 1: Reversibly photoswitching protein Dathail



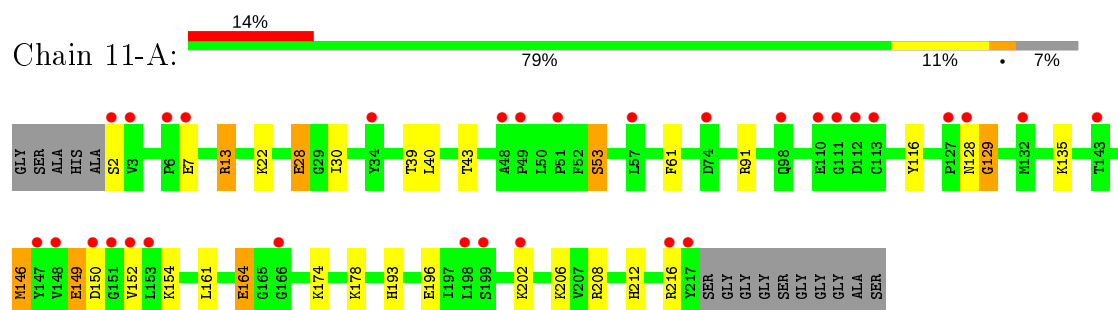
- Molecule 1: Reversibly photoswitching protein Dathail



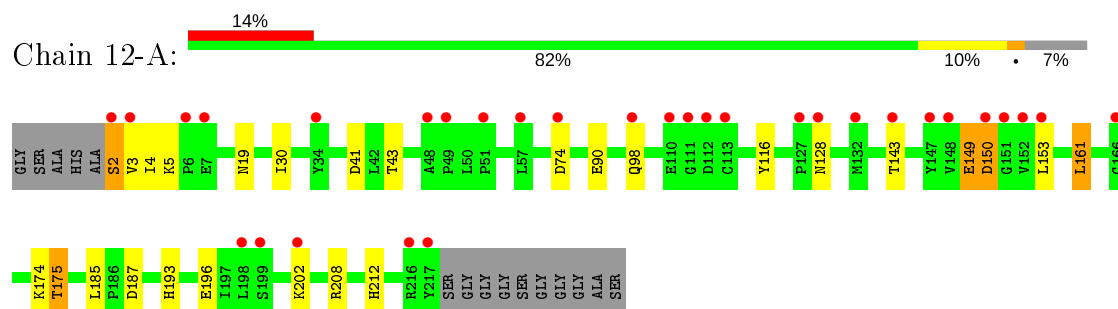
- Molecule 1: Reversibly photoswitching protein Dathail



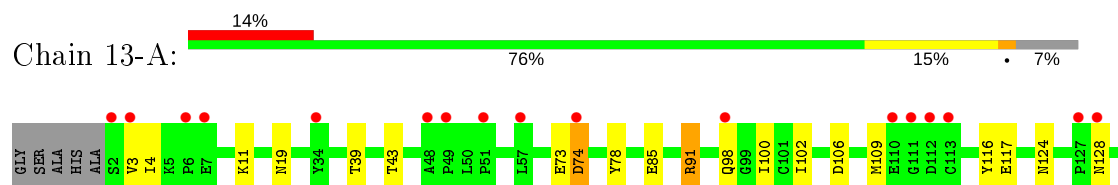
- Molecule 1: Reversibly photoswitching protein Dathail



- Molecule 1: Reversibly photoswitching protein Dathail

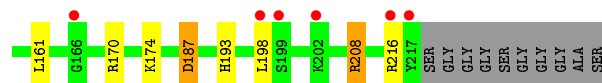
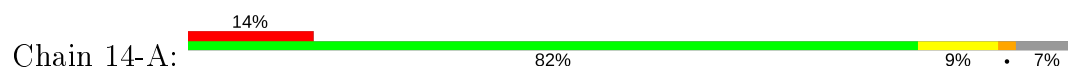


- Molecule 1: Reversibly photoswitching protein Dathail

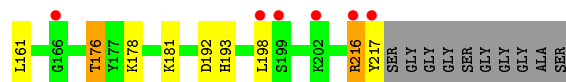
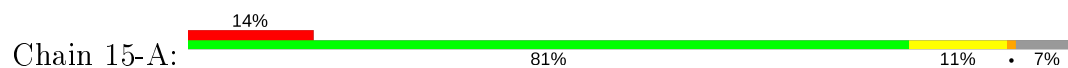




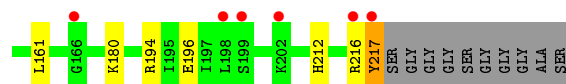
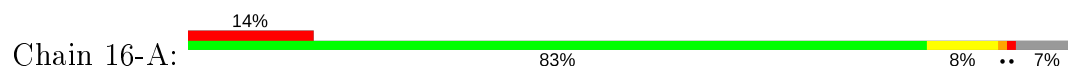
- Molecule 1: Reversibly photoswitching protein Dathail



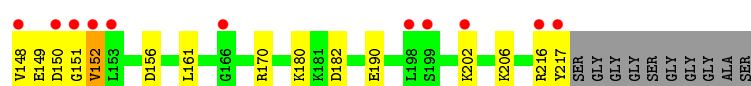
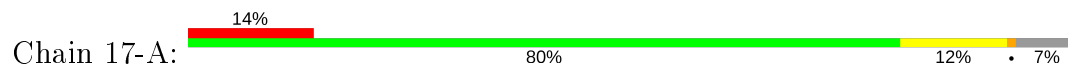
- Molecule 1: Reversibly photoswitching protein Dathail



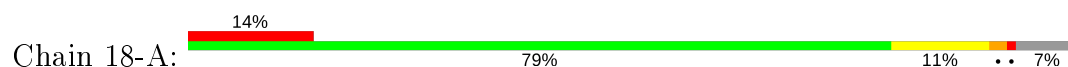
- Molecule 1: Reversibly photoswitching protein Dathail

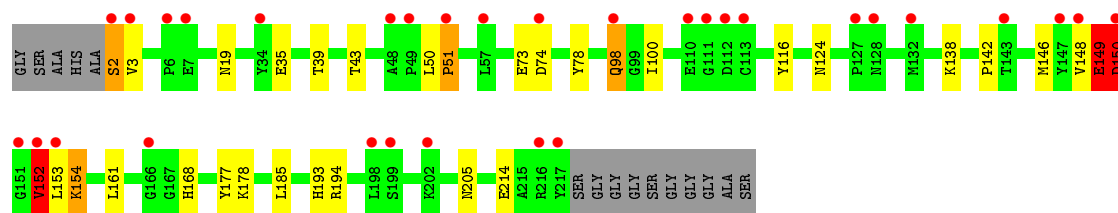


- Molecule 1: Reversibly photoswitching protein Dathail

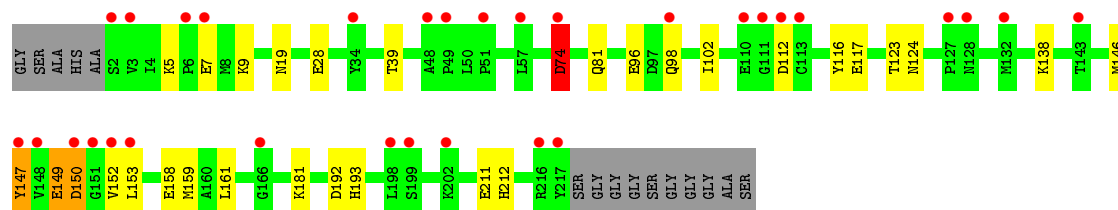
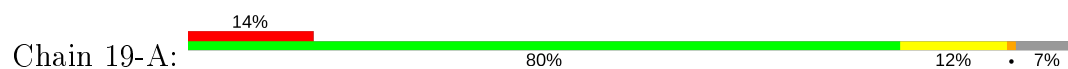


- Molecule 1: Reversibly photoswitching protein Dathail

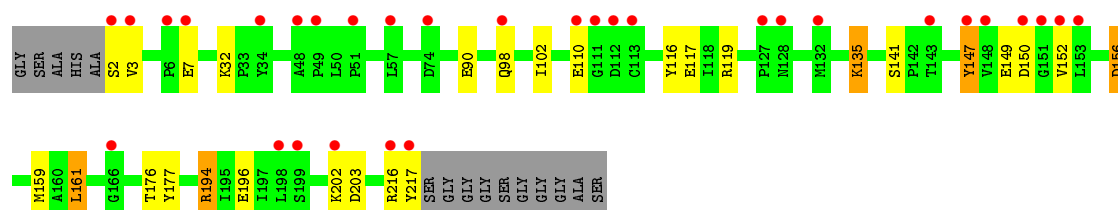
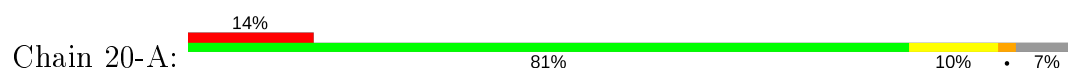




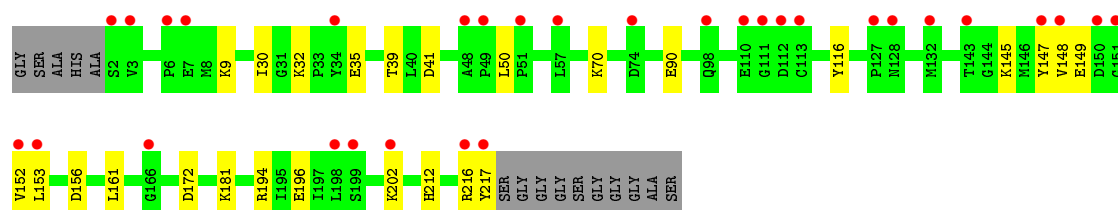
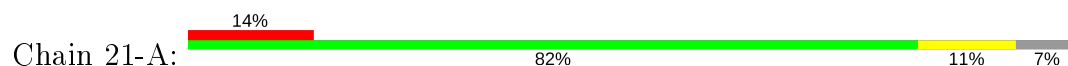
- Molecule 1: Reversibly photoswitching protein Dathail



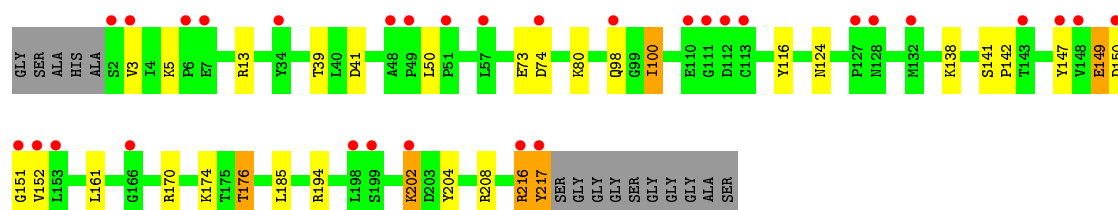
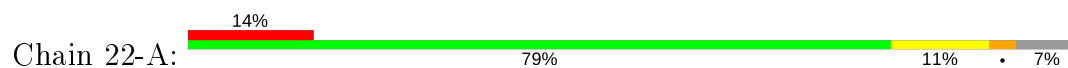
- Molecule 1: Reversibly photoswitching protein Dathail



- Molecule 1: Reversibly photoswitching protein Dathail

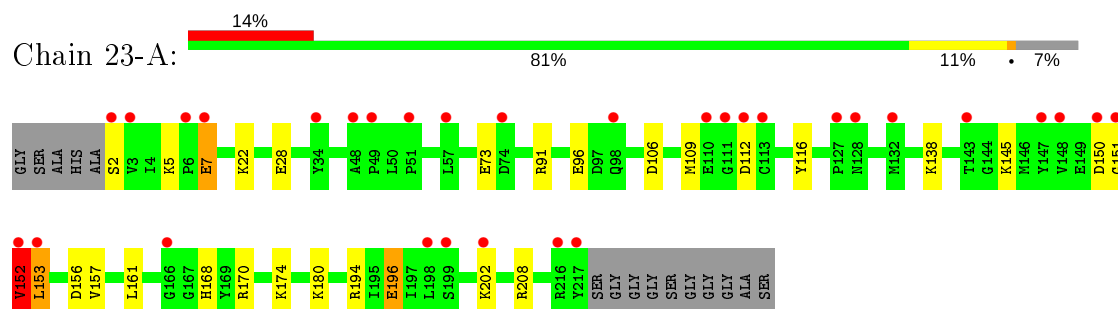


- Molecule 1: Reversibly photoswitching protein Dathail



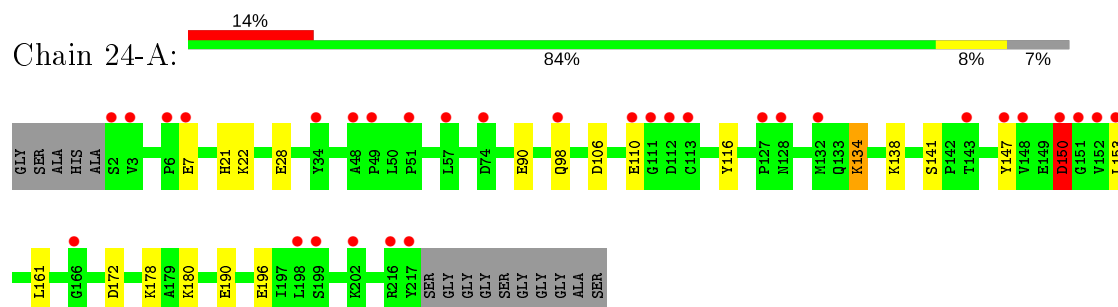
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 23-A:



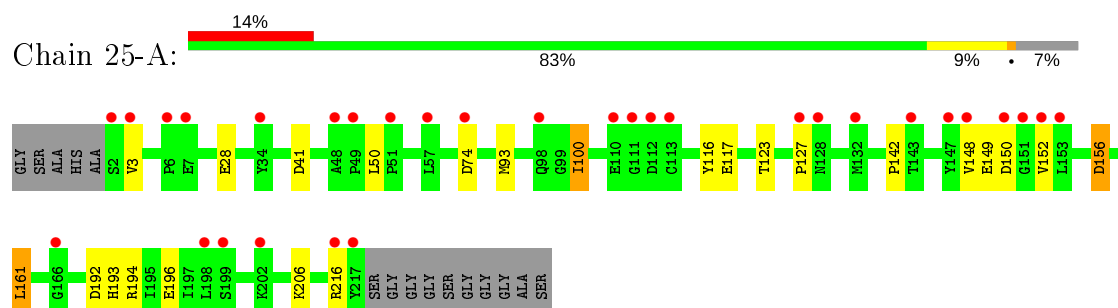
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 24-A:



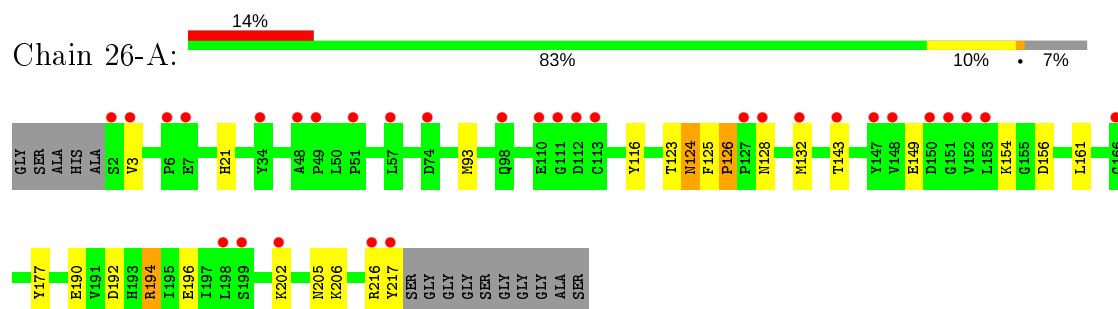
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 25-A:



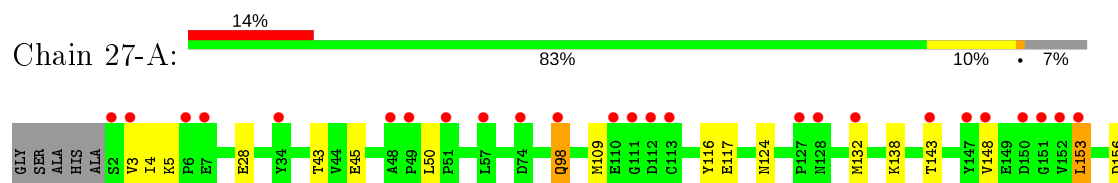
- Molecule 1: Reversibly photoswitching protein Dathail

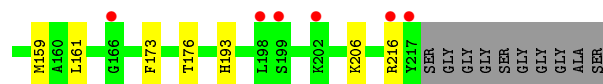
Chain 26-A:



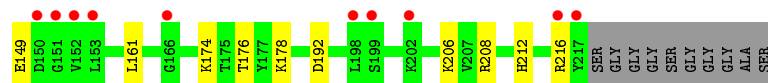
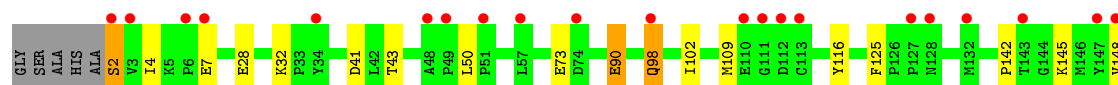
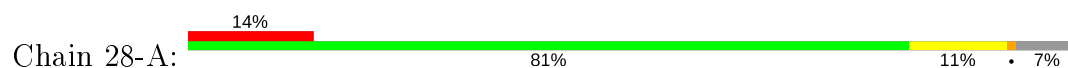
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 27-A:

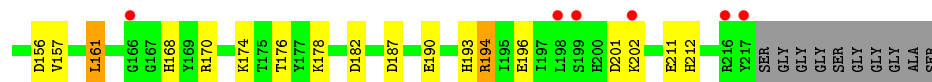
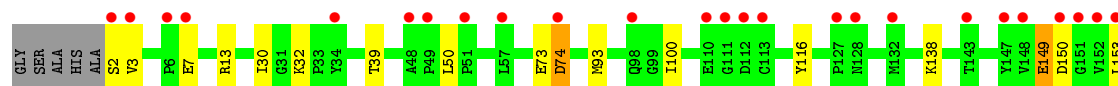
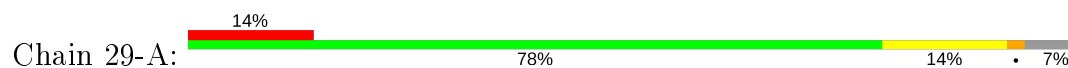




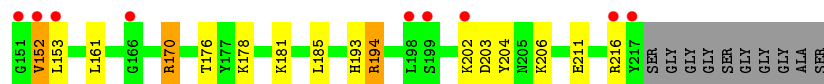
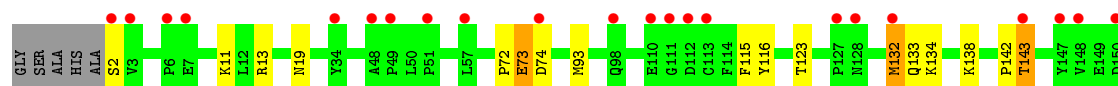
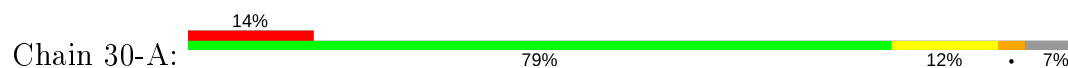
- Molecule 1: Reversibly photoswitching protein Dathail



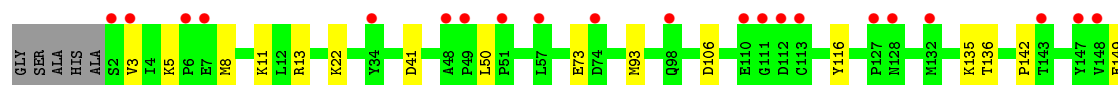
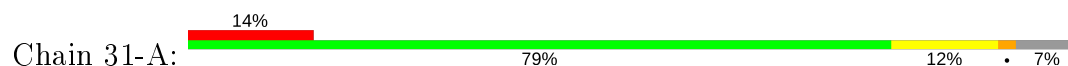
- Molecule 1: Reversibly photoswitching protein Dathail



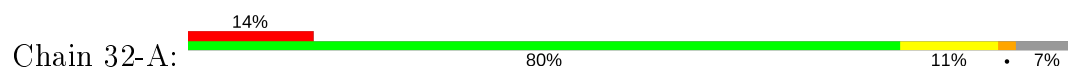
- Molecule 1: Reversibly photoswitching protein Dathail



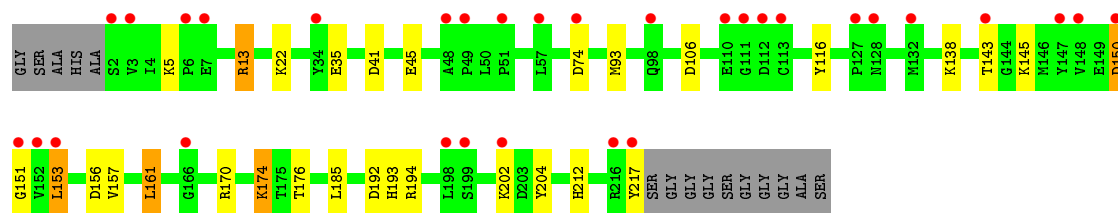
- Molecule 1: Reversibly photoswitching protein Dathail



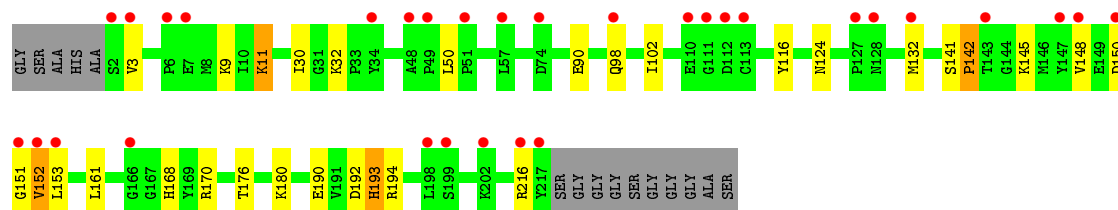
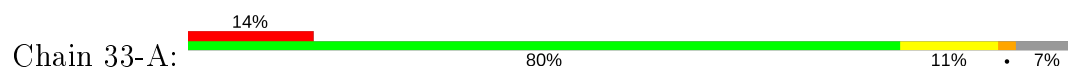
- Molecule 1: Reversibly photoswitching protein Dathail



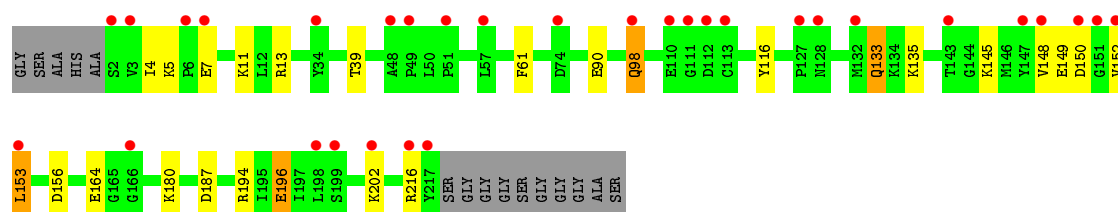
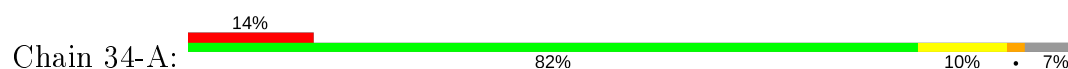




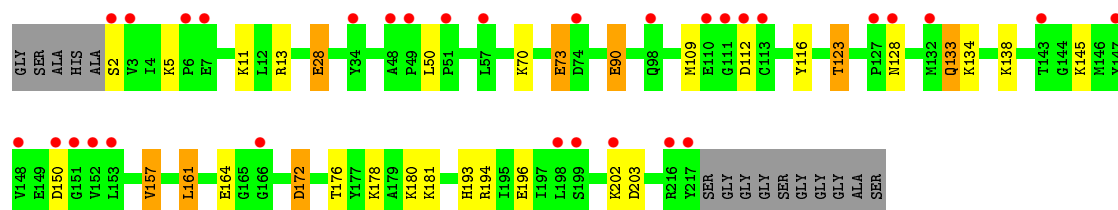
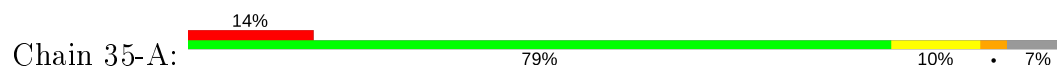
- Molecule 1: Reversibly photoswitching protein Dathail



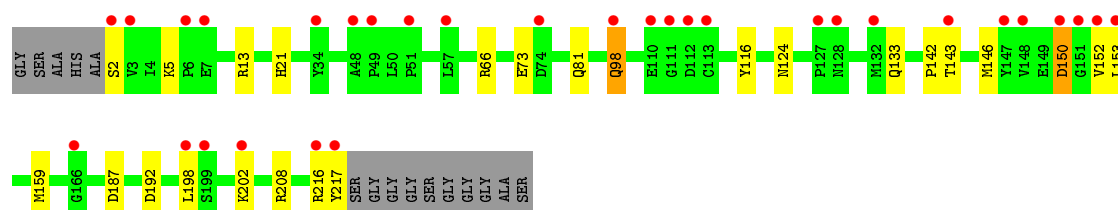
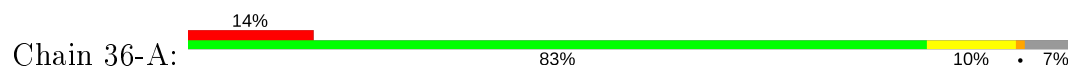
- Molecule 1: Reversibly photoswitching protein Dathail



- Molecule 1: Reversibly photoswitching protein Dathail

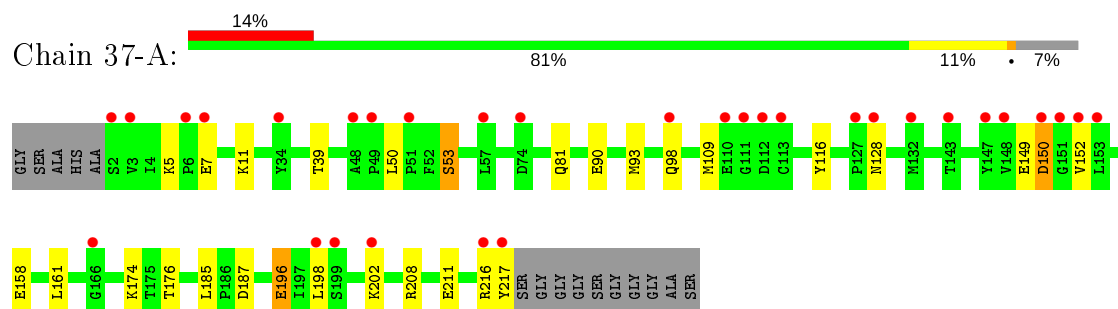


- Molecule 1: Reversibly photoswitching protein Dathail



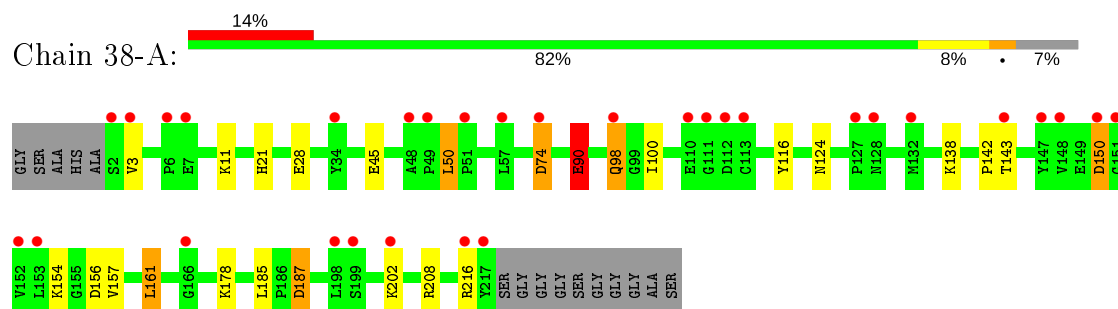
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 37-A:



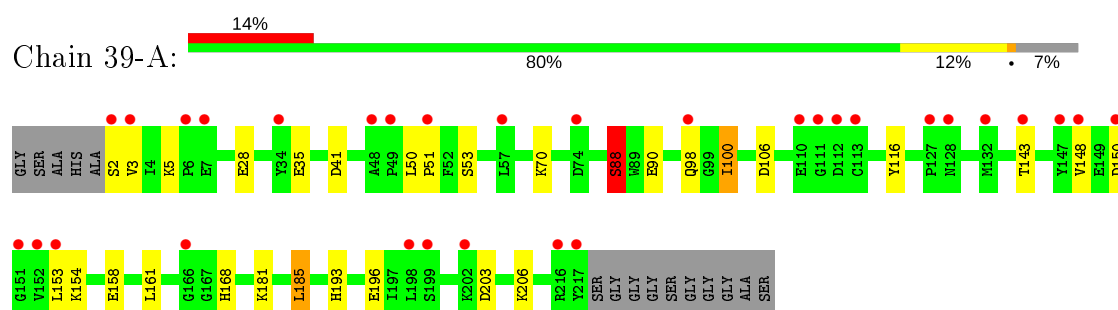
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 38-A:



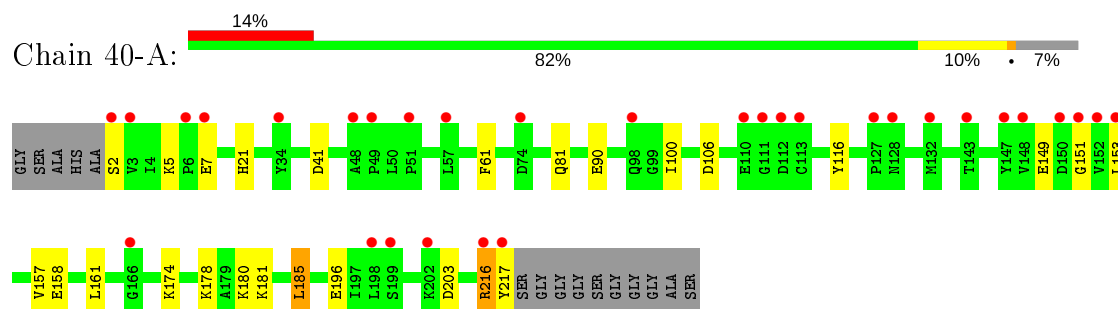
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 39-A:



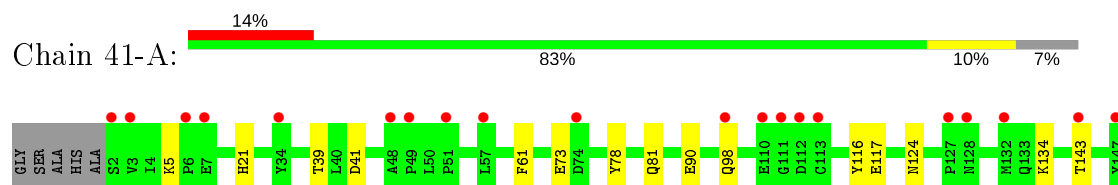
- Molecule 1: Reversibly photoswitching protein Dathail

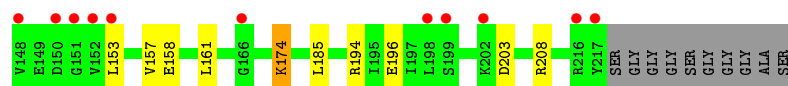
Chain 40-A:



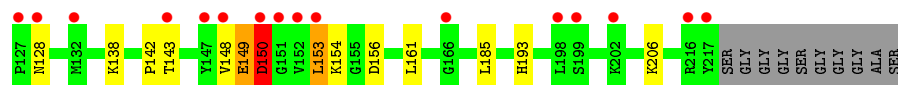
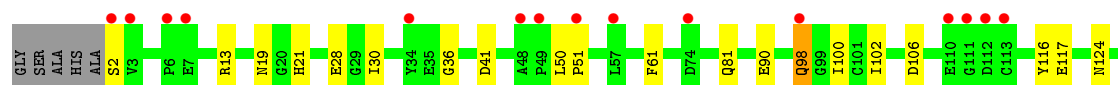
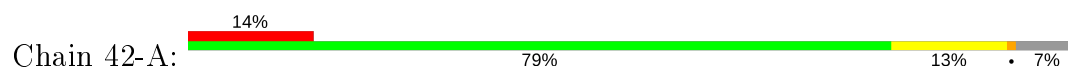
- Molecule 1: Reversibly photoswitching protein Dathail

Chain 41-A:

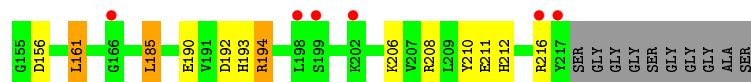
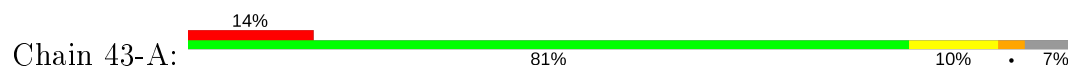




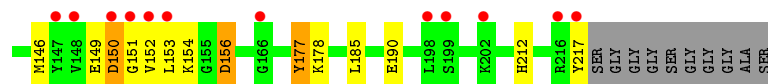
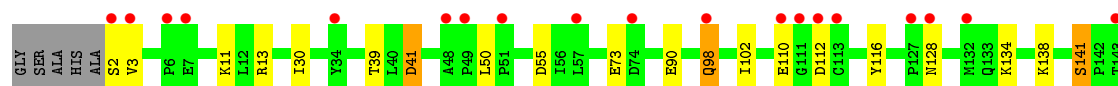
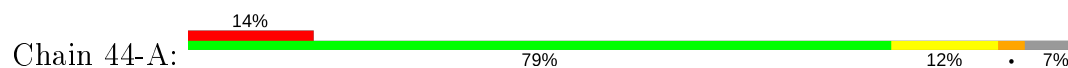
- Molecule 1: Reversibly photoswitching protein Dathail



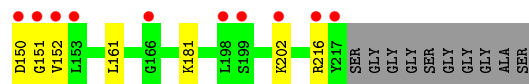
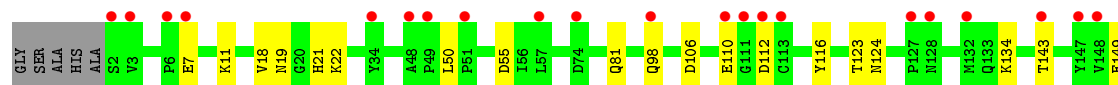
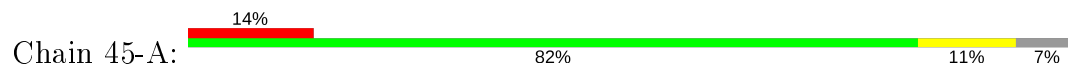
- Molecule 1: Reversibly photoswitching protein Dathail



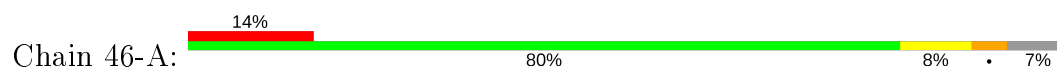
- Molecule 1: Reversibly photoswitching protein Dathail

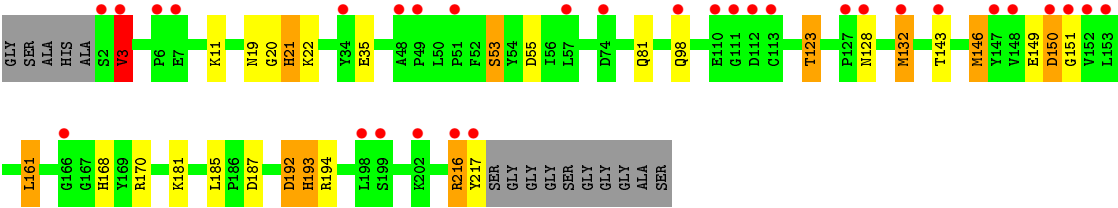


- Molecule 1: Reversibly photoswitching protein Dathail

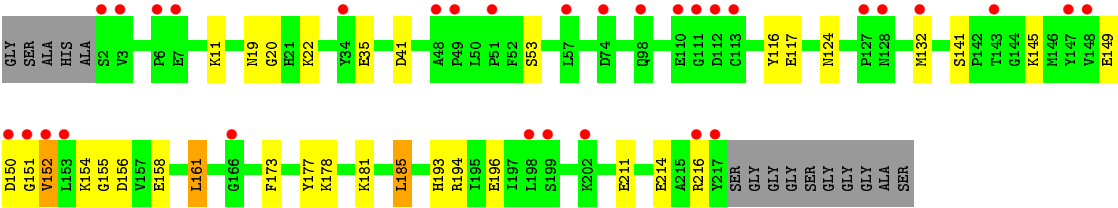
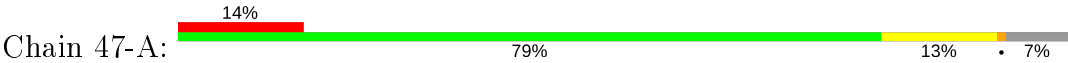


- Molecule 1: Reversibly photoswitching protein Dathail





- Molecule 1: Reversibly photoswitching protein Dathail



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 75.97Å 81.09Å 39.44Å<br>90.00° 90.00° 90.00°                | Depositor        |
| Resolution (Å)  | 28.27 – 1.65<br>32.14 – 1.65                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.4 (28.27-1.65)<br>95.6 (32.14-1.65)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.04  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.47 (at 1.65Å)   | Xtriage          |
| Refinement program  | PHENIX 1.9_1692   | Depositor        |
| R, $R_{free}$   | 0.151 , 0.194<br>0.169 , 0.204                              | Depositor<br>DCC |
| $R_{free}$ test set   | 1888 reflections (6.43%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 25.4  | Xtriage          |
| Anisotropy  | 0.565   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.22 , 357.5  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.96  | EDS              |
| Total number of atoms   | 167541  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 29.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5        |
| 1   | 1-A   | 0.90         | 7/1766 (0.4%) | 0.99        | 6/2382 (0.3%)  |
| 1   | 2-A   | 0.91         | 3/1766 (0.2%) | 1.01        | 3/2382 (0.1%)  |
| 1   | 3-A   | 0.99         | 7/1766 (0.4%) | 1.06        | 9/2382 (0.4%)  |
| 1   | 4-A   | 0.91         | 5/1766 (0.3%) | 1.03        | 6/2382 (0.3%)  |
| 1   | 5-A   | 0.88         | 3/1766 (0.2%) | 1.05        | 11/2382 (0.5%) |
| 1   | 6-A   | 0.91         | 5/1766 (0.3%) | 1.04        | 6/2382 (0.3%)  |
| 1   | 7-A   | 0.89         | 4/1766 (0.2%) | 1.02        | 7/2382 (0.3%)  |
| 1   | 8-A   | 1.00         | 6/1766 (0.3%) | 1.09        | 10/2382 (0.4%) |
| 1   | 9-A   | 0.90         | 6/1766 (0.3%) | 0.96        | 1/2382 (0.0%)  |
| 1   | 10-A  | 0.85         | 2/1766 (0.1%) | 0.99        | 6/2382 (0.3%)  |
| 1   | 11-A  | 0.98         | 8/1766 (0.5%) | 1.11        | 12/2382 (0.5%) |
| 1   | 12-A  | 0.84         | 2/1766 (0.1%) | 0.98        | 3/2382 (0.1%)  |
| 1   | 13-A  | 0.88         | 1/1766 (0.1%) | 1.08        | 8/2382 (0.3%)  |
| 1   | 14-A  | 0.89         | 1/1766 (0.1%) | 1.07        | 9/2382 (0.4%)  |
| 1   | 15-A  | 0.89         | 3/1766 (0.2%) | 1.00        | 2/2382 (0.1%)  |
| 1   | 16-A  | 0.83         | 3/1766 (0.2%) | 0.97        | 3/2382 (0.1%)  |
| 1   | 17-A  | 0.88         | 2/1766 (0.1%) | 1.00        | 3/2382 (0.1%)  |
| 1   | 18-A  | 0.91         | 6/1766 (0.3%) | 1.02        | 5/2382 (0.2%)  |
| 1   | 19-A  | 0.88         | 2/1766 (0.1%) | 1.00        | 9/2382 (0.4%)  |
| 1   | 20-A  | 0.89         | 3/1766 (0.2%) | 1.04        | 7/2382 (0.3%)  |
| 1   | 21-A  | 0.90         | 3/1766 (0.2%) | 1.06        | 4/2382 (0.2%)  |
| 1   | 22-A  | 0.84         | 4/1766 (0.2%) | 0.97        | 5/2382 (0.2%)  |
| 1   | 23-A  | 0.90         | 3/1766 (0.2%) | 1.02        | 8/2382 (0.3%)  |
| 1   | 24-A  | 0.89         | 3/1766 (0.2%) | 0.96        | 4/2382 (0.2%)  |
| 1   | 25-A  | 0.87         | 1/1766 (0.1%) | 1.00        | 4/2382 (0.2%)  |
| 1   | 26-A  | 0.91         | 4/1766 (0.2%) | 1.00        | 8/2382 (0.3%)  |
| 1   | 27-A  | 0.85         | 4/1766 (0.2%) | 1.01        | 7/2382 (0.3%)  |
| 1   | 28-A  | 0.90         | 4/1766 (0.2%) | 0.97        | 3/2382 (0.1%)  |
| 1   | 29-A  | 0.88         | 3/1766 (0.2%) | 1.02        | 7/2382 (0.3%)  |
| 1   | 30-A  | 0.87         | 3/1766 (0.2%) | 1.05        | 4/2382 (0.2%)  |
| 1   | 31-A  | 0.85         | 2/1766 (0.1%) | 0.99        | 6/2382 (0.3%)  |
| 1   | 32-A  | 0.87         | 2/1766 (0.1%) | 1.06        | 11/2382 (0.5%) |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 1   | 33-A  | 0.97         | 5/1766 (0.3%)    | 1.03        | 7/2382 (0.3%)     |
| 1   | 34-A  | 0.83         | 3/1766 (0.2%)    | 0.97        | 3/2382 (0.1%)     |
| 1   | 35-A  | 0.91         | 6/1766 (0.3%)    | 1.03        | 7/2382 (0.3%)     |
| 1   | 36-A  | 0.86         | 0/1766           | 1.01        | 5/2382 (0.2%)     |
| 1   | 37-A  | 0.89         | 3/1766 (0.2%)    | 0.96        | 2/2382 (0.1%)     |
| 1   | 38-A  | 0.88         | 3/1766 (0.2%)    | 0.96        | 4/2382 (0.2%)     |
| 1   | 39-A  | 0.85         | 3/1766 (0.2%)    | 0.99        | 5/2382 (0.2%)     |
| 1   | 40-A  | 0.82         | 1/1766 (0.1%)    | 0.97        | 4/2382 (0.2%)     |
| 1   | 41-A  | 0.87         | 4/1766 (0.2%)    | 0.99        | 7/2382 (0.3%)     |
| 1   | 42-A  | 0.75         | 0/1766           | 0.95        | 2/2382 (0.1%)     |
| 1   | 43-A  | 0.90         | 6/1766 (0.3%)    | 1.09        | 13/2382 (0.5%)    |
| 1   | 44-A  | 0.89         | 3/1766 (0.2%)    | 0.99        | 5/2382 (0.2%)     |
| 1   | 45-A  | 0.88         | 1/1766 (0.1%)    | 1.01        | 3/2382 (0.1%)     |
| 1   | 46-A  | 0.83         | 2/1766 (0.1%)    | 1.00        | 7/2382 (0.3%)     |
| 1   | 47-A  | 0.89         | 4/1766 (0.2%)    | 1.00        | 6/2382 (0.3%)     |
| All | All   | 0.89         | 159/83002 (0.2%) | 1.01        | 277/111954 (0.2%) |

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   | 2-A   | 0                   | 4                   |
| 1   | 3-A   | 0                   | 6                   |
| 1   | 4-A   | 0                   | 2                   |
| 1   | 5-A   | 0                   | 1                   |
| 1   | 6-A   | 0                   | 4                   |
| 1   | 7-A   | 0                   | 2                   |
| 1   | 8-A   | 0                   | 2                   |
| 1   | 9-A   | 0                   | 3                   |
| 1   | 10-A  | 0                   | 4                   |
| 1   | 11-A  | 0                   | 2                   |
| 1   | 12-A  | 0                   | 4                   |
| 1   | 14-A  | 0                   | 5                   |
| 1   | 15-A  | 0                   | 1                   |
| 1   | 17-A  | 0                   | 3                   |
| 1   | 18-A  | 0                   | 5                   |
| 1   | 19-A  | 0                   | 1                   |
| 1   | 22-A  | 0                   | 1                   |
| 1   | 23-A  | 0                   | 2                   |
| 1   | 25-A  | 0                   | 2                   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | 26-A  | 0                   | 1                   |
| 1   | 28-A  | 0                   | 1                   |
| 1   | 30-A  | 0                   | 1                   |
| 1   | 31-A  | 0                   | 2                   |
| 1   | 32-A  | 0                   | 1                   |
| 1   | 34-A  | 0                   | 1                   |
| 1   | 36-A  | 0                   | 1                   |
| 1   | 37-A  | 0                   | 1                   |
| 1   | 38-A  | 0                   | 2                   |
| 1   | 39-A  | 0                   | 1                   |
| 1   | 40-A  | 0                   | 2                   |
| 1   | 41-A  | 0                   | 1                   |
| 1   | 42-A  | 0                   | 5                   |
| 1   | 43-A  | 0                   | 2                   |
| 1   | 44-A  | 0                   | 1                   |
| 1   | 45-A  | 0                   | 4                   |
| 1   | 46-A  | 0                   | 4                   |
| 1   | 47-A  | 0                   | 1                   |
| All | All   | 0                   | 86                  |

All (159) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | 8-A   | 152 | VAL  | CB-CG2 | -10.82 | 1.30        | 1.52     |
| 1   | 8-A   | 73  | GLU  | CB-CG  | -10.15 | 1.32        | 1.52     |
| 1   | 41-A  | 41  | ASP  | CB-CG  | 9.69   | 1.72        | 1.51     |
| 1   | 35-A  | 164 | GLU  | CB-CG  | 9.36   | 1.70        | 1.52     |
| 1   | 21-A  | 196 | GLU  | CB-CG  | 9.32   | 1.69        | 1.52     |
| 1   | 35-A  | 164 | GLU  | CG-CD  | 9.21   | 1.65        | 1.51     |
| 1   | 35-A  | 133 | GLN  | CB-CG  | 9.09   | 1.77        | 1.52     |
| 1   | 24-A  | 90  | GLU  | CG-CD  | 8.63   | 1.65        | 1.51     |
| 1   | 32-A  | 157 | VAL  | CB-CG2 | -8.36  | 1.35        | 1.52     |
| 1   | 15-A  | 176 | THR  | CA-CB  | 8.32   | 1.75        | 1.53     |
| 1   | 43-A  | 154 | LYS  | CG-CD  | 8.10   | 1.79        | 1.52     |
| 1   | 26-A  | 128 | ASN  | CB-CG  | 8.06   | 1.69        | 1.51     |
| 1   | 28-A  | 174 | LYS  | CD-CE  | 8.05   | 1.71        | 1.51     |
| 1   | 3-A   | 85  | GLU  | CB-CG  | -8.00  | 1.36        | 1.52     |
| 1   | 38-A  | 90  | GLU  | CG-CD  | 7.93   | 1.63        | 1.51     |
| 1   | 33-A  | 90  | GLU  | CG-CD  | 7.81   | 1.63        | 1.51     |
| 1   | 11-A  | 164 | GLU  | CB-CG  | 7.76   | 1.66        | 1.52     |
| 1   | 33-A  | 161 | LEU  | CG-CD2 | -7.66  | 1.23        | 1.51     |
| 1   | 29-A  | 196 | GLU  | CD-OE2 | -7.62  | 1.17        | 1.25     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | 40-A  | 161 | LEU  | CG-CD2  | -7.55 | 1.24        | 1.51     |
| 1   | 44-A  | 177 | TYR  | CD2-CE2 | -7.47 | 1.28        | 1.39     |
| 1   | 39-A  | 196 | GLU  | CB-CG   | 7.39  | 1.66        | 1.52     |
| 1   | 33-A  | 11  | LYS  | CE-NZ   | -7.26 | 1.30        | 1.49     |
| 1   | 14-A  | 161 | LEU  | CG-CD2  | -7.25 | 1.25        | 1.51     |
| 1   | 39-A  | 88  | SER  | CB-OG   | -7.17 | 1.32        | 1.42     |
| 1   | 10-A  | 152 | VAL  | CB-CG2  | 7.14  | 1.67        | 1.52     |
| 1   | 23-A  | 161 | LEU  | CG-CD2  | -7.10 | 1.25        | 1.51     |
| 1   | 30-A  | 161 | LEU  | CG-CD2  | -7.05 | 1.25        | 1.51     |
| 1   | 13-A  | 154 | LYS  | CG-CD   | 7.02  | 1.76        | 1.52     |
| 1   | 6-A   | 78  | TYR  | CD2-CE2 | 6.96  | 1.49        | 1.39     |
| 1   | 34-A  | 196 | GLU  | CB-CG   | 6.90  | 1.65        | 1.52     |
| 1   | 26-A  | 132 | MET  | CB-CG   | 6.89  | 1.73        | 1.51     |
| 1   | 37-A  | 161 | LEU  | CG-CD2  | -6.88 | 1.26        | 1.51     |
| 1   | 7-A   | 161 | LEU  | CG-CD2  | -6.85 | 1.26        | 1.51     |
| 1   | 11-A  | 164 | GLU  | CG-CD   | 6.83  | 1.62        | 1.51     |
| 1   | 27-A  | 161 | LEU  | CG-CD2  | -6.81 | 1.26        | 1.51     |
| 1   | 47-A  | 158 | GLU  | CB-CG   | -6.79 | 1.39        | 1.52     |
| 1   | 3-A   | 85  | GLU  | CG-CD   | -6.72 | 1.41        | 1.51     |
| 1   | 19-A  | 161 | LEU  | CG-CD2  | -6.70 | 1.27        | 1.51     |
| 1   | 4-A   | 149 | GLU  | CB-CG   | 6.69  | 1.64        | 1.52     |
| 1   | 37-A  | 196 | GLU  | CG-CD   | 6.69  | 1.61        | 1.51     |
| 1   | 18-A  | 177 | TYR  | CD1-CE1 | -6.67 | 1.29        | 1.39     |
| 1   | 9-A   | 191 | VAL  | CB-CG2  | -6.64 | 1.39        | 1.52     |
| 1   | 25-A  | 196 | GLU  | CB-CG   | 6.61  | 1.64        | 1.52     |
| 1   | 17-A  | 73  | GLU  | CB-CG   | 6.59  | 1.64        | 1.52     |
| 1   | 1-A   | 81  | GLN  | CB-CG   | 6.57  | 1.70        | 1.52     |
| 1   | 2-A   | 135 | LYS  | CD-CE   | 6.56  | 1.67        | 1.51     |
| 1   | 41-A  | 90  | GLU  | CG-CD   | 6.48  | 1.61        | 1.51     |
| 1   | 22-A  | 161 | LEU  | CG-CD2  | -6.47 | 1.27        | 1.51     |
| 1   | 34-A  | 133 | GLN  | CB-CG   | 6.43  | 1.70        | 1.52     |
| 1   | 11-A  | 161 | LEU  | CG-CD2  | -6.40 | 1.28        | 1.51     |
| 1   | 3-A   | 161 | LEU  | CG-CD2  | -6.39 | 1.28        | 1.51     |
| 1   | 20-A  | 90  | GLU  | CB-CG   | -6.39 | 1.40        | 1.52     |
| 1   | 23-A  | 196 | GLU  | CG-CD   | 6.36  | 1.61        | 1.51     |
| 1   | 21-A  | 196 | GLU  | CG-CD   | 6.36  | 1.61        | 1.51     |
| 1   | 9-A   | 214 | GLU  | CB-CG   | 6.30  | 1.64        | 1.52     |
| 1   | 11-A  | 28  | GLU  | CB-CG   | 6.30  | 1.64        | 1.52     |
| 1   | 20-A  | 177 | TYR  | CD1-CE1 | -6.30 | 1.29        | 1.39     |
| 1   | 46-A  | 123 | THR  | CA-CB   | 6.26  | 1.69        | 1.53     |
| 1   | 45-A  | 161 | LEU  | CG-CD2  | -6.26 | 1.28        | 1.51     |
| 1   | 35-A  | 73  | GLU  | CB-CG   | 6.24  | 1.64        | 1.52     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | 19-A  | 74  | ASP  | CB-CG   | 6.23  | 1.64        | 1.51     |
| 1   | 18-A  | 154 | LYS  | CD-CE   | 6.23  | 1.66        | 1.51     |
| 1   | 9-A   | 196 | GLU  | CB-CG   | 6.22  | 1.64        | 1.52     |
| 1   | 26-A  | 161 | LEU  | CG-CD2  | -6.15 | 1.29        | 1.51     |
| 1   | 6-A   | 90  | GLU  | CB-CG   | 6.15  | 1.63        | 1.52     |
| 1   | 8-A   | 211 | GLU  | CB-CG   | 6.14  | 1.63        | 1.52     |
| 1   | 21-A  | 32  | LYS  | CD-CE   | 6.11  | 1.66        | 1.51     |
| 1   | 5-A   | 152 | VAL  | CB-CG2  | 6.11  | 1.65        | 1.52     |
| 1   | 11-A  | 28  | GLU  | CG-CD   | 6.08  | 1.61        | 1.51     |
| 1   | 20-A  | 135 | LYS  | CB-CG   | 6.07  | 1.69        | 1.52     |
| 1   | 44-A  | 156 | ASP  | CB-CG   | 6.05  | 1.64        | 1.51     |
| 1   | 22-A  | 149 | GLU  | CG-CD   | 6.03  | 1.60        | 1.51     |
| 1   | 22-A  | 176 | THR  | CB-CG2  | -5.99 | 1.32        | 1.52     |
| 1   | 27-A  | 138 | LYS  | CD-CE   | 5.99  | 1.66        | 1.51     |
| 1   | 6-A   | 194 | ARG  | CG-CD   | 5.96  | 1.66        | 1.51     |
| 1   | 11-A  | 196 | GLU  | CB-CG   | 5.94  | 1.63        | 1.52     |
| 1   | 7-A   | 117 | GLU  | CG-CD   | 5.92  | 1.60        | 1.51     |
| 1   | 1-A   | 177 | TYR  | CD1-CE1 | -5.92 | 1.30        | 1.39     |
| 1   | 38-A  | 157 | VAL  | CB-CG2  | 5.89  | 1.65        | 1.52     |
| 1   | 44-A  | 90  | GLU  | CB-CG   | -5.89 | 1.41        | 1.52     |
| 1   | 43-A  | 53  | SER  | CB-OG   | 5.88  | 1.49        | 1.42     |
| 1   | 33-A  | 102 | ILE  | CB-CG2  | -5.86 | 1.34        | 1.52     |
| 1   | 27-A  | 117 | GLU  | CG-CD   | 5.85  | 1.60        | 1.51     |
| 1   | 3-A   | 150 | ASP  | CB-CG   | 5.83  | 1.64        | 1.51     |
| 1   | 15-A  | 192 | ASP  | CB-CG   | -5.82 | 1.39        | 1.51     |
| 1   | 18-A  | 149 | GLU  | CG-CD   | 5.78  | 1.60        | 1.51     |
| 1   | 29-A  | 161 | LEU  | CG-CD1  | -5.78 | 1.30        | 1.51     |
| 1   | 4-A   | 152 | VAL  | CB-CG2  | 5.76  | 1.65        | 1.52     |
| 1   | 8-A   | 211 | GLU  | CG-CD   | 5.76  | 1.60        | 1.51     |
| 1   | 43-A  | 53  | SER  | CA-CB   | 5.76  | 1.61        | 1.52     |
| 1   | 3-A   | 74  | ASP  | CB-CG   | 5.74  | 1.63        | 1.51     |
| 1   | 28-A  | 102 | ILE  | CB-CG2  | -5.70 | 1.35        | 1.52     |
| 1   | 9-A   | 149 | GLU  | CG-CD   | 5.70  | 1.60        | 1.51     |
| 1   | 15-A  | 110 | GLU  | CB-CG   | 5.69  | 1.62        | 1.52     |
| 1   | 9-A   | 158 | GLU  | CB-CG   | -5.68 | 1.41        | 1.52     |
| 1   | 11-A  | 135 | LYS  | CB-CG   | 5.68  | 1.67        | 1.52     |
| 1   | 43-A  | 154 | LYS  | CD-CE   | -5.67 | 1.37        | 1.51     |
| 1   | 27-A  | 138 | LYS  | CE-NZ   | 5.65  | 1.63        | 1.49     |
| 1   | 11-A  | 53  | SER  | CA-CB   | 5.64  | 1.61        | 1.52     |
| 1   | 2-A   | 192 | ASP  | CB-CG   | -5.63 | 1.40        | 1.51     |
| 1   | 34-A  | 196 | GLU  | CG-CD   | 5.63  | 1.60        | 1.51     |
| 1   | 7-A   | 211 | GLU  | CB-CG   | 5.62  | 1.62        | 1.52     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | 30-A  | 194 | ARG  | CB-CG   | 5.60  | 1.67        | 1.52     |
| 1   | 30-A  | 194 | ARG  | CG-CD   | 5.59  | 1.66        | 1.51     |
| 1   | 43-A  | 138 | LYS  | CB-CG   | -5.58 | 1.37        | 1.52     |
| 1   | 2-A   | 177 | TYR  | CD1-CE1 | -5.55 | 1.31        | 1.39     |
| 1   | 46-A  | 123 | THR  | CB-CG2  | -5.53 | 1.34        | 1.52     |
| 1   | 4-A   | 149 | GLU  | N-CA    | 5.52  | 1.57        | 1.46     |
| 1   | 47-A  | 117 | GLU  | CG-CD   | 5.52  | 1.60        | 1.51     |
| 1   | 28-A  | 98  | GLN  | CB-CG   | 5.50  | 1.67        | 1.52     |
| 1   | 31-A  | 73  | GLU  | CB-CG   | 5.47  | 1.62        | 1.52     |
| 1   | 3-A   | 13  | ARG  | CG-CD   | 5.46  | 1.65        | 1.51     |
| 1   | 47-A  | 177 | TYR  | CD1-CE1 | -5.46 | 1.31        | 1.39     |
| 1   | 1-A   | 149 | GLU  | CG-CD   | 5.45  | 1.60        | 1.51     |
| 1   | 16-A  | 35  | GLU  | CB-CG   | 5.42  | 1.62        | 1.52     |
| 1   | 5-A   | 78  | TYR  | CB-CG   | 5.40  | 1.59        | 1.51     |
| 1   | 1-A   | 157 | VAL  | CB-CG2  | -5.39 | 1.41        | 1.52     |
| 1   | 8-A   | 176 | THR  | CB-CG2  | -5.38 | 1.34        | 1.52     |
| 1   | 38-A  | 187 | ASP  | CB-CG   | 5.38  | 1.63        | 1.51     |
| 1   | 41-A  | 157 | VAL  | CB-CG1  | -5.38 | 1.41        | 1.52     |
| 1   | 8-A   | 196 | GLU  | CB-CG   | 5.37  | 1.62        | 1.52     |
| 1   | 23-A  | 7   | GLU  | CG-CD   | 5.37  | 1.60        | 1.51     |
| 1   | 6-A   | 78  | TYR  | CB-CG   | -5.35 | 1.43        | 1.51     |
| 1   | 33-A  | 170 | ARG  | CZ-NH1  | 5.34  | 1.40        | 1.33     |
| 1   | 1-A   | 133 | GLN  | CG-CD   | 5.29  | 1.63        | 1.51     |
| 1   | 28-A  | 90  | GLU  | CG-CD   | 5.26  | 1.59        | 1.51     |
| 1   | 35-A  | 28  | GLU  | CB-CG   | 5.25  | 1.62        | 1.52     |
| 1   | 18-A  | 149 | GLU  | N-CA    | 5.24  | 1.56        | 1.46     |
| 1   | 43-A  | 194 | ARG  | CB-CG   | 5.24  | 1.66        | 1.52     |
| 1   | 18-A  | 161 | LEU  | CG-CD1  | -5.24 | 1.32        | 1.51     |
| 1   | 5-A   | 152 | VAL  | CB-CG1  | 5.23  | 1.63        | 1.52     |
| 1   | 6-A   | 161 | LEU  | CG-CD1  | -5.22 | 1.32        | 1.51     |
| 1   | 24-A  | 28  | GLU  | CB-CG   | 5.22  | 1.62        | 1.52     |
| 1   | 35-A  | 196 | GLU  | CG-CD   | 5.19  | 1.59        | 1.51     |
| 1   | 31-A  | 135 | LYS  | CE-NZ   | 5.19  | 1.62        | 1.49     |
| 1   | 41-A  | 174 | LYS  | CE-NZ   | 5.19  | 1.62        | 1.49     |
| 1   | 4-A   | 152 | VAL  | N-CA    | 5.18  | 1.56        | 1.46     |
| 1   | 9-A   | 178 | LYS  | CE-NZ   | 5.17  | 1.61        | 1.49     |
| 1   | 1-A   | 81  | GLN  | CG-CD   | 5.16  | 1.62        | 1.51     |
| 1   | 26-A  | 177 | TYR  | CD1-CE1 | -5.15 | 1.31        | 1.39     |
| 1   | 47-A  | 211 | GLU  | CB-CG   | -5.14 | 1.42        | 1.52     |
| 1   | 16-A  | 196 | GLU  | CB-CG   | 5.13  | 1.61        | 1.52     |
| 1   | 37-A  | 187 | ASP  | CB-CG   | 5.13  | 1.62        | 1.51     |
| 1   | 3-A   | 90  | GLU  | CB-CG   | 5.13  | 1.61        | 1.52     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | 32-A  | 174 | LYS  | CG-CD  | -5.12 | 1.35        | 1.52     |
| 1   | 4-A   | 152 | VAL  | CB-CG1 | 5.12  | 1.63        | 1.52     |
| 1   | 16-A  | 152 | VAL  | CB-CG2 | 5.12  | 1.63        | 1.52     |
| 1   | 17-A  | 123 | THR  | CA-CB  | 5.12  | 1.66        | 1.53     |
| 1   | 7-A   | 91  | ARG  | CZ-NH1 | 5.10  | 1.39        | 1.33     |
| 1   | 12-A  | 196 | GLU  | CG-CD  | 5.10  | 1.59        | 1.51     |
| 1   | 29-A  | 196 | GLU  | CD-OE1 | -5.10 | 1.20        | 1.25     |
| 1   | 12-A  | 90  | GLU  | CG-CD  | 5.08  | 1.59        | 1.51     |
| 1   | 18-A  | 150 | ASP  | CB-CG  | 5.07  | 1.62        | 1.51     |
| 1   | 10-A  | 146 | MET  | CG-SD  | -5.06 | 1.68        | 1.81     |
| 1   | 24-A  | 196 | GLU  | CG-CD  | 5.05  | 1.59        | 1.51     |
| 1   | 22-A  | 13  | ARG  | CG-CD  | 5.04  | 1.64        | 1.51     |
| 1   | 1-A   | 152 | VAL  | CB-CG2 | 5.04  | 1.63        | 1.52     |
| 1   | 39-A  | 196 | GLU  | CG-CD  | 5.03  | 1.59        | 1.51     |

All (277) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | 17-A  | 170 | ARG  | NE-CZ-NH1 | 14.47  | 127.53      | 120.30   |
| 1   | 13-A  | 91  | ARG  | NE-CZ-NH1 | 13.14  | 126.87      | 120.30   |
| 1   | 11-A  | 91  | ARG  | NE-CZ-NH1 | 12.58  | 126.59      | 120.30   |
| 1   | 46-A  | 55  | ASP  | CB-CG-OD1 | -12.49 | 107.06      | 118.30   |
| 1   | 3-A   | 146 | MET  | CB-CG-SD  | -11.64 | 77.48       | 112.40   |
| 1   | 21-A  | 194 | ARG  | NE-CZ-NH2 | -11.34 | 114.63      | 120.30   |
| 1   | 7-A   | 91  | ARG  | NE-CZ-NH2 | -11.06 | 114.77      | 120.30   |
| 1   | 14-A  | 153 | LEU  | CB-CG-CD1 | -10.69 | 92.83       | 111.00   |
| 1   | 11-A  | 91  | ARG  | NE-CZ-NH2 | -10.50 | 115.05      | 120.30   |
| 1   | 21-A  | 194 | ARG  | NE-CZ-NH1 | 10.49  | 125.55      | 120.30   |
| 1   | 33-A  | 170 | ARG  | NE-CZ-NH2 | -10.14 | 115.23      | 120.30   |
| 1   | 29-A  | 93  | MET  | CG-SD-CE  | 9.71   | 115.73      | 100.20   |
| 1   | 35-A  | 157 | VAL  | CB-CA-C   | -9.66  | 93.04       | 111.40   |
| 1   | 32-A  | 93  | MET  | CG-SD-CE  | 9.62   | 115.58      | 100.20   |
| 1   | 20-A  | 194 | ARG  | NE-CZ-NH1 | 9.45   | 125.02      | 120.30   |
| 1   | 43-A  | 53  | SER  | CB-CA-C   | -9.33  | 92.38       | 110.10   |
| 1   | 32-A  | 170 | ARG  | NE-CZ-NH2 | -8.96  | 115.82      | 120.30   |
| 1   | 8-A   | 172 | ASP  | CB-CG-OD1 | -8.79  | 110.39      | 118.30   |
| 1   | 17-A  | 151 | GLY  | N-CA-C    | -8.71  | 91.33       | 113.10   |
| 1   | 11-A  | 53  | SER  | N-CA-CB   | 8.59   | 123.39      | 110.50   |
| 1   | 32-A  | 156 | ASP  | CB-CG-OD1 | -8.59  | 110.57      | 118.30   |
| 1   | 33-A  | 170 | ARG  | NE-CZ-NH1 | 8.56   | 124.58      | 120.30   |
| 1   | 14-A  | 208 | ARG  | NE-CZ-NH1 | 8.51   | 124.56      | 120.30   |
| 1   | 12-A  | 150 | ASP  | CB-CG-OD1 | 8.41   | 125.87      | 118.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | 5-A   | 217 | TYR  | CB-CG-CD1  | 8.41  | 126.04      | 121.00   |
| 1   | 30-A  | 152 | VAL  | CB-CA-C    | -8.28 | 95.66       | 111.40   |
| 1   | 43-A  | 53  | SER  | N-CA-CB    | 8.24  | 122.86      | 110.50   |
| 1   | 4-A   | 149 | GLU  | N-CA-C     | 8.23  | 133.21      | 111.00   |
| 1   | 39-A  | 185 | LEU  | CA-CB-CG   | 8.21  | 134.18      | 115.30   |
| 1   | 7-A   | 138 | LYS  | CD-CE-NZ   | 8.18  | 130.52      | 111.70   |
| 1   | 36-A  | 208 | ARG  | NE-CZ-NH2  | -8.04 | 116.28      | 120.30   |
| 1   | 12-A  | 175 | THR  | CB-CA-C    | -8.03 | 89.92       | 111.60   |
| 1   | 8-A   | 152 | VAL  | CB-CA-C    | -8.01 | 96.17       | 111.40   |
| 1   | 18-A  | 194 | ARG  | NE-CZ-NH1  | 7.84  | 124.22      | 120.30   |
| 1   | 8-A   | 170 | ARG  | NE-CZ-NH2  | -7.81 | 116.40      | 120.30   |
| 1   | 43-A  | 150 | ASP  | CB-CG-OD2  | 7.79  | 125.31      | 118.30   |
| 1   | 11-A  | 152 | VAL  | N-CA-C     | -7.78 | 90.01       | 111.00   |
| 1   | 24-A  | 134 | LYS  | CD-CE-NZ   | 7.76  | 129.55      | 111.70   |
| 1   | 45-A  | 106 | ASP  | CB-CG-OD1  | 7.74  | 125.26      | 118.30   |
| 1   | 43-A  | 208 | ARG  | NE-CZ-NH1  | 7.66  | 124.13      | 120.30   |
| 1   | 42-A  | 153 | LEU  | CB-CG-CD1  | -7.64 | 98.02       | 111.00   |
| 1   | 2-A   | 174 | LYS  | CD-CE-NZ   | 7.62  | 129.23      | 111.70   |
| 1   | 33-A  | 102 | ILE  | CB-CA-C    | 7.61  | 126.83      | 111.60   |
| 1   | 5-A   | 217 | TYR  | CB-CG-CD2  | -7.57 | 116.46      | 121.00   |
| 1   | 8-A   | 161 | LEU  | CA-CB-CG   | 7.54  | 132.65      | 115.30   |
| 1   | 25-A  | 93  | MET  | CG-SD-CE   | 7.45  | 112.12      | 100.20   |
| 1   | 7-A   | 91  | ARG  | NE-CZ-NH1  | 7.39  | 123.99      | 120.30   |
| 1   | 19-A  | 159 | MET  | CG-SD-CE   | 7.36  | 111.98      | 100.20   |
| 1   | 22-A  | 151 | GLY  | N-CA-C     | -7.33 | 94.77       | 113.10   |
| 1   | 43-A  | 185 | LEU  | CA-CB-CG   | 7.31  | 132.11      | 115.30   |
| 1   | 29-A  | 196 | GLU  | OE1-CD-OE2 | -7.29 | 114.55      | 123.30   |
| 1   | 27-A  | 159 | MET  | CG-SD-CE   | -7.29 | 88.53       | 100.20   |
| 1   | 15-A  | 176 | THR  | CB-CA-C    | 7.28  | 131.26      | 111.60   |
| 1   | 10-A  | 152 | VAL  | CB-CA-C    | 7.28  | 125.22      | 111.40   |
| 1   | 40-A  | 185 | LEU  | CA-CB-CG   | 7.27  | 132.03      | 115.30   |
| 1   | 47-A  | 185 | LEU  | CB-CG-CD1  | 7.26  | 123.34      | 111.00   |
| 1   | 32-A  | 170 | ARG  | NE-CZ-NH1  | 7.24  | 123.92      | 120.30   |
| 1   | 16-A  | 161 | LEU  | CB-CG-CD1  | -7.17 | 98.82       | 111.00   |
| 1   | 11-A  | 13  | ARG  | NE-CZ-NH1  | -7.13 | 116.73      | 120.30   |
| 1   | 14-A  | 170 | ARG  | NE-CZ-NH2  | -7.13 | 116.73      | 120.30   |
| 1   | 1-A   | 154 | LYS  | CD-CE-NZ   | 7.08  | 127.99      | 111.70   |
| 1   | 43-A  | 216 | ARG  | NE-CZ-NH1  | 7.05  | 123.83      | 120.30   |
| 1   | 5-A   | 170 | ARG  | NE-CZ-NH2  | -7.02 | 116.79      | 120.30   |
| 1   | 3-A   | 194 | ARG  | NE-CZ-NH2  | -7.00 | 116.80      | 120.30   |
| 1   | 30-A  | 170 | ARG  | NE-CZ-NH2  | 6.97  | 123.79      | 120.30   |
| 1   | 24-A  | 196 | GLU  | OE1-CD-OE2 | -6.94 | 114.97      | 123.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | 4-A   | 14  | MET  | CG-SD-CE  | 6.93  | 111.28      | 100.20   |
| 1   | 26-A  | 93  | MET  | CG-SD-CE  | 6.92  | 111.28      | 100.20   |
| 1   | 24-A  | 150 | ASP  | CB-CG-OD2 | 6.89  | 124.50      | 118.30   |
| 1   | 10-A  | 194 | ARG  | NE-CZ-NH2 | -6.88 | 116.86      | 120.30   |
| 1   | 31-A  | 170 | ARG  | NE-CZ-NH1 | -6.86 | 116.87      | 120.30   |
| 1   | 11-A  | 13  | ARG  | NE-CZ-NH2 | 6.81  | 123.71      | 120.30   |
| 1   | 35-A  | 172 | ASP  | CB-CG-OD2 | -6.81 | 112.17      | 118.30   |
| 1   | 33-A  | 132 | MET  | CG-SD-CE  | 6.77  | 111.03      | 100.20   |
| 1   | 3-A   | 150 | ASP  | N-CA-C    | -6.73 | 92.84       | 111.00   |
| 1   | 7-A   | 151 | GLY  | N-CA-C    | 6.72  | 129.91      | 113.10   |
| 1   | 35-A  | 123 | THR  | CB-CA-C   | -6.72 | 93.46       | 111.60   |
| 1   | 33-A  | 193 | HIS  | CB-CA-C   | -6.71 | 96.98       | 110.40   |
| 1   | 10-A  | 208 | ARG  | NE-CZ-NH2 | -6.67 | 116.97      | 120.30   |
| 1   | 14-A  | 13  | ARG  | NE-CZ-NH1 | 6.67  | 123.63      | 120.30   |
| 1   | 47-A  | 41  | ASP  | CB-CG-OD1 | 6.63  | 124.27      | 118.30   |
| 1   | 5-A   | 217 | TYR  | CA-CB-CG  | 6.63  | 125.99      | 113.40   |
| 1   | 43-A  | 208 | ARG  | NE-CZ-NH2 | -6.63 | 116.99      | 120.30   |
| 1   | 14-A  | 154 | LYS  | N-CA-CB   | 6.61  | 122.49      | 110.60   |
| 1   | 39-A  | 185 | LEU  | CB-CG-CD2 | 6.58  | 122.19      | 111.00   |
| 1   | 44-A  | 152 | VAL  | N-CA-C    | -6.52 | 93.39       | 111.00   |
| 1   | 6-A   | 175 | THR  | CB-CA-C   | -6.48 | 94.11       | 111.60   |
| 1   | 47-A  | 152 | VAL  | N-CA-C    | -6.47 | 93.53       | 111.00   |
| 1   | 44-A  | 138 | LYS  | CD-CE-NZ  | 6.46  | 126.57      | 111.70   |
| 1   | 8-A   | 158 | GLU  | CB-CA-C   | -6.46 | 97.47       | 110.40   |
| 1   | 13-A  | 161 | LEU  | CB-CG-CD1 | 6.46  | 121.97      | 111.00   |
| 1   | 37-A  | 93  | MET  | CG-SD-CE  | 6.44  | 110.50      | 100.20   |
| 1   | 2-A   | 151 | GLY  | N-CA-C    | -6.41 | 97.07       | 113.10   |
| 1   | 23-A  | 170 | ARG  | NE-CZ-NH2 | -6.41 | 117.10      | 120.30   |
| 1   | 32-A  | 106 | ASP  | CB-CG-OD2 | 6.41  | 124.06      | 118.30   |
| 1   | 3-A   | 161 | LEU  | CB-CG-CD2 | -6.40 | 100.11      | 111.00   |
| 1   | 28-A  | 102 | ILE  | CB-CA-C   | 6.38  | 124.37      | 111.60   |
| 1   | 37-A  | 53  | SER  | N-CA-CB   | 6.34  | 120.00      | 110.50   |
| 1   | 29-A  | 190 | GLU  | CB-CA-C   | -6.32 | 97.75       | 110.40   |
| 1   | 9-A   | 191 | VAL  | CB-CA-C   | -6.31 | 99.42       | 111.40   |
| 1   | 45-A  | 55  | ASP  | CB-CG-OD1 | -6.27 | 112.66      | 118.30   |
| 1   | 1-A   | 185 | LEU  | CB-CG-CD2 | -6.26 | 100.36      | 111.00   |
| 1   | 46-A  | 53  | SER  | N-CA-CB   | -6.26 | 101.12      | 110.50   |
| 1   | 46-A  | 21  | HIS  | CB-CA-C   | 6.24  | 122.87      | 110.40   |
| 1   | 23-A  | 91  | ARG  | NE-CZ-NH2 | -6.18 | 117.21      | 120.30   |
| 1   | 26-A  | 156 | ASP  | CB-CG-OD2 | -6.17 | 112.75      | 118.30   |
| 1   | 13-A  | 91  | ARG  | NE-CZ-NH2 | -6.16 | 117.22      | 120.30   |
| 1   | 31-A  | 161 | LEU  | CA-CB-CG  | 6.15  | 129.44      | 115.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | 14-A  | 170 | ARG  | NE-CZ-NH1  | 6.13  | 123.36      | 120.30   |
| 1   | 8-A   | 100 | ILE  | CB-CA-C    | -6.12 | 99.37       | 111.60   |
| 1   | 20-A  | 156 | ASP  | CB-CG-OD1  | -6.12 | 112.79      | 118.30   |
| 1   | 19-A  | 147 | TYR  | CA-CB-CG   | 6.10  | 125.00      | 113.40   |
| 1   | 27-A  | 161 | LEU  | CB-CG-CD2  | -6.10 | 100.63      | 111.00   |
| 1   | 44-A  | 102 | ILE  | CB-CA-C    | -6.09 | 99.43       | 111.60   |
| 1   | 41-A  | 41  | ASP  | CB-CG-OD1  | 6.07  | 123.76      | 118.30   |
| 1   | 28-A  | 208 | ARG  | NE-CZ-NH1  | 6.06  | 123.33      | 120.30   |
| 1   | 8-A   | 170 | ARG  | NE-CZ-NH1  | 6.05  | 123.33      | 120.30   |
| 1   | 11-A  | 91  | ARG  | CD-NE-CZ   | 6.05  | 132.07      | 123.60   |
| 1   | 3-A   | 150 | ASP  | CB-CG-OD1  | 6.05  | 123.74      | 118.30   |
| 1   | 5-A   | 170 | ARG  | NE-CZ-NH1  | 6.04  | 123.32      | 120.30   |
| 1   | 34-A  | 90  | GLU  | OE1-CD-OE2 | -6.03 | 116.06      | 123.30   |
| 1   | 10-A  | 192 | ASP  | CB-CG-OD1  | -6.03 | 112.88      | 118.30   |
| 1   | 32-A  | 13  | ARG  | NE-CZ-NH1  | 6.03  | 123.31      | 120.30   |
| 1   | 14-A  | 20  | GLY  | N-CA-C     | -6.02 | 98.06       | 113.10   |
| 1   | 32-A  | 106 | ASP  | CB-CG-OD1  | -5.99 | 112.91      | 118.30   |
| 1   | 43-A  | 156 | ASP  | CB-CA-C    | 5.98  | 122.37      | 110.40   |
| 1   | 20-A  | 147 | TYR  | CA-CB-CG   | 5.96  | 124.72      | 113.40   |
| 1   | 25-A  | 156 | ASP  | N-CA-CB    | 5.96  | 121.32      | 110.60   |
| 1   | 13-A  | 146 | MET  | CG-SD-CE   | -5.96 | 90.67       | 100.20   |
| 1   | 15-A  | 161 | LEU  | CB-CG-CD2  | -5.94 | 100.90      | 111.00   |
| 1   | 29-A  | 194 | ARG  | NE-CZ-NH1  | 5.94  | 123.27      | 120.30   |
| 1   | 41-A  | 161 | LEU  | CB-CG-CD2  | -5.91 | 100.95      | 111.00   |
| 1   | 46-A  | 3   | VAL  | N-CA-C     | 5.91  | 126.96      | 111.00   |
| 1   | 3-A   | 150 | ASP  | CB-CA-C    | 5.91  | 122.22      | 110.40   |
| 1   | 26-A  | 194 | ARG  | NE-CZ-NH2  | -5.90 | 117.35      | 120.30   |
| 1   | 29-A  | 74  | ASP  | N-CA-CB    | -5.89 | 100.00      | 110.60   |
| 1   | 36-A  | 159 | MET  | CG-SD-CE   | -5.89 | 90.78       | 100.20   |
| 1   | 42-A  | 150 | ASP  | N-CA-C     | -5.89 | 95.11       | 111.00   |
| 1   | 13-A  | 91  | ARG  | CB-CA-C    | -5.88 | 98.63       | 110.40   |
| 1   | 26-A  | 124 | ASN  | CA-C-N     | -5.88 | 104.27      | 117.20   |
| 1   | 33-A  | 152 | VAL  | N-CA-C     | -5.86 | 95.19       | 111.00   |
| 1   | 47-A  | 149 | GLU  | CB-CA-C    | 5.85  | 122.11      | 110.40   |
| 1   | 23-A  | 138 | LYS  | CD-CE-NZ   | 5.85  | 125.15      | 111.70   |
| 1   | 4-A   | 170 | ARG  | NE-CZ-NH1  | -5.84 | 117.38      | 120.30   |
| 1   | 17-A  | 170 | ARG  | NE-CZ-NH2  | -5.84 | 117.38      | 120.30   |
| 1   | 20-A  | 194 | ARG  | NE-CZ-NH2  | -5.83 | 117.38      | 120.30   |
| 1   | 23-A  | 153 | LEU  | CB-CG-CD2  | -5.80 | 101.13      | 111.00   |
| 1   | 13-A  | 74  | ASP  | CB-CG-OD1  | 5.79  | 123.51      | 118.30   |
| 1   | 16-A  | 149 | GLU  | N-CA-C     | 5.78  | 126.61      | 111.00   |
| 1   | 43-A  | 149 | GLU  | N-CA-C     | -5.78 | 95.40       | 111.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | 46-A  | 132 | MET  | CG-SD-CE   | -5.77 | 90.97       | 100.20   |
| 1   | 35-A  | 90  | GLU  | CB-CA-C    | 5.75  | 121.91      | 110.40   |
| 1   | 29-A  | 149 | GLU  | N-CA-C     | -5.74 | 95.50       | 111.00   |
| 1   | 5-A   | 161 | LEU  | CB-CG-CD1  | 5.73  | 120.75      | 111.00   |
| 1   | 41-A  | 208 | ARG  | NE-CZ-NH2  | -5.73 | 117.43      | 120.30   |
| 1   | 22-A  | 100 | ILE  | CB-CA-C    | -5.73 | 100.15      | 111.60   |
| 1   | 5-A   | 153 | LEU  | CB-CG-CD2  | 5.72  | 120.73      | 111.00   |
| 1   | 20-A  | 119 | ARG  | NE-CZ-NH2  | -5.72 | 117.44      | 120.30   |
| 1   | 33-A  | 192 | ASP  | CB-CG-OD1  | 5.72  | 123.45      | 118.30   |
| 1   | 12-A  | 161 | LEU  | CB-CG-CD1  | 5.71  | 120.71      | 111.00   |
| 1   | 23-A  | 170 | ARG  | NE-CZ-NH1  | 5.71  | 123.16      | 120.30   |
| 1   | 38-A  | 50  | LEU  | CB-CG-CD1  | 5.71  | 120.71      | 111.00   |
| 1   | 4-A   | 151 | GLY  | N-CA-C     | -5.69 | 98.87       | 113.10   |
| 1   | 34-A  | 153 | LEU  | CB-CG-CD2  | 5.67  | 120.65      | 111.00   |
| 1   | 11-A  | 146 | MET  | CA-CB-CG   | 5.66  | 122.92      | 113.30   |
| 1   | 5-A   | 194 | ARG  | NE-CZ-NH1  | 5.65  | 123.12      | 120.30   |
| 1   | 47-A  | 161 | LEU  | CB-CG-CD1  | 5.62  | 120.55      | 111.00   |
| 1   | 19-A  | 102 | ILE  | CB-CA-C    | -5.60 | 100.39      | 111.60   |
| 1   | 5-A   | 156 | ASP  | CB-CG-OD1  | 5.60  | 123.34      | 118.30   |
| 1   | 19-A  | 193 | HIS  | CB-CA-C    | -5.60 | 99.20       | 110.40   |
| 1   | 41-A  | 208 | ARG  | NE-CZ-NH1  | 5.60  | 123.10      | 120.30   |
| 1   | 23-A  | 208 | ARG  | NE-CZ-NH1  | 5.60  | 123.10      | 120.30   |
| 1   | 21-A  | 196 | GLU  | CA-CB-CG   | 5.59  | 125.70      | 113.40   |
| 1   | 11-A  | 154 | LYS  | CD-CE-NZ   | 5.54  | 124.44      | 111.70   |
| 1   | 32-A  | 150 | ASP  | CB-CG-OD1  | 5.54  | 123.28      | 118.30   |
| 1   | 26-A  | 125 | PHE  | N-CA-C     | -5.53 | 96.06       | 111.00   |
| 1   | 30-A  | 143 | THR  | N-CA-C     | -5.51 | 96.12       | 111.00   |
| 1   | 43-A  | 161 | LEU  | CB-CG-CD1  | 5.50  | 120.36      | 111.00   |
| 1   | 8-A   | 106 | ASP  | CB-CG-OD1  | -5.50 | 113.35      | 118.30   |
| 1   | 7-A   | 161 | LEU  | CB-CG-CD2  | -5.49 | 101.67      | 111.00   |
| 1   | 11-A  | 164 | GLU  | OE1-CD-OE2 | -5.49 | 116.72      | 123.30   |
| 1   | 18-A  | 161 | LEU  | CB-CG-CD1  | -5.48 | 101.68      | 111.00   |
| 1   | 18-A  | 150 | ASP  | CB-CA-C    | 5.47  | 121.34      | 110.40   |
| 1   | 25-A  | 100 | ILE  | CG1-CB-CG2 | -5.45 | 99.42       | 111.40   |
| 1   | 45-A  | 98  | GLN  | CA-CB-CG   | 5.45  | 125.38      | 113.40   |
| 1   | 27-A  | 153 | LEU  | CA-CB-CG   | 5.44  | 127.82      | 115.30   |
| 1   | 40-A  | 157 | VAL  | CB-CA-C    | -5.44 | 101.06      | 111.40   |
| 1   | 6-A   | 156 | ASP  | CB-CG-OD1  | 5.43  | 123.19      | 118.30   |
| 1   | 41-A  | 158 | GLU  | CA-CB-CG   | 5.42  | 125.33      | 113.40   |
| 1   | 20-A  | 159 | MET  | CG-SD-CE   | -5.42 | 91.53       | 100.20   |
| 1   | 13-A  | 78  | TYR  | OH-CZ-CE2  | -5.42 | 105.48      | 120.10   |
| 1   | 27-A  | 153 | LEU  | CB-CA-C    | 5.42  | 120.49      | 110.20   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | 31-A  | 185 | LEU  | CA-CB-CG  | 5.41  | 127.75      | 115.30   |
| 1   | 8-A   | 153 | LEU  | CB-CG-CD2 | -5.41 | 101.80      | 111.00   |
| 1   | 26-A  | 3   | VAL  | CB-CA-C   | -5.38 | 101.18      | 111.40   |
| 1   | 10-A  | 208 | ARG  | NE-CZ-NH1 | 5.38  | 122.99      | 120.30   |
| 1   | 27-A  | 138 | LYS  | CD-CE-NZ  | 5.38  | 124.07      | 111.70   |
| 1   | 19-A  | 161 | LEU  | CB-CG-CD2 | -5.37 | 101.87      | 111.00   |
| 1   | 6-A   | 161 | LEU  | CB-CG-CD1 | -5.37 | 101.88      | 111.00   |
| 1   | 7-A   | 13  | ARG  | NE-CZ-NH1 | 5.36  | 122.98      | 120.30   |
| 1   | 44-A  | 41  | ASP  | CB-CG-OD1 | 5.36  | 123.12      | 118.30   |
| 1   | 28-A  | 174 | LYS  | CD-CE-NZ  | 5.36  | 124.02      | 111.70   |
| 1   | 32-A  | 161 | LEU  | CA-CB-CG  | 5.36  | 127.62      | 115.30   |
| 1   | 43-A  | 216 | ARG  | NE-CZ-NH2 | -5.35 | 117.62      | 120.30   |
| 1   | 38-A  | 161 | LEU  | CA-CB-CG  | 5.35  | 127.61      | 115.30   |
| 1   | 3-A   | 173 | PHE  | CB-CG-CD2 | -5.33 | 117.07      | 120.80   |
| 1   | 32-A  | 161 | LEU  | CB-CG-CD1 | 5.33  | 120.05      | 111.00   |
| 1   | 40-A  | 41  | ASP  | CB-CG-OD1 | 5.32  | 123.09      | 118.30   |
| 1   | 25-A  | 161 | LEU  | CB-CG-CD1 | 5.30  | 120.01      | 111.00   |
| 1   | 41-A  | 41  | ASP  | N-CA-CB   | 5.29  | 120.12      | 110.60   |
| 1   | 39-A  | 100 | ILE  | CB-CA-C   | -5.29 | 101.02      | 111.60   |
| 1   | 11-A  | 129 | GLY  | N-CA-C    | 5.29  | 126.32      | 113.10   |
| 1   | 46-A  | 161 | LEU  | CA-CB-CG  | 5.28  | 127.45      | 115.30   |
| 1   | 4-A   | 217 | TYR  | CA-CB-CG  | 5.28  | 123.43      | 113.40   |
| 1   | 26-A  | 156 | ASP  | CB-CG-OD1 | 5.27  | 123.04      | 118.30   |
| 1   | 1-A   | 157 | VAL  | CB-CA-C   | -5.27 | 101.39      | 111.40   |
| 1   | 38-A  | 90  | GLU  | CB-CA-C   | 5.26  | 120.92      | 110.40   |
| 1   | 39-A  | 53  | SER  | CB-CA-C   | -5.26 | 100.11      | 110.10   |
| 1   | 21-A  | 156 | ASP  | CB-CG-OD1 | 5.25  | 123.03      | 118.30   |
| 1   | 27-A  | 98  | GLN  | CB-CA-C   | -5.25 | 99.89       | 110.40   |
| 1   | 46-A  | 146 | MET  | CB-CG-SD  | 5.25  | 128.16      | 112.40   |
| 1   | 1-A   | 161 | LEU  | CA-CB-CG  | 5.23  | 127.34      | 115.30   |
| 1   | 14-A  | 154 | LYS  | CB-CG-CD  | 5.23  | 125.20      | 111.60   |
| 1   | 41-A  | 90  | GLU  | CB-CA-C   | -5.23 | 99.94       | 110.40   |
| 1   | 38-A  | 208 | ARG  | NE-CZ-NH2 | -5.23 | 117.69      | 120.30   |
| 1   | 40-A  | 106 | ASP  | CB-CA-C   | 5.23  | 120.85      | 110.40   |
| 1   | 16-A  | 217 | TYR  | CA-CB-CG  | 5.21  | 123.31      | 113.40   |
| 1   | 35-A  | 133 | GLN  | CA-CB-CG  | 5.21  | 124.87      | 113.40   |
| 1   | 6-A   | 150 | ASP  | CB-CG-OD2 | 5.21  | 122.99      | 118.30   |
| 1   | 22-A  | 13  | ARG  | NE-CZ-NH1 | 5.20  | 122.90      | 120.30   |
| 1   | 4-A   | 153 | LEU  | CB-CG-CD1 | 5.20  | 119.84      | 111.00   |
| 1   | 35-A  | 161 | LEU  | CA-CB-CG  | 5.19  | 127.24      | 115.30   |
| 1   | 27-A  | 173 | PHE  | CB-CG-CD2 | -5.19 | 117.17      | 120.80   |
| 1   | 10-A  | 194 | ARG  | NE-CZ-NH1 | 5.19  | 122.89      | 120.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | 24-A  | 90  | GLU  | OE1-CD-OE2 | -5.19 | 117.08      | 123.30   |
| 1   | 19-A  | 146 | MET  | CB-CG-SD   | -5.18 | 96.84       | 112.40   |
| 1   | 23-A  | 161 | LEU  | CB-CG-CD2  | -5.18 | 102.20      | 111.00   |
| 1   | 31-A  | 152 | VAL  | CA-CB-CG2  | 5.18  | 118.66      | 110.90   |
| 1   | 1-A   | 178 | LYS  | N-CA-C     | 5.16  | 124.93      | 111.00   |
| 1   | 47-A  | 173 | PHE  | CB-CA-C    | -5.16 | 100.08      | 110.40   |
| 1   | 3-A   | 74  | ASP  | CB-CG-OD2  | 5.16  | 122.94      | 118.30   |
| 1   | 34-A  | 194 | ARG  | CG-CD-NE   | 5.15  | 122.62      | 111.80   |
| 1   | 39-A  | 88  | SER  | CB-CA-C    | -5.15 | 100.31      | 110.10   |
| 1   | 43-A  | 210 | TYR  | CA-CB-CG   | 5.15  | 123.18      | 113.40   |
| 1   | 26-A  | 125 | PHE  | N-CA-CB    | -5.14 | 101.34      | 110.60   |
| 1   | 36-A  | 208 | ARG  | NE-CZ-NH1  | 5.14  | 122.87      | 120.30   |
| 1   | 6-A   | 74  | ASP  | CB-CG-OD1  | -5.14 | 113.67      | 118.30   |
| 1   | 14-A  | 146 | MET  | CG-SD-CE   | 5.14  | 108.42      | 100.20   |
| 1   | 18-A  | 194 | ARG  | NE-CZ-NH2  | -5.14 | 117.73      | 120.30   |
| 1   | 30-A  | 132 | MET  | CB-CG-SD   | 5.14  | 127.81      | 112.40   |
| 1   | 7-A   | 170 | ARG  | NE-CZ-NH1  | -5.13 | 117.73      | 120.30   |
| 1   | 32-A  | 153 | LEU  | CA-CB-CG   | 5.13  | 127.11      | 115.30   |
| 1   | 43-A  | 161 | LEU  | CA-CB-CG   | 5.13  | 127.11      | 115.30   |
| 1   | 19-A  | 153 | LEU  | CB-CG-CD1  | -5.13 | 102.28      | 111.00   |
| 1   | 22-A  | 217 | TYR  | N-CA-CB    | 5.13  | 119.84      | 110.60   |
| 1   | 5-A   | 161 | LEU  | CA-CB-CG   | 5.13  | 127.09      | 115.30   |
| 1   | 1-A   | 81  | GLN  | CB-CG-CD   | 5.12  | 124.91      | 111.60   |
| 1   | 13-A  | 106 | ASP  | CB-CG-OD1  | 5.12  | 122.91      | 118.30   |
| 1   | 29-A  | 194 | ARG  | NE-CZ-NH2  | -5.12 | 117.74      | 120.30   |
| 1   | 31-A  | 161 | LEU  | CB-CG-CD1  | 5.11  | 119.69      | 111.00   |
| 1   | 11-A  | 193 | HIS  | CB-CA-C    | -5.10 | 100.19      | 110.40   |
| 1   | 36-A  | 66  | ARG  | NE-CZ-NH2  | 5.10  | 122.85      | 120.30   |
| 1   | 31-A  | 93  | MET  | CG-SD-CE   | -5.09 | 92.06       | 100.20   |
| 1   | 20-A  | 161 | LEU  | CA-CB-CG   | 5.08  | 126.98      | 115.30   |
| 1   | 23-A  | 152 | VAL  | N-CA-C     | 5.07  | 124.68      | 111.00   |
| 1   | 35-A  | 157 | VAL  | CG1-CB-CG2 | 5.07  | 119.00      | 110.90   |
| 1   | 6-A   | 149 | GLU  | N-CA-C     | 5.06  | 124.67      | 111.00   |
| 1   | 22-A  | 80  | LYS  | CD-CE-NZ   | -5.06 | 100.06      | 111.70   |
| 1   | 2-A   | 135 | LYS  | CD-CE-NZ   | 5.06  | 123.34      | 111.70   |
| 1   | 36-A  | 146 | MET  | CG-SD-CE   | -5.06 | 92.10       | 100.20   |
| 1   | 3-A   | 194 | ARG  | NE-CZ-NH1  | 5.05  | 122.82      | 120.30   |
| 1   | 18-A  | 149 | GLU  | N-CA-C     | 5.05  | 124.62      | 111.00   |
| 1   | 19-A  | 153 | LEU  | N-CA-C     | 5.04  | 124.62      | 111.00   |
| 1   | 44-A  | 146 | MET  | CG-SD-CE   | 5.04  | 108.26      | 100.20   |
| 1   | 5-A   | 194 | ARG  | NE-CZ-NH2  | -5.03 | 117.78      | 120.30   |
| 1   | 19-A  | 153 | LEU  | CB-CA-C    | -5.03 | 100.64      | 110.20   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 1   | 8-A   | 146 | MET  | CB-CG-SD | 5.01 | 127.44      | 112.40   |

There are no chirality outliers.

All (86) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | 10-A  | 129 | GLY  | Peptide   |
| 1   | 10-A  | 148 | VAL  | Peptide   |
| 1   | 10-A  | 149 | GLU  | Peptide   |
| 1   | 10-A  | 61  | PHE  | Mainchain |
| 1   | 11-A  | 149 | GLU  | Peptide   |
| 1   | 11-A  | 61  | PHE  | Mainchain |
| 1   | 12-A  | 128 | ASN  | Peptide   |
| 1   | 12-A  | 149 | GLU  | Peptide   |
| 1   | 12-A  | 2   | SER  | Peptide   |
| 1   | 12-A  | 74  | ASP  | Peptide   |
| 1   | 14-A  | 149 | GLU  | Peptide   |
| 1   | 14-A  | 150 | ASP  | Peptide   |
| 1   | 14-A  | 151 | GLY  | Peptide   |
| 1   | 14-A  | 19  | ASN  | Peptide   |
| 1   | 14-A  | 21  | HIS  | Peptide   |
| 1   | 15-A  | 216 | ARG  | Peptide   |
| 1   | 17-A  | 148 | VAL  | Peptide   |
| 1   | 17-A  | 216 | ARG  | Peptide   |
| 1   | 17-A  | 61  | PHE  | Mainchain |
| 1   | 18-A  | 148 | VAL  | Peptide   |
| 1   | 18-A  | 150 | ASP  | Peptide   |
| 1   | 18-A  | 152 | VAL  | Peptide   |
| 1   | 18-A  | 2   | SER  | Peptide   |
| 1   | 18-A  | 98  | GLN  | Peptide   |
| 1   | 19-A  | 149 | GLU  | Peptide   |
| 1   | 2-A   | 149 | GLU  | Peptide   |
| 1   | 2-A   | 150 | ASP  | Peptide   |
| 1   | 2-A   | 179 | ALA  | Peptide   |
| 1   | 2-A   | 2   | SER  | Peptide   |
| 1   | 22-A  | 216 | ARG  | Peptide   |
| 1   | 23-A  | 150 | ASP  | Peptide   |
| 1   | 23-A  | 151 | GLY  | Peptide   |
| 1   | 25-A  | 149 | GLU  | Peptide   |
| 1   | 25-A  | 152 | VAL  | Peptide   |
| 1   | 26-A  | 123 | THR  | Peptide   |
| 1   | 28-A  | 2   | SER  | Peptide   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | 3-A   | 148 | VAL  | Peptide   |
| 1   | 3-A   | 150 | ASP  | Peptide   |
| 1   | 3-A   | 151 | GLY  | Peptide   |
| 1   | 3-A   | 178 | LYS  | Peptide   |
| 1   | 3-A   | 2   | SER  | Peptide   |
| 1   | 3-A   | 3   | VAL  | Peptide   |
| 1   | 30-A  | 73  | GLU  | Peptide   |
| 1   | 31-A  | 150 | ASP  | Peptide   |
| 1   | 31-A  | 216 | ARG  | Peptide   |
| 1   | 32-A  | 151 | GLY  | Peptide   |
| 1   | 34-A  | 61  | PHE  | Mainchain |
| 1   | 36-A  | 150 | ASP  | Peptide   |
| 1   | 37-A  | 149 | GLU  | Peptide   |
| 1   | 38-A  | 74  | ASP  | Peptide   |
| 1   | 38-A  | 90  | GLU  | Peptide   |
| 1   | 39-A  | 88  | SER  | Peptide   |
| 1   | 4-A   | 148 | VAL  | Peptide   |
| 1   | 4-A   | 150 | ASP  | Peptide   |
| 1   | 40-A  | 216 | ARG  | Peptide   |
| 1   | 40-A  | 61  | PHE  | Mainchain |
| 1   | 41-A  | 61  | PHE  | Mainchain |
| 1   | 42-A  | 149 | GLU  | Peptide   |
| 1   | 42-A  | 150 | ASP  | Peptide   |
| 1   | 42-A  | 21  | HIS  | Peptide   |
| 1   | 42-A  | 61  | PHE  | Mainchain |
| 1   | 42-A  | 98  | GLN  | Peptide   |
| 1   | 43-A  | 20  | GLY  | Peptide   |
| 1   | 43-A  | 74  | ASP  | Peptide   |
| 1   | 44-A  | 149 | GLU  | Peptide   |
| 1   | 45-A  | 123 | THR  | Peptide   |
| 1   | 45-A  | 149 | GLU  | Peptide   |
| 1   | 45-A  | 152 | VAL  | Peptide   |
| 1   | 45-A  | 18  | VAL  | Peptide   |
| 1   | 46-A  | 149 | GLU  | Peptide   |
| 1   | 46-A  | 192 | ASP  | Peptide   |
| 1   | 46-A  | 20  | GLY  | Peptide   |
| 1   | 46-A  | 216 | ARG  | Peptide   |
| 1   | 47-A  | 155 | GLY  | Peptide   |
| 1   | 5-A   | 148 | VAL  | Peptide   |
| 1   | 6-A   | 148 | VAL  | Peptide   |
| 1   | 6-A   | 149 | GLU  | Peptide   |
| 1   | 6-A   | 27  | GLY  | Peptide   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | 6-A   | 98  | GLN  | Peptide |
| 1   | 7-A   | 148 | VAL  | Peptide |
| 1   | 7-A   | 149 | GLU  | Peptide |
| 1   | 8-A   | 148 | VAL  | Peptide |
| 1   | 8-A   | 149 | GLU  | Peptide |
| 1   | 9-A   | 148 | VAL  | Peptide |
| 1   | 9-A   | 149 | GLU  | Peptide |
| 1   | 9-A   | 2   | SER  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1-A   | 1745  | 1665     | 1678     | 0       | 0            |
| 1   | 2-A   | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 3-A   | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 4-A   | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 5-A   | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 6-A   | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 7-A   | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 8-A   | 1745  | 1665     | 1677     | 0       | 0            |
| 1   | 9-A   | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 10-A  | 1745  | 1665     | 1678     | 0       | 0            |
| 1   | 11-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 12-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 13-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 14-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 15-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 16-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 17-A  | 1745  | 1665     | 1678     | 0       | 0            |
| 1   | 18-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 19-A  | 1745  | 1665     | 1678     | 0       | 0            |
| 1   | 20-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 21-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 22-A  | 1745  | 1665     | 1678     | 0       | 0            |
| 1   | 23-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 24-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 25-A  | 1745  | 1665     | 1679     | 0       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 26-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 27-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 28-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 29-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 30-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 31-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 32-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 33-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 34-A  | 1745  | 1665     | 1678     | 0       | 0            |
| 1   | 35-A  | 1745  | 1665     | 1678     | 0       | 0            |
| 1   | 36-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 37-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 38-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 39-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 40-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 41-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 42-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 43-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 44-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 45-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 46-A  | 1745  | 1665     | 1679     | 0       | 0            |
| 1   | 47-A  | 1745  | 1665     | 1678     | 0       | 0            |
| 2   | 1-A   | 165   | 0        | 0        | 0       | 0            |
| 2   | 2-A   | 173   | 0        | 0        | 0       | 0            |
| 2   | 3-A   | 140   | 0        | 0        | 0       | 0            |
| 2   | 4-A   | 153   | 0        | 0        | 0       | 0            |
| 2   | 5-A   | 167   | 0        | 0        | 0       | 0            |
| 2   | 6-A   | 150   | 0        | 0        | 0       | 0            |
| 2   | 7-A   | 150   | 0        | 0        | 0       | 0            |
| 2   | 8-A   | 160   | 0        | 0        | 0       | 0            |
| 2   | 9-A   | 160   | 0        | 0        | 0       | 0            |
| 2   | 10-A  | 152   | 0        | 0        | 0       | 0            |
| 2   | 11-A  | 173   | 0        | 0        | 0       | 0            |
| 2   | 12-A  | 160   | 0        | 0        | 0       | 0            |
| 2   | 13-A  | 152   | 0        | 0        | 0       | 0            |
| 2   | 14-A  | 157   | 0        | 0        | 0       | 0            |
| 2   | 15-A  | 148   | 0        | 0        | 0       | 0            |
| 2   | 16-A  | 152   | 0        | 0        | 0       | 0            |
| 2   | 17-A  | 147   | 0        | 0        | 0       | 0            |
| 2   | 18-A  | 156   | 0        | 0        | 0       | 0            |
| 2   | 19-A  | 151   | 0        | 0        | 0       | 0            |
| 2   | 20-A  | 147   | 0        | 0        | 0       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | 21-A  | 148   | 0        | 0        | 0       | 0            |
| 2   | 22-A  | 169   | 0        | 0        | 0       | 0            |
| 2   | 23-A  | 144   | 0        | 0        | 0       | 0            |
| 2   | 24-A  | 138   | 0        | 0        | 0       | 0            |
| 2   | 25-A  | 149   | 0        | 0        | 0       | 0            |
| 2   | 26-A  | 143   | 0        | 0        | 0       | 0            |
| 2   | 27-A  | 148   | 0        | 0        | 0       | 0            |
| 2   | 28-A  | 165   | 0        | 0        | 0       | 0            |
| 2   | 29-A  | 146   | 0        | 0        | 0       | 0            |
| 2   | 30-A  | 165   | 0        | 0        | 0       | 0            |
| 2   | 31-A  | 163   | 0        | 0        | 0       | 0            |
| 2   | 32-A  | 163   | 0        | 0        | 0       | 0            |
| 2   | 33-A  | 154   | 0        | 0        | 0       | 0            |
| 2   | 34-A  | 147   | 0        | 0        | 0       | 0            |
| 2   | 35-A  | 135   | 0        | 0        | 0       | 0            |
| 2   | 36-A  | 160   | 0        | 0        | 0       | 0            |
| 2   | 37-A  | 156   | 0        | 0        | 0       | 0            |
| 2   | 38-A  | 149   | 0        | 0        | 0       | 0            |
| 2   | 39-A  | 154   | 0        | 0        | 0       | 0            |
| 2   | 40-A  | 164   | 0        | 0        | 0       | 0            |
| 2   | 41-A  | 156   | 0        | 0        | 0       | 0            |
| 2   | 42-A  | 142   | 0        | 0        | 0       | 0            |
| 2   | 43-A  | 162   | 0        | 0        | 0       | 0            |
| 2   | 44-A  | 159   | 0        | 0        | 0       | 0            |
| 2   | 45-A  | 143   | 0        | 0        | 0       | 0            |
| 2   | 46-A  | 174   | 0        | 0        | 0       | 0            |
| 2   | 47-A  | 162   | 0        | 0        | 0       | 0            |
| All | All   | 89286 | 78255    | 78903    | 0       | 0            |

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

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles [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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1   | 1-A   | 211/229 (92%) | 196 (93%) | 9 (4%)  | 6 (3%)   | 5           | 0  |
| 1   | 2-A   | 211/229 (92%) | 195 (92%) | 13 (6%) | 3 (1%)   | 11          | 1  |
| 1   | 3-A   | 211/229 (92%) | 194 (92%) | 11 (5%) | 6 (3%)   | 5           | 0  |
| 1   | 4-A   | 211/229 (92%) | 200 (95%) | 7 (3%)  | 4 (2%)   | 8           | 0  |
| 1   | 5-A   | 211/229 (92%) | 200 (95%) | 5 (2%)  | 6 (3%)   | 5           | 0  |
| 1   | 6-A   | 211/229 (92%) | 196 (93%) | 6 (3%)  | 9 (4%)   | 2           | 0  |
| 1   | 7-A   | 211/229 (92%) | 199 (94%) | 8 (4%)  | 4 (2%)   | 8           | 0  |
| 1   | 8-A   | 211/229 (92%) | 201 (95%) | 3 (1%)  | 7 (3%)   | 4           | 0  |
| 1   | 9-A   | 211/229 (92%) | 200 (95%) | 7 (3%)  | 4 (2%)   | 8           | 0  |
| 1   | 10-A  | 211/229 (92%) | 202 (96%) | 7 (3%)  | 2 (1%)   | 17          | 4  |
| 1   | 11-A  | 211/229 (92%) | 199 (94%) | 9 (4%)  | 3 (1%)   | 11          | 1  |
| 1   | 12-A  | 211/229 (92%) | 198 (94%) | 11 (5%) | 2 (1%)   | 17          | 4  |
| 1   | 13-A  | 211/229 (92%) | 197 (93%) | 10 (5%) | 4 (2%)   | 8           | 0  |
| 1   | 14-A  | 211/229 (92%) | 199 (94%) | 9 (4%)  | 3 (1%)   | 11          | 1  |
| 1   | 15-A  | 211/229 (92%) | 200 (95%) | 8 (4%)  | 3 (1%)   | 11          | 1  |
| 1   | 16-A  | 211/229 (92%) | 199 (94%) | 8 (4%)  | 4 (2%)   | 8           | 0  |
| 1   | 17-A  | 211/229 (92%) | 197 (93%) | 10 (5%) | 4 (2%)   | 8           | 0  |
| 1   | 18-A  | 211/229 (92%) | 200 (95%) | 6 (3%)  | 5 (2%)   | 6           | 0  |
| 1   | 19-A  | 211/229 (92%) | 199 (94%) | 7 (3%)  | 5 (2%)   | 6           | 0  |
| 1   | 20-A  | 211/229 (92%) | 201 (95%) | 7 (3%)  | 3 (1%)   | 11          | 1  |
| 1   | 21-A  | 211/229 (92%) | 199 (94%) | 11 (5%) | 1 (0%)   | 29          | 11 |
| 1   | 22-A  | 211/229 (92%) | 196 (93%) | 8 (4%)  | 7 (3%)   | 4           | 0  |
| 1   | 23-A  | 211/229 (92%) | 202 (96%) | 8 (4%)  | 1 (0%)   | 29          | 11 |
| 1   | 24-A  | 211/229 (92%) | 201 (95%) | 7 (3%)  | 3 (1%)   | 11          | 1  |
| 1   | 25-A  | 211/229 (92%) | 200 (95%) | 9 (4%)  | 2 (1%)   | 17          | 4  |
| 1   | 26-A  | 211/229 (92%) | 196 (93%) | 13 (6%) | 2 (1%)   | 17          | 4  |
| 1   | 27-A  | 211/229 (92%) | 202 (96%) | 7 (3%)  | 2 (1%)   | 17          | 4  |
| 1   | 28-A  | 211/229 (92%) | 204 (97%) | 5 (2%)  | 2 (1%)   | 17          | 4  |
| 1   | 29-A  | 211/229 (92%) | 201 (95%) | 9 (4%)  | 1 (0%)   | 29          | 11 |
| 1   | 30-A  | 211/229 (92%) | 191 (90%) | 13 (6%) | 7 (3%)   | 4           | 0  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|----------|-------------|----|
| 1   | 31-A  | 211/229 (92%)    | 200 (95%)  | 7 (3%)   | 4 (2%)   | 8           | 0  |
| 1   | 32-A  | 211/229 (92%)    | 202 (96%)  | 8 (4%)   | 1 (0%)   | 29          | 11 |
| 1   | 33-A  | 211/229 (92%)    | 194 (92%)  | 13 (6%)  | 4 (2%)   | 8           | 0  |
| 1   | 34-A  | 211/229 (92%)    | 198 (94%)  | 10 (5%)  | 3 (1%)   | 11          | 1  |
| 1   | 35-A  | 211/229 (92%)    | 202 (96%)  | 8 (4%)   | 1 (0%)   | 29          | 11 |
| 1   | 36-A  | 211/229 (92%)    | 197 (93%)  | 11 (5%)  | 3 (1%)   | 11          | 1  |
| 1   | 37-A  | 211/229 (92%)    | 200 (95%)  | 10 (5%)  | 1 (0%)   | 29          | 11 |
| 1   | 38-A  | 211/229 (92%)    | 199 (94%)  | 9 (4%)   | 3 (1%)   | 11          | 1  |
| 1   | 39-A  | 211/229 (92%)    | 199 (94%)  | 9 (4%)   | 3 (1%)   | 11          | 1  |
| 1   | 40-A  | 211/229 (92%)    | 206 (98%)  | 4 (2%)   | 1 (0%)   | 29          | 11 |
| 1   | 41-A  | 211/229 (92%)    | 204 (97%)  | 6 (3%)   | 1 (0%)   | 29          | 11 |
| 1   | 42-A  | 211/229 (92%)    | 192 (91%)  | 14 (7%)  | 5 (2%)   | 6           | 0  |
| 1   | 43-A  | 211/229 (92%)    | 200 (95%)  | 10 (5%)  | 1 (0%)   | 29          | 11 |
| 1   | 44-A  | 211/229 (92%)    | 200 (95%)  | 7 (3%)   | 4 (2%)   | 8           | 0  |
| 1   | 45-A  | 211/229 (92%)    | 199 (94%)  | 6 (3%)   | 6 (3%)   | 5           | 0  |
| 1   | 46-A  | 211/229 (92%)    | 193 (92%)  | 11 (5%)  | 7 (3%)   | 4           | 0  |
| 1   | 47-A  | 211/229 (92%)    | 197 (93%)  | 10 (5%)  | 4 (2%)   | 8           | 0  |
| All | All   | 9917/10763 (92%) | 9346 (94%) | 404 (4%) | 167 (2%) | 9           | 1  |

All (167) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-A   | 98  | GLN  |
| 1   | 1-A   | 149 | GLU  |
| 1   | 1-A   | 151 | GLY  |
| 1   | 1-A   | 152 | VAL  |
| 1   | 1-A   | 179 | ALA  |
| 1   | 2-A   | 150 | ASP  |
| 1   | 2-A   | 152 | VAL  |
| 1   | 3-A   | 3   | VAL  |
| 1   | 3-A   | 179 | ALA  |
| 1   | 4-A   | 3   | VAL  |
| 1   | 4-A   | 150 | ASP  |
| 1   | 5-A   | 3   | VAL  |
| 1   | 5-A   | 98  | GLN  |
| 1   | 5-A   | 152 | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 6-A   | 98  | GLN  |
| 1   | 6-A   | 149 | GLU  |
| 1   | 6-A   | 150 | ASP  |
| 1   | 6-A   | 152 | VAL  |
| 1   | 7-A   | 149 | GLU  |
| 1   | 7-A   | 150 | ASP  |
| 1   | 8-A   | 149 | GLU  |
| 1   | 9-A   | 149 | GLU  |
| 1   | 10-A  | 149 | GLU  |
| 1   | 11-A  | 128 | ASN  |
| 1   | 11-A  | 129 | GLY  |
| 1   | 11-A  | 149 | GLU  |
| 1   | 12-A  | 150 | ASP  |
| 1   | 13-A  | 98  | GLN  |
| 1   | 13-A  | 149 | GLU  |
| 1   | 13-A  | 152 | VAL  |
| 1   | 14-A  | 19  | ASN  |
| 1   | 14-A  | 152 | VAL  |
| 1   | 15-A  | 151 | GLY  |
| 1   | 17-A  | 149 | GLU  |
| 1   | 17-A  | 152 | VAL  |
| 1   | 18-A  | 98  | GLN  |
| 1   | 18-A  | 149 | GLU  |
| 1   | 19-A  | 150 | ASP  |
| 1   | 20-A  | 150 | ASP  |
| 1   | 20-A  | 152 | VAL  |
| 1   | 21-A  | 152 | VAL  |
| 1   | 22-A  | 142 | PRO  |
| 1   | 22-A  | 152 | VAL  |
| 1   | 23-A  | 152 | VAL  |
| 1   | 24-A  | 150 | ASP  |
| 1   | 25-A  | 142 | PRO  |
| 1   | 25-A  | 150 | ASP  |
| 1   | 26-A  | 124 | ASN  |
| 1   | 27-A  | 4   | ILE  |
| 1   | 27-A  | 5   | LYS  |
| 1   | 30-A  | 19  | ASN  |
| 1   | 30-A  | 72  | PRO  |
| 1   | 31-A  | 203 | ASP  |
| 1   | 32-A  | 204 | TYR  |
| 1   | 34-A  | 5   | LYS  |
| 1   | 35-A  | 203 | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 38-A  | 150 | ASP  |
| 1   | 42-A  | 19  | ASN  |
| 1   | 43-A  | 21  | HIS  |
| 1   | 44-A  | 150 | ASP  |
| 1   | 45-A  | 19  | ASN  |
| 1   | 45-A  | 21  | HIS  |
| 1   | 45-A  | 22  | LYS  |
| 1   | 45-A  | 150 | ASP  |
| 1   | 45-A  | 151 | GLY  |
| 1   | 46-A  | 3   | VAL  |
| 1   | 46-A  | 21  | HIS  |
| 1   | 46-A  | 151 | GLY  |
| 1   | 47-A  | 22  | LYS  |
| 1   | 3-A   | 149 | GLU  |
| 1   | 5-A   | 28  | GLU  |
| 1   | 6-A   | 3   | VAL  |
| 1   | 6-A   | 151 | GLY  |
| 1   | 7-A   | 3   | VAL  |
| 1   | 7-A   | 202 | LYS  |
| 1   | 8-A   | 151 | GLY  |
| 1   | 9-A   | 150 | ASP  |
| 1   | 13-A  | 151 | GLY  |
| 1   | 15-A  | 152 | VAL  |
| 1   | 16-A  | 3   | VAL  |
| 1   | 16-A  | 149 | GLU  |
| 1   | 16-A  | 152 | VAL  |
| 1   | 18-A  | 152 | VAL  |
| 1   | 19-A  | 74  | ASP  |
| 1   | 19-A  | 98  | GLN  |
| 1   | 22-A  | 204 | TYR  |
| 1   | 28-A  | 98  | GLN  |
| 1   | 30-A  | 73  | GLU  |
| 1   | 30-A  | 74  | ASP  |
| 1   | 30-A  | 133 | GLN  |
| 1   | 31-A  | 150 | ASP  |
| 1   | 31-A  | 151 | GLY  |
| 1   | 33-A  | 150 | ASP  |
| 1   | 34-A  | 98  | GLN  |
| 1   | 36-A  | 98  | GLN  |
| 1   | 37-A  | 150 | ASP  |
| 1   | 39-A  | 150 | ASP  |
| 1   | 41-A  | 98  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 42-A  | 36  | GLY  |
| 1   | 44-A  | 151 | GLY  |
| 1   | 45-A  | 124 | ASN  |
| 1   | 1-A   | 150 | ASP  |
| 1   | 3-A   | 150 | ASP  |
| 1   | 4-A   | 28  | GLU  |
| 1   | 5-A   | 51  | PRO  |
| 1   | 5-A   | 151 | GLY  |
| 1   | 6-A   | 22  | LYS  |
| 1   | 8-A   | 4   | ILE  |
| 1   | 8-A   | 19  | ASN  |
| 1   | 14-A  | 187 | ASP  |
| 1   | 15-A  | 111 | GLY  |
| 1   | 17-A  | 150 | ASP  |
| 1   | 22-A  | 124 | ASN  |
| 1   | 22-A  | 149 | GLU  |
| 1   | 28-A  | 142 | PRO  |
| 1   | 29-A  | 74  | ASP  |
| 1   | 30-A  | 204 | TYR  |
| 1   | 34-A  | 4   | ILE  |
| 1   | 38-A  | 98  | GLN  |
| 1   | 38-A  | 124 | ASN  |
| 1   | 2-A   | 98  | GLN  |
| 1   | 3-A   | 153 | LEU  |
| 1   | 6-A   | 23  | PHE  |
| 1   | 8-A   | 3   | VAL  |
| 1   | 16-A  | 98  | GLN  |
| 1   | 18-A  | 142 | PRO  |
| 1   | 19-A  | 19  | ASN  |
| 1   | 19-A  | 152 | VAL  |
| 1   | 22-A  | 98  | GLN  |
| 1   | 24-A  | 98  | GLN  |
| 1   | 33-A  | 98  | GLN  |
| 1   | 36-A  | 142 | PRO  |
| 1   | 36-A  | 150 | ASP  |
| 1   | 39-A  | 181 | LYS  |
| 1   | 40-A  | 151 | GLY  |
| 1   | 42-A  | 51  | PRO  |
| 1   | 46-A  | 98  | GLN  |
| 1   | 47-A  | 20  | GLY  |
| 1   | 3-A   | 142 | PRO  |
| 1   | 8-A   | 51  | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 12-A  | 98  | GLN  |
| 1   | 33-A  | 142 | PRO  |
| 1   | 33-A  | 151 | GLY  |
| 1   | 42-A  | 98  | GLN  |
| 1   | 46-A  | 22  | LYS  |
| 1   | 46-A  | 193 | HIS  |
| 1   | 47-A  | 193 | HIS  |
| 1   | 4-A   | 152 | VAL  |
| 1   | 9-A   | 129 | GLY  |
| 1   | 17-A  | 3   | VAL  |
| 1   | 20-A  | 141 | SER  |
| 1   | 22-A  | 202 | LYS  |
| 1   | 42-A  | 142 | PRO  |
| 1   | 44-A  | 98  | GLN  |
| 1   | 46-A  | 150 | ASP  |
| 1   | 26-A  | 126 | PRO  |
| 1   | 47-A  | 151 | GLY  |
| 1   | 9-A   | 151 | GLY  |
| 1   | 18-A  | 51  | PRO  |
| 1   | 30-A  | 142 | PRO  |
| 1   | 31-A  | 142 | PRO  |
| 1   | 39-A  | 51  | PRO  |
| 1   | 6-A   | 142 | PRO  |
| 1   | 8-A   | 142 | PRO  |
| 1   | 10-A  | 142 | PRO  |
| 1   | 24-A  | 141 | SER  |
| 1   | 44-A  | 141 | SER  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |   |
|-----|-------|---------------|-----------|----------|-------------|---|
| 1   | 1-A   | 184/189 (97%) | 164 (89%) | 20 (11%) | 6           | 1 |
| 1   | 2-A   | 184/189 (97%) | 162 (88%) | 22 (12%) | 5           | 0 |
| 1   | 3-A   | 184/189 (97%) | 163 (89%) | 21 (11%) | 5           | 1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |   |
|-----|-------|---------------|-----------|----------|-------------|---|
| 1   | 4-A   | 184/189 (97%) | 158 (86%) | 26 (14%) | 3           | 0 |
| 1   | 5-A   | 184/189 (97%) | 157 (85%) | 27 (15%) | 3           | 0 |
| 1   | 6-A   | 184/189 (97%) | 161 (88%) | 23 (12%) | 4           | 0 |
| 1   | 7-A   | 184/189 (97%) | 166 (90%) | 18 (10%) | 8           | 1 |
| 1   | 8-A   | 184/189 (97%) | 160 (87%) | 24 (13%) | 4           | 0 |
| 1   | 9-A   | 184/189 (97%) | 163 (89%) | 21 (11%) | 5           | 1 |
| 1   | 10-A  | 184/189 (97%) | 161 (88%) | 23 (12%) | 4           | 0 |
| 1   | 11-A  | 184/189 (97%) | 163 (89%) | 21 (11%) | 5           | 1 |
| 1   | 12-A  | 184/189 (97%) | 163 (89%) | 21 (11%) | 5           | 1 |
| 1   | 13-A  | 184/189 (97%) | 152 (83%) | 32 (17%) | 2           | 0 |
| 1   | 14-A  | 184/189 (97%) | 168 (91%) | 16 (9%)  | 10          | 1 |
| 1   | 15-A  | 184/189 (97%) | 161 (88%) | 23 (12%) | 4           | 0 |
| 1   | 16-A  | 184/189 (97%) | 165 (90%) | 19 (10%) | 7           | 1 |
| 1   | 17-A  | 184/189 (97%) | 162 (88%) | 22 (12%) | 5           | 0 |
| 1   | 18-A  | 184/189 (97%) | 157 (85%) | 27 (15%) | 3           | 0 |
| 1   | 19-A  | 184/189 (97%) | 162 (88%) | 22 (12%) | 5           | 0 |
| 1   | 20-A  | 184/189 (97%) | 163 (89%) | 21 (11%) | 5           | 1 |
| 1   | 21-A  | 184/189 (97%) | 163 (89%) | 21 (11%) | 5           | 1 |
| 1   | 22-A  | 184/189 (97%) | 162 (88%) | 22 (12%) | 5           | 0 |
| 1   | 23-A  | 184/189 (97%) | 162 (88%) | 22 (12%) | 5           | 0 |
| 1   | 24-A  | 184/189 (97%) | 168 (91%) | 16 (9%)  | 10          | 1 |
| 1   | 25-A  | 184/189 (97%) | 166 (90%) | 18 (10%) | 8           | 1 |
| 1   | 26-A  | 184/189 (97%) | 169 (92%) | 15 (8%)  | 11          | 2 |
| 1   | 27-A  | 184/189 (97%) | 166 (90%) | 18 (10%) | 8           | 1 |
| 1   | 28-A  | 184/189 (97%) | 161 (88%) | 23 (12%) | 4           | 0 |
| 1   | 29-A  | 184/189 (97%) | 153 (83%) | 31 (17%) | 2           | 0 |
| 1   | 30-A  | 184/189 (97%) | 159 (86%) | 25 (14%) | 3           | 0 |
| 1   | 31-A  | 184/189 (97%) | 161 (88%) | 23 (12%) | 4           | 0 |
| 1   | 32-A  | 184/189 (97%) | 161 (88%) | 23 (12%) | 4           | 0 |
| 1   | 33-A  | 184/189 (97%) | 163 (89%) | 21 (11%) | 5           | 1 |
| 1   | 34-A  | 184/189 (97%) | 163 (89%) | 21 (11%) | 5           | 1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Rotameric  | Outliers   | Percentiles |   |
|-----|-------|-----------------|------------|------------|-------------|---|
| 1   | 35-A  | 184/189 (97%)   | 155 (84%)  | 29 (16%)   | 2           | 0 |
| 1   | 36-A  | 184/189 (97%)   | 165 (90%)  | 19 (10%)   | 7           | 1 |
| 1   | 37-A  | 184/189 (97%)   | 159 (86%)  | 25 (14%)   | 3           | 0 |
| 1   | 38-A  | 184/189 (97%)   | 161 (88%)  | 23 (12%)   | 4           | 0 |
| 1   | 39-A  | 184/189 (97%)   | 159 (86%)  | 25 (14%)   | 3           | 0 |
| 1   | 40-A  | 184/189 (97%)   | 164 (89%)  | 20 (11%)   | 6           | 1 |
| 1   | 41-A  | 184/189 (97%)   | 167 (91%)  | 17 (9%)    | 9           | 1 |
| 1   | 42-A  | 184/189 (97%)   | 157 (85%)  | 27 (15%)   | 3           | 0 |
| 1   | 43-A  | 184/189 (97%)   | 164 (89%)  | 20 (11%)   | 6           | 1 |
| 1   | 44-A  | 184/189 (97%)   | 157 (85%)  | 27 (15%)   | 3           | 0 |
| 1   | 45-A  | 184/189 (97%)   | 172 (94%)  | 12 (6%)    | 17          | 3 |
| 1   | 46-A  | 184/189 (97%)   | 161 (88%)  | 23 (12%)   | 4           | 0 |
| 1   | 47-A  | 184/189 (97%)   | 163 (89%)  | 21 (11%)   | 5           | 1 |
| All | All   | 8648/8883 (97%) | 7612 (88%) | 1036 (12%) | 5           | 0 |

All (1036) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-A   | 2   | SER  |
| 1   | 1-A   | 19  | ASN  |
| 1   | 1-A   | 28  | GLU  |
| 1   | 1-A   | 73  | GLU  |
| 1   | 1-A   | 81  | GLN  |
| 1   | 1-A   | 85  | GLU  |
| 1   | 1-A   | 116 | TYR  |
| 1   | 1-A   | 143 | THR  |
| 1   | 1-A   | 147 | TYR  |
| 1   | 1-A   | 148 | VAL  |
| 1   | 1-A   | 150 | ASP  |
| 1   | 1-A   | 161 | LEU  |
| 1   | 1-A   | 174 | LYS  |
| 1   | 1-A   | 176 | THR  |
| 1   | 1-A   | 178 | LYS  |
| 1   | 1-A   | 185 | LEU  |
| 1   | 1-A   | 191 | VAL  |
| 1   | 1-A   | 193 | HIS  |
| 1   | 1-A   | 211 | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-A   | 216 | ARG  |
| 1   | 2-A   | 4   | ILE  |
| 1   | 2-A   | 9   | LYS  |
| 1   | 2-A   | 39  | THR  |
| 1   | 2-A   | 45  | GLU  |
| 1   | 2-A   | 81  | GLN  |
| 1   | 2-A   | 100 | ILE  |
| 1   | 2-A   | 116 | TYR  |
| 1   | 2-A   | 123 | THR  |
| 1   | 2-A   | 133 | GLN  |
| 1   | 2-A   | 145 | LYS  |
| 1   | 2-A   | 146 | MET  |
| 1   | 2-A   | 148 | VAL  |
| 1   | 2-A   | 150 | ASP  |
| 1   | 2-A   | 153 | LEU  |
| 1   | 2-A   | 156 | ASP  |
| 1   | 2-A   | 178 | LYS  |
| 1   | 2-A   | 180 | LYS  |
| 1   | 2-A   | 181 | LYS  |
| 1   | 2-A   | 187 | ASP  |
| 1   | 2-A   | 192 | ASP  |
| 1   | 2-A   | 216 | ARG  |
| 1   | 2-A   | 217 | TYR  |
| 1   | 3-A   | 9   | LYS  |
| 1   | 3-A   | 11  | LYS  |
| 1   | 3-A   | 41  | ASP  |
| 1   | 3-A   | 96  | GLU  |
| 1   | 3-A   | 110 | GLU  |
| 1   | 3-A   | 116 | TYR  |
| 1   | 3-A   | 138 | LYS  |
| 1   | 3-A   | 146 | MET  |
| 1   | 3-A   | 148 | VAL  |
| 1   | 3-A   | 149 | GLU  |
| 1   | 3-A   | 150 | ASP  |
| 1   | 3-A   | 152 | VAL  |
| 1   | 3-A   | 153 | LEU  |
| 1   | 3-A   | 156 | ASP  |
| 1   | 3-A   | 158 | GLU  |
| 1   | 3-A   | 176 | THR  |
| 1   | 3-A   | 178 | LYS  |
| 1   | 3-A   | 180 | LYS  |
| 1   | 3-A   | 187 | ASP  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 3-A   | 193 | HIS  |
| 1   | 3-A   | 194 | ARG  |
| 1   | 4-A   | 9   | LYS  |
| 1   | 4-A   | 13  | ARG  |
| 1   | 4-A   | 19  | ASN  |
| 1   | 4-A   | 28  | GLU  |
| 1   | 4-A   | 74  | ASP  |
| 1   | 4-A   | 100 | ILE  |
| 1   | 4-A   | 110 | GLU  |
| 1   | 4-A   | 116 | TYR  |
| 1   | 4-A   | 134 | LYS  |
| 1   | 4-A   | 138 | LYS  |
| 1   | 4-A   | 140 | LYS  |
| 1   | 4-A   | 145 | LYS  |
| 1   | 4-A   | 150 | ASP  |
| 1   | 4-A   | 153 | LEU  |
| 1   | 4-A   | 161 | LEU  |
| 1   | 4-A   | 163 | LEU  |
| 1   | 4-A   | 170 | ARG  |
| 1   | 4-A   | 174 | LYS  |
| 1   | 4-A   | 178 | LYS  |
| 1   | 4-A   | 180 | LYS  |
| 1   | 4-A   | 185 | LEU  |
| 1   | 4-A   | 192 | ASP  |
| 1   | 4-A   | 193 | HIS  |
| 1   | 4-A   | 194 | ARG  |
| 1   | 4-A   | 216 | ARG  |
| 1   | 4-A   | 217 | TYR  |
| 1   | 5-A   | 2   | SER  |
| 1   | 5-A   | 13  | ARG  |
| 1   | 5-A   | 30  | ILE  |
| 1   | 5-A   | 70  | LYS  |
| 1   | 5-A   | 78  | TYR  |
| 1   | 5-A   | 90  | GLU  |
| 1   | 5-A   | 100 | ILE  |
| 1   | 5-A   | 110 | GLU  |
| 1   | 5-A   | 116 | TYR  |
| 1   | 5-A   | 133 | GLN  |
| 1   | 5-A   | 134 | LYS  |
| 1   | 5-A   | 136 | THR  |
| 1   | 5-A   | 138 | LYS  |
| 1   | 5-A   | 145 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 5-A   | 148 | VAL  |
| 1   | 5-A   | 149 | GLU  |
| 1   | 5-A   | 152 | VAL  |
| 1   | 5-A   | 153 | LEU  |
| 1   | 5-A   | 161 | LEU  |
| 1   | 5-A   | 170 | ARG  |
| 1   | 5-A   | 174 | LYS  |
| 1   | 5-A   | 176 | THR  |
| 1   | 5-A   | 178 | LYS  |
| 1   | 5-A   | 183 | VAL  |
| 1   | 5-A   | 203 | ASP  |
| 1   | 5-A   | 216 | ARG  |
| 1   | 5-A   | 217 | TYR  |
| 1   | 6-A   | 5   | LYS  |
| 1   | 6-A   | 11  | LYS  |
| 1   | 6-A   | 19  | ASN  |
| 1   | 6-A   | 30  | ILE  |
| 1   | 6-A   | 39  | THR  |
| 1   | 6-A   | 74  | ASP  |
| 1   | 6-A   | 78  | TYR  |
| 1   | 6-A   | 81  | GLN  |
| 1   | 6-A   | 91  | ARG  |
| 1   | 6-A   | 98  | GLN  |
| 1   | 6-A   | 100 | ILE  |
| 1   | 6-A   | 110 | GLU  |
| 1   | 6-A   | 116 | TYR  |
| 1   | 6-A   | 117 | GLU  |
| 1   | 6-A   | 158 | GLU  |
| 1   | 6-A   | 172 | ASP  |
| 1   | 6-A   | 174 | LYS  |
| 1   | 6-A   | 175 | THR  |
| 1   | 6-A   | 176 | THR  |
| 1   | 6-A   | 180 | LYS  |
| 1   | 6-A   | 191 | VAL  |
| 1   | 6-A   | 194 | ARG  |
| 1   | 6-A   | 202 | LYS  |
| 1   | 7-A   | 5   | LYS  |
| 1   | 7-A   | 19  | ASN  |
| 1   | 7-A   | 22  | LYS  |
| 1   | 7-A   | 28  | GLU  |
| 1   | 7-A   | 30  | ILE  |
| 1   | 7-A   | 32  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 7-A   | 42  | LEU  |
| 1   | 7-A   | 74  | ASP  |
| 1   | 7-A   | 89  | TRP  |
| 1   | 7-A   | 109 | MET  |
| 1   | 7-A   | 112 | ASP  |
| 1   | 7-A   | 116 | TYR  |
| 1   | 7-A   | 149 | GLU  |
| 1   | 7-A   | 178 | LYS  |
| 1   | 7-A   | 180 | LYS  |
| 1   | 7-A   | 190 | GLU  |
| 1   | 7-A   | 216 | ARG  |
| 1   | 7-A   | 217 | TYR  |
| 1   | 8-A   | 4   | ILE  |
| 1   | 8-A   | 42  | LEU  |
| 1   | 8-A   | 73  | GLU  |
| 1   | 8-A   | 74  | ASP  |
| 1   | 8-A   | 98  | GLN  |
| 1   | 8-A   | 100 | ILE  |
| 1   | 8-A   | 112 | ASP  |
| 1   | 8-A   | 116 | TYR  |
| 1   | 8-A   | 128 | ASN  |
| 1   | 8-A   | 153 | LEU  |
| 1   | 8-A   | 156 | ASP  |
| 1   | 8-A   | 157 | VAL  |
| 1   | 8-A   | 158 | GLU  |
| 1   | 8-A   | 170 | ARG  |
| 1   | 8-A   | 176 | THR  |
| 1   | 8-A   | 177 | TYR  |
| 1   | 8-A   | 178 | LYS  |
| 1   | 8-A   | 180 | LYS  |
| 1   | 8-A   | 181 | LYS  |
| 1   | 8-A   | 187 | ASP  |
| 1   | 8-A   | 193 | HIS  |
| 1   | 8-A   | 212 | HIS  |
| 1   | 8-A   | 214 | GLU  |
| 1   | 8-A   | 216 | ARG  |
| 1   | 9-A   | 19  | ASN  |
| 1   | 9-A   | 21  | HIS  |
| 1   | 9-A   | 22  | LYS  |
| 1   | 9-A   | 28  | GLU  |
| 1   | 9-A   | 39  | THR  |
| 1   | 9-A   | 42  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 9-A   | 45  | GLU  |
| 1   | 9-A   | 53  | SER  |
| 1   | 9-A   | 85  | GLU  |
| 1   | 9-A   | 116 | TYR  |
| 1   | 9-A   | 123 | THR  |
| 1   | 9-A   | 128 | ASN  |
| 1   | 9-A   | 130 | PRO  |
| 1   | 9-A   | 146 | MET  |
| 1   | 9-A   | 149 | GLU  |
| 1   | 9-A   | 152 | VAL  |
| 1   | 9-A   | 161 | LEU  |
| 1   | 9-A   | 180 | LYS  |
| 1   | 9-A   | 192 | ASP  |
| 1   | 9-A   | 214 | GLU  |
| 1   | 9-A   | 216 | ARG  |
| 1   | 10-A  | 7   | GLU  |
| 1   | 10-A  | 9   | LYS  |
| 1   | 10-A  | 13  | ARG  |
| 1   | 10-A  | 21  | HIS  |
| 1   | 10-A  | 22  | LYS  |
| 1   | 10-A  | 28  | GLU  |
| 1   | 10-A  | 53  | SER  |
| 1   | 10-A  | 70  | LYS  |
| 1   | 10-A  | 88  | SER  |
| 1   | 10-A  | 102 | ILE  |
| 1   | 10-A  | 116 | TYR  |
| 1   | 10-A  | 128 | ASN  |
| 1   | 10-A  | 143 | THR  |
| 1   | 10-A  | 149 | GLU  |
| 1   | 10-A  | 153 | LEU  |
| 1   | 10-A  | 158 | GLU  |
| 1   | 10-A  | 161 | LEU  |
| 1   | 10-A  | 164 | GLU  |
| 1   | 10-A  | 174 | LYS  |
| 1   | 10-A  | 178 | LYS  |
| 1   | 10-A  | 185 | LEU  |
| 1   | 10-A  | 193 | HIS  |
| 1   | 10-A  | 216 | ARG  |
| 1   | 11-A  | 2   | SER  |
| 1   | 11-A  | 7   | GLU  |
| 1   | 11-A  | 13  | ARG  |
| 1   | 11-A  | 22  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 11-A  | 28  | GLU  |
| 1   | 11-A  | 30  | ILE  |
| 1   | 11-A  | 39  | THR  |
| 1   | 11-A  | 40  | LEU  |
| 1   | 11-A  | 43  | THR  |
| 1   | 11-A  | 53  | SER  |
| 1   | 11-A  | 116 | TYR  |
| 1   | 11-A  | 146 | MET  |
| 1   | 11-A  | 150 | ASP  |
| 1   | 11-A  | 164 | GLU  |
| 1   | 11-A  | 174 | LYS  |
| 1   | 11-A  | 178 | LYS  |
| 1   | 11-A  | 202 | LYS  |
| 1   | 11-A  | 206 | LYS  |
| 1   | 11-A  | 208 | ARG  |
| 1   | 11-A  | 212 | HIS  |
| 1   | 11-A  | 216 | ARG  |
| 1   | 12-A  | 2   | SER  |
| 1   | 12-A  | 3   | VAL  |
| 1   | 12-A  | 4   | ILE  |
| 1   | 12-A  | 5   | LYS  |
| 1   | 12-A  | 19  | ASN  |
| 1   | 12-A  | 30  | ILE  |
| 1   | 12-A  | 41  | ASP  |
| 1   | 12-A  | 43  | THR  |
| 1   | 12-A  | 116 | TYR  |
| 1   | 12-A  | 143 | THR  |
| 1   | 12-A  | 149 | GLU  |
| 1   | 12-A  | 153 | LEU  |
| 1   | 12-A  | 161 | LEU  |
| 1   | 12-A  | 174 | LYS  |
| 1   | 12-A  | 175 | THR  |
| 1   | 12-A  | 185 | LEU  |
| 1   | 12-A  | 187 | ASP  |
| 1   | 12-A  | 193 | HIS  |
| 1   | 12-A  | 202 | LYS  |
| 1   | 12-A  | 208 | ARG  |
| 1   | 12-A  | 212 | HIS  |
| 1   | 13-A  | 3   | VAL  |
| 1   | 13-A  | 4   | ILE  |
| 1   | 13-A  | 11  | LYS  |
| 1   | 13-A  | 19  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 13-A  | 39  | THR  |
| 1   | 13-A  | 43  | THR  |
| 1   | 13-A  | 73  | GLU  |
| 1   | 13-A  | 74  | ASP  |
| 1   | 13-A  | 85  | GLU  |
| 1   | 13-A  | 91  | ARG  |
| 1   | 13-A  | 100 | ILE  |
| 1   | 13-A  | 102 | ILE  |
| 1   | 13-A  | 109 | MET  |
| 1   | 13-A  | 116 | TYR  |
| 1   | 13-A  | 117 | GLU  |
| 1   | 13-A  | 124 | ASN  |
| 1   | 13-A  | 128 | ASN  |
| 1   | 13-A  | 134 | LYS  |
| 1   | 13-A  | 142 | PRO  |
| 1   | 13-A  | 150 | ASP  |
| 1   | 13-A  | 153 | LEU  |
| 1   | 13-A  | 154 | LYS  |
| 1   | 13-A  | 156 | ASP  |
| 1   | 13-A  | 161 | LEU  |
| 1   | 13-A  | 170 | ARG  |
| 1   | 13-A  | 176 | THR  |
| 1   | 13-A  | 193 | HIS  |
| 1   | 13-A  | 202 | LYS  |
| 1   | 13-A  | 205 | ASN  |
| 1   | 13-A  | 206 | LYS  |
| 1   | 13-A  | 212 | HIS  |
| 1   | 13-A  | 214 | GLU  |
| 1   | 14-A  | 4   | ILE  |
| 1   | 14-A  | 11  | LYS  |
| 1   | 14-A  | 19  | ASN  |
| 1   | 14-A  | 96  | GLU  |
| 1   | 14-A  | 110 | GLU  |
| 1   | 14-A  | 116 | TYR  |
| 1   | 14-A  | 128 | ASN  |
| 1   | 14-A  | 135 | LYS  |
| 1   | 14-A  | 153 | LEU  |
| 1   | 14-A  | 154 | LYS  |
| 1   | 14-A  | 174 | LYS  |
| 1   | 14-A  | 187 | ASP  |
| 1   | 14-A  | 193 | HIS  |
| 1   | 14-A  | 198 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 14-A  | 208 | ARG  |
| 1   | 14-A  | 216 | ARG  |
| 1   | 15-A  | 2   | SER  |
| 1   | 15-A  | 3   | VAL  |
| 1   | 15-A  | 4   | ILE  |
| 1   | 15-A  | 11  | LYS  |
| 1   | 15-A  | 39  | THR  |
| 1   | 15-A  | 90  | GLU  |
| 1   | 15-A  | 110 | GLU  |
| 1   | 15-A  | 116 | TYR  |
| 1   | 15-A  | 128 | ASN  |
| 1   | 15-A  | 134 | LYS  |
| 1   | 15-A  | 138 | LYS  |
| 1   | 15-A  | 143 | THR  |
| 1   | 15-A  | 147 | TYR  |
| 1   | 15-A  | 153 | LEU  |
| 1   | 15-A  | 154 | LYS  |
| 1   | 15-A  | 158 | GLU  |
| 1   | 15-A  | 176 | THR  |
| 1   | 15-A  | 178 | LYS  |
| 1   | 15-A  | 181 | LYS  |
| 1   | 15-A  | 193 | HIS  |
| 1   | 15-A  | 198 | LEU  |
| 1   | 15-A  | 216 | ARG  |
| 1   | 15-A  | 217 | TYR  |
| 1   | 16-A  | 4   | ILE  |
| 1   | 16-A  | 13  | ARG  |
| 1   | 16-A  | 19  | ASN  |
| 1   | 16-A  | 39  | THR  |
| 1   | 16-A  | 74  | ASP  |
| 1   | 16-A  | 98  | GLN  |
| 1   | 16-A  | 100 | ILE  |
| 1   | 16-A  | 106 | ASP  |
| 1   | 16-A  | 116 | TYR  |
| 1   | 16-A  | 149 | GLU  |
| 1   | 16-A  | 150 | ASP  |
| 1   | 16-A  | 152 | VAL  |
| 1   | 16-A  | 154 | LYS  |
| 1   | 16-A  | 157 | VAL  |
| 1   | 16-A  | 180 | LYS  |
| 1   | 16-A  | 194 | ARG  |
| 1   | 16-A  | 212 | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 16-A  | 216 | ARG  |
| 1   | 16-A  | 217 | TYR  |
| 1   | 17-A  | 9   | LYS  |
| 1   | 17-A  | 19  | ASN  |
| 1   | 17-A  | 28  | GLU  |
| 1   | 17-A  | 41  | ASP  |
| 1   | 17-A  | 50  | LEU  |
| 1   | 17-A  | 70  | LYS  |
| 1   | 17-A  | 73  | GLU  |
| 1   | 17-A  | 78  | TYR  |
| 1   | 17-A  | 98  | GLN  |
| 1   | 17-A  | 116 | TYR  |
| 1   | 17-A  | 123 | THR  |
| 1   | 17-A  | 138 | LYS  |
| 1   | 17-A  | 145 | LYS  |
| 1   | 17-A  | 152 | VAL  |
| 1   | 17-A  | 156 | ASP  |
| 1   | 17-A  | 161 | LEU  |
| 1   | 17-A  | 180 | LYS  |
| 1   | 17-A  | 182 | ASP  |
| 1   | 17-A  | 190 | GLU  |
| 1   | 17-A  | 202 | LYS  |
| 1   | 17-A  | 206 | LYS  |
| 1   | 17-A  | 217 | TYR  |
| 1   | 18-A  | 2   | SER  |
| 1   | 18-A  | 3   | VAL  |
| 1   | 18-A  | 19  | ASN  |
| 1   | 18-A  | 35  | GLU  |
| 1   | 18-A  | 39  | THR  |
| 1   | 18-A  | 43  | THR  |
| 1   | 18-A  | 50  | LEU  |
| 1   | 18-A  | 51  | PRO  |
| 1   | 18-A  | 73  | GLU  |
| 1   | 18-A  | 74  | ASP  |
| 1   | 18-A  | 78  | TYR  |
| 1   | 18-A  | 100 | ILE  |
| 1   | 18-A  | 116 | TYR  |
| 1   | 18-A  | 124 | ASN  |
| 1   | 18-A  | 138 | LYS  |
| 1   | 18-A  | 146 | MET  |
| 1   | 18-A  | 149 | GLU  |
| 1   | 18-A  | 150 | ASP  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 18-A  | 152 | VAL  |
| 1   | 18-A  | 153 | LEU  |
| 1   | 18-A  | 154 | LYS  |
| 1   | 18-A  | 168 | HIS  |
| 1   | 18-A  | 178 | LYS  |
| 1   | 18-A  | 185 | LEU  |
| 1   | 18-A  | 193 | HIS  |
| 1   | 18-A  | 205 | ASN  |
| 1   | 18-A  | 214 | GLU  |
| 1   | 19-A  | 5   | LYS  |
| 1   | 19-A  | 7   | GLU  |
| 1   | 19-A  | 9   | LYS  |
| 1   | 19-A  | 28  | GLU  |
| 1   | 19-A  | 39  | THR  |
| 1   | 19-A  | 74  | ASP  |
| 1   | 19-A  | 81  | GLN  |
| 1   | 19-A  | 96  | GLU  |
| 1   | 19-A  | 112 | ASP  |
| 1   | 19-A  | 116 | TYR  |
| 1   | 19-A  | 117 | GLU  |
| 1   | 19-A  | 123 | THR  |
| 1   | 19-A  | 124 | ASN  |
| 1   | 19-A  | 138 | LYS  |
| 1   | 19-A  | 147 | TYR  |
| 1   | 19-A  | 149 | GLU  |
| 1   | 19-A  | 150 | ASP  |
| 1   | 19-A  | 158 | GLU  |
| 1   | 19-A  | 181 | LYS  |
| 1   | 19-A  | 192 | ASP  |
| 1   | 19-A  | 211 | GLU  |
| 1   | 19-A  | 212 | HIS  |
| 1   | 20-A  | 2   | SER  |
| 1   | 20-A  | 3   | VAL  |
| 1   | 20-A  | 7   | GLU  |
| 1   | 20-A  | 32  | LYS  |
| 1   | 20-A  | 98  | GLN  |
| 1   | 20-A  | 102 | ILE  |
| 1   | 20-A  | 110 | GLU  |
| 1   | 20-A  | 116 | TYR  |
| 1   | 20-A  | 117 | GLU  |
| 1   | 20-A  | 135 | LYS  |
| 1   | 20-A  | 147 | TYR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 20-A  | 149 | GLU  |
| 1   | 20-A  | 156 | ASP  |
| 1   | 20-A  | 161 | LEU  |
| 1   | 20-A  | 176 | THR  |
| 1   | 20-A  | 194 | ARG  |
| 1   | 20-A  | 196 | GLU  |
| 1   | 20-A  | 202 | LYS  |
| 1   | 20-A  | 203 | ASP  |
| 1   | 20-A  | 216 | ARG  |
| 1   | 20-A  | 217 | TYR  |
| 1   | 21-A  | 9   | LYS  |
| 1   | 21-A  | 30  | ILE  |
| 1   | 21-A  | 35  | GLU  |
| 1   | 21-A  | 39  | THR  |
| 1   | 21-A  | 41  | ASP  |
| 1   | 21-A  | 50  | LEU  |
| 1   | 21-A  | 70  | LYS  |
| 1   | 21-A  | 90  | GLU  |
| 1   | 21-A  | 116 | TYR  |
| 1   | 21-A  | 145 | LYS  |
| 1   | 21-A  | 147 | TYR  |
| 1   | 21-A  | 148 | VAL  |
| 1   | 21-A  | 149 | GLU  |
| 1   | 21-A  | 153 | LEU  |
| 1   | 21-A  | 161 | LEU  |
| 1   | 21-A  | 172 | ASP  |
| 1   | 21-A  | 181 | LYS  |
| 1   | 21-A  | 202 | LYS  |
| 1   | 21-A  | 212 | HIS  |
| 1   | 21-A  | 216 | ARG  |
| 1   | 21-A  | 217 | TYR  |
| 1   | 22-A  | 3   | VAL  |
| 1   | 22-A  | 5   | LYS  |
| 1   | 22-A  | 39  | THR  |
| 1   | 22-A  | 41  | ASP  |
| 1   | 22-A  | 50  | LEU  |
| 1   | 22-A  | 73  | GLU  |
| 1   | 22-A  | 74  | ASP  |
| 1   | 22-A  | 100 | ILE  |
| 1   | 22-A  | 116 | TYR  |
| 1   | 22-A  | 138 | LYS  |
| 1   | 22-A  | 141 | SER  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 22-A  | 147 | TYR  |
| 1   | 22-A  | 150 | ASP  |
| 1   | 22-A  | 170 | ARG  |
| 1   | 22-A  | 174 | LYS  |
| 1   | 22-A  | 176 | THR  |
| 1   | 22-A  | 185 | LEU  |
| 1   | 22-A  | 194 | ARG  |
| 1   | 22-A  | 202 | LYS  |
| 1   | 22-A  | 208 | ARG  |
| 1   | 22-A  | 216 | ARG  |
| 1   | 22-A  | 217 | TYR  |
| 1   | 23-A  | 2   | SER  |
| 1   | 23-A  | 5   | LYS  |
| 1   | 23-A  | 7   | GLU  |
| 1   | 23-A  | 22  | LYS  |
| 1   | 23-A  | 28  | GLU  |
| 1   | 23-A  | 73  | GLU  |
| 1   | 23-A  | 96  | GLU  |
| 1   | 23-A  | 106 | ASP  |
| 1   | 23-A  | 109 | MET  |
| 1   | 23-A  | 112 | ASP  |
| 1   | 23-A  | 116 | TYR  |
| 1   | 23-A  | 145 | LYS  |
| 1   | 23-A  | 152 | VAL  |
| 1   | 23-A  | 153 | LEU  |
| 1   | 23-A  | 156 | ASP  |
| 1   | 23-A  | 157 | VAL  |
| 1   | 23-A  | 168 | HIS  |
| 1   | 23-A  | 174 | LYS  |
| 1   | 23-A  | 180 | LYS  |
| 1   | 23-A  | 194 | ARG  |
| 1   | 23-A  | 196 | GLU  |
| 1   | 23-A  | 202 | LYS  |
| 1   | 24-A  | 7   | GLU  |
| 1   | 24-A  | 21  | HIS  |
| 1   | 24-A  | 22  | LYS  |
| 1   | 24-A  | 106 | ASP  |
| 1   | 24-A  | 110 | GLU  |
| 1   | 24-A  | 116 | TYR  |
| 1   | 24-A  | 134 | LYS  |
| 1   | 24-A  | 138 | LYS  |
| 1   | 24-A  | 147 | TYR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 24-A  | 150 | ASP  |
| 1   | 24-A  | 153 | LEU  |
| 1   | 24-A  | 161 | LEU  |
| 1   | 24-A  | 172 | ASP  |
| 1   | 24-A  | 178 | LYS  |
| 1   | 24-A  | 180 | LYS  |
| 1   | 24-A  | 190 | GLU  |
| 1   | 25-A  | 3   | VAL  |
| 1   | 25-A  | 28  | GLU  |
| 1   | 25-A  | 41  | ASP  |
| 1   | 25-A  | 50  | LEU  |
| 1   | 25-A  | 74  | ASP  |
| 1   | 25-A  | 100 | ILE  |
| 1   | 25-A  | 116 | TYR  |
| 1   | 25-A  | 117 | GLU  |
| 1   | 25-A  | 123 | THR  |
| 1   | 25-A  | 127 | PRO  |
| 1   | 25-A  | 148 | VAL  |
| 1   | 25-A  | 156 | ASP  |
| 1   | 25-A  | 161 | LEU  |
| 1   | 25-A  | 192 | ASP  |
| 1   | 25-A  | 193 | HIS  |
| 1   | 25-A  | 194 | ARG  |
| 1   | 25-A  | 206 | LYS  |
| 1   | 25-A  | 216 | ARG  |
| 1   | 26-A  | 21  | HIS  |
| 1   | 26-A  | 116 | TYR  |
| 1   | 26-A  | 126 | PRO  |
| 1   | 26-A  | 143 | THR  |
| 1   | 26-A  | 149 | GLU  |
| 1   | 26-A  | 154 | LYS  |
| 1   | 26-A  | 190 | GLU  |
| 1   | 26-A  | 192 | ASP  |
| 1   | 26-A  | 194 | ARG  |
| 1   | 26-A  | 196 | GLU  |
| 1   | 26-A  | 202 | LYS  |
| 1   | 26-A  | 205 | ASN  |
| 1   | 26-A  | 206 | LYS  |
| 1   | 26-A  | 216 | ARG  |
| 1   | 26-A  | 217 | TYR  |
| 1   | 27-A  | 3   | VAL  |
| 1   | 27-A  | 28  | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 27-A  | 43  | THR  |
| 1   | 27-A  | 45  | GLU  |
| 1   | 27-A  | 50  | LEU  |
| 1   | 27-A  | 98  | GLN  |
| 1   | 27-A  | 109 | MET  |
| 1   | 27-A  | 116 | TYR  |
| 1   | 27-A  | 124 | ASN  |
| 1   | 27-A  | 132 | MET  |
| 1   | 27-A  | 143 | THR  |
| 1   | 27-A  | 148 | VAL  |
| 1   | 27-A  | 153 | LEU  |
| 1   | 27-A  | 156 | ASP  |
| 1   | 27-A  | 176 | THR  |
| 1   | 27-A  | 193 | HIS  |
| 1   | 27-A  | 206 | LYS  |
| 1   | 27-A  | 216 | ARG  |
| 1   | 28-A  | 2   | SER  |
| 1   | 28-A  | 4   | ILE  |
| 1   | 28-A  | 7   | GLU  |
| 1   | 28-A  | 28  | GLU  |
| 1   | 28-A  | 32  | LYS  |
| 1   | 28-A  | 41  | ASP  |
| 1   | 28-A  | 43  | THR  |
| 1   | 28-A  | 50  | LEU  |
| 1   | 28-A  | 73  | GLU  |
| 1   | 28-A  | 90  | GLU  |
| 1   | 28-A  | 109 | MET  |
| 1   | 28-A  | 116 | TYR  |
| 1   | 28-A  | 125 | PHE  |
| 1   | 28-A  | 145 | LYS  |
| 1   | 28-A  | 148 | VAL  |
| 1   | 28-A  | 149 | GLU  |
| 1   | 28-A  | 161 | LEU  |
| 1   | 28-A  | 176 | THR  |
| 1   | 28-A  | 178 | LYS  |
| 1   | 28-A  | 192 | ASP  |
| 1   | 28-A  | 206 | LYS  |
| 1   | 28-A  | 212 | HIS  |
| 1   | 28-A  | 216 | ARG  |
| 1   | 29-A  | 2   | SER  |
| 1   | 29-A  | 3   | VAL  |
| 1   | 29-A  | 7   | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 29-A  | 13  | ARG  |
| 1   | 29-A  | 30  | ILE  |
| 1   | 29-A  | 32  | LYS  |
| 1   | 29-A  | 39  | THR  |
| 1   | 29-A  | 50  | LEU  |
| 1   | 29-A  | 73  | GLU  |
| 1   | 29-A  | 100 | ILE  |
| 1   | 29-A  | 116 | TYR  |
| 1   | 29-A  | 138 | LYS  |
| 1   | 29-A  | 149 | GLU  |
| 1   | 29-A  | 150 | ASP  |
| 1   | 29-A  | 153 | LEU  |
| 1   | 29-A  | 156 | ASP  |
| 1   | 29-A  | 157 | VAL  |
| 1   | 29-A  | 161 | LEU  |
| 1   | 29-A  | 168 | HIS  |
| 1   | 29-A  | 170 | ARG  |
| 1   | 29-A  | 174 | LYS  |
| 1   | 29-A  | 176 | THR  |
| 1   | 29-A  | 178 | LYS  |
| 1   | 29-A  | 182 | ASP  |
| 1   | 29-A  | 187 | ASP  |
| 1   | 29-A  | 193 | HIS  |
| 1   | 29-A  | 194 | ARG  |
| 1   | 29-A  | 201 | ASP  |
| 1   | 29-A  | 202 | LYS  |
| 1   | 29-A  | 211 | GLU  |
| 1   | 29-A  | 212 | HIS  |
| 1   | 30-A  | 2   | SER  |
| 1   | 30-A  | 11  | LYS  |
| 1   | 30-A  | 13  | ARG  |
| 1   | 30-A  | 93  | MET  |
| 1   | 30-A  | 115 | PHE  |
| 1   | 30-A  | 116 | TYR  |
| 1   | 30-A  | 123 | THR  |
| 1   | 30-A  | 132 | MET  |
| 1   | 30-A  | 134 | LYS  |
| 1   | 30-A  | 138 | LYS  |
| 1   | 30-A  | 143 | THR  |
| 1   | 30-A  | 152 | VAL  |
| 1   | 30-A  | 153 | LEU  |
| 1   | 30-A  | 170 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 30-A  | 176 | THR  |
| 1   | 30-A  | 178 | LYS  |
| 1   | 30-A  | 181 | LYS  |
| 1   | 30-A  | 185 | LEU  |
| 1   | 30-A  | 193 | HIS  |
| 1   | 30-A  | 194 | ARG  |
| 1   | 30-A  | 202 | LYS  |
| 1   | 30-A  | 203 | ASP  |
| 1   | 30-A  | 206 | LYS  |
| 1   | 30-A  | 211 | GLU  |
| 1   | 30-A  | 216 | ARG  |
| 1   | 31-A  | 3   | VAL  |
| 1   | 31-A  | 5   | LYS  |
| 1   | 31-A  | 8   | MET  |
| 1   | 31-A  | 11  | LYS  |
| 1   | 31-A  | 13  | ARG  |
| 1   | 31-A  | 22  | LYS  |
| 1   | 31-A  | 41  | ASP  |
| 1   | 31-A  | 50  | LEU  |
| 1   | 31-A  | 106 | ASP  |
| 1   | 31-A  | 116 | TYR  |
| 1   | 31-A  | 136 | THR  |
| 1   | 31-A  | 149 | GLU  |
| 1   | 31-A  | 153 | LEU  |
| 1   | 31-A  | 156 | ASP  |
| 1   | 31-A  | 158 | GLU  |
| 1   | 31-A  | 161 | LEU  |
| 1   | 31-A  | 174 | LYS  |
| 1   | 31-A  | 185 | LEU  |
| 1   | 31-A  | 190 | GLU  |
| 1   | 31-A  | 192 | ASP  |
| 1   | 31-A  | 203 | ASP  |
| 1   | 31-A  | 208 | ARG  |
| 1   | 31-A  | 217 | TYR  |
| 1   | 32-A  | 5   | LYS  |
| 1   | 32-A  | 13  | ARG  |
| 1   | 32-A  | 22  | LYS  |
| 1   | 32-A  | 35  | GLU  |
| 1   | 32-A  | 41  | ASP  |
| 1   | 32-A  | 45  | GLU  |
| 1   | 32-A  | 74  | ASP  |
| 1   | 32-A  | 116 | TYR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 32-A  | 138 | LYS  |
| 1   | 32-A  | 143 | THR  |
| 1   | 32-A  | 145 | LYS  |
| 1   | 32-A  | 150 | ASP  |
| 1   | 32-A  | 153 | LEU  |
| 1   | 32-A  | 161 | LEU  |
| 1   | 32-A  | 174 | LYS  |
| 1   | 32-A  | 176 | THR  |
| 1   | 32-A  | 185 | LEU  |
| 1   | 32-A  | 192 | ASP  |
| 1   | 32-A  | 193 | HIS  |
| 1   | 32-A  | 194 | ARG  |
| 1   | 32-A  | 202 | LYS  |
| 1   | 32-A  | 212 | HIS  |
| 1   | 32-A  | 217 | TYR  |
| 1   | 33-A  | 3   | VAL  |
| 1   | 33-A  | 9   | LYS  |
| 1   | 33-A  | 11  | LYS  |
| 1   | 33-A  | 30  | ILE  |
| 1   | 33-A  | 32  | LYS  |
| 1   | 33-A  | 50  | LEU  |
| 1   | 33-A  | 116 | TYR  |
| 1   | 33-A  | 124 | ASN  |
| 1   | 33-A  | 141 | SER  |
| 1   | 33-A  | 142 | PRO  |
| 1   | 33-A  | 145 | LYS  |
| 1   | 33-A  | 148 | VAL  |
| 1   | 33-A  | 152 | VAL  |
| 1   | 33-A  | 153 | LEU  |
| 1   | 33-A  | 168 | HIS  |
| 1   | 33-A  | 176 | THR  |
| 1   | 33-A  | 180 | LYS  |
| 1   | 33-A  | 190 | GLU  |
| 1   | 33-A  | 193 | HIS  |
| 1   | 33-A  | 194 | ARG  |
| 1   | 33-A  | 216 | ARG  |
| 1   | 34-A  | 7   | GLU  |
| 1   | 34-A  | 11  | LYS  |
| 1   | 34-A  | 13  | ARG  |
| 1   | 34-A  | 39  | THR  |
| 1   | 34-A  | 98  | GLN  |
| 1   | 34-A  | 116 | TYR  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 34-A  | 133 | GLN  |
| 1   | 34-A  | 135 | LYS  |
| 1   | 34-A  | 145 | LYS  |
| 1   | 34-A  | 148 | VAL  |
| 1   | 34-A  | 149 | GLU  |
| 1   | 34-A  | 150 | ASP  |
| 1   | 34-A  | 152 | VAL  |
| 1   | 34-A  | 153 | LEU  |
| 1   | 34-A  | 156 | ASP  |
| 1   | 34-A  | 164 | GLU  |
| 1   | 34-A  | 180 | LYS  |
| 1   | 34-A  | 187 | ASP  |
| 1   | 34-A  | 196 | GLU  |
| 1   | 34-A  | 202 | LYS  |
| 1   | 34-A  | 216 | ARG  |
| 1   | 35-A  | 2   | SER  |
| 1   | 35-A  | 5   | LYS  |
| 1   | 35-A  | 11  | LYS  |
| 1   | 35-A  | 13  | ARG  |
| 1   | 35-A  | 28  | GLU  |
| 1   | 35-A  | 50  | LEU  |
| 1   | 35-A  | 70  | LYS  |
| 1   | 35-A  | 73  | GLU  |
| 1   | 35-A  | 90  | GLU  |
| 1   | 35-A  | 109 | MET  |
| 1   | 35-A  | 112 | ASP  |
| 1   | 35-A  | 116 | TYR  |
| 1   | 35-A  | 123 | THR  |
| 1   | 35-A  | 128 | ASN  |
| 1   | 35-A  | 133 | GLN  |
| 1   | 35-A  | 134 | LYS  |
| 1   | 35-A  | 138 | LYS  |
| 1   | 35-A  | 145 | LYS  |
| 1   | 35-A  | 150 | ASP  |
| 1   | 35-A  | 157 | VAL  |
| 1   | 35-A  | 161 | LEU  |
| 1   | 35-A  | 172 | ASP  |
| 1   | 35-A  | 176 | THR  |
| 1   | 35-A  | 178 | LYS  |
| 1   | 35-A  | 180 | LYS  |
| 1   | 35-A  | 181 | LYS  |
| 1   | 35-A  | 193 | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 35-A  | 194 | ARG  |
| 1   | 35-A  | 202 | LYS  |
| 1   | 36-A  | 2   | SER  |
| 1   | 36-A  | 5   | LYS  |
| 1   | 36-A  | 13  | ARG  |
| 1   | 36-A  | 21  | HIS  |
| 1   | 36-A  | 73  | GLU  |
| 1   | 36-A  | 81  | GLN  |
| 1   | 36-A  | 98  | GLN  |
| 1   | 36-A  | 116 | TYR  |
| 1   | 36-A  | 124 | ASN  |
| 1   | 36-A  | 133 | GLN  |
| 1   | 36-A  | 143 | THR  |
| 1   | 36-A  | 152 | VAL  |
| 1   | 36-A  | 153 | LEU  |
| 1   | 36-A  | 187 | ASP  |
| 1   | 36-A  | 192 | ASP  |
| 1   | 36-A  | 198 | LEU  |
| 1   | 36-A  | 202 | LYS  |
| 1   | 36-A  | 216 | ARG  |
| 1   | 36-A  | 217 | TYR  |
| 1   | 37-A  | 5   | LYS  |
| 1   | 37-A  | 7   | GLU  |
| 1   | 37-A  | 11  | LYS  |
| 1   | 37-A  | 39  | THR  |
| 1   | 37-A  | 50  | LEU  |
| 1   | 37-A  | 53  | SER  |
| 1   | 37-A  | 81  | GLN  |
| 1   | 37-A  | 90  | GLU  |
| 1   | 37-A  | 98  | GLN  |
| 1   | 37-A  | 109 | MET  |
| 1   | 37-A  | 116 | TYR  |
| 1   | 37-A  | 128 | ASN  |
| 1   | 37-A  | 150 | ASP  |
| 1   | 37-A  | 152 | VAL  |
| 1   | 37-A  | 158 | GLU  |
| 1   | 37-A  | 174 | LYS  |
| 1   | 37-A  | 176 | THR  |
| 1   | 37-A  | 185 | LEU  |
| 1   | 37-A  | 196 | GLU  |
| 1   | 37-A  | 198 | LEU  |
| 1   | 37-A  | 202 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 37-A  | 208 | ARG  |
| 1   | 37-A  | 211 | GLU  |
| 1   | 37-A  | 216 | ARG  |
| 1   | 37-A  | 217 | TYR  |
| 1   | 38-A  | 3   | VAL  |
| 1   | 38-A  | 11  | LYS  |
| 1   | 38-A  | 21  | HIS  |
| 1   | 38-A  | 28  | GLU  |
| 1   | 38-A  | 45  | GLU  |
| 1   | 38-A  | 50  | LEU  |
| 1   | 38-A  | 74  | ASP  |
| 1   | 38-A  | 90  | GLU  |
| 1   | 38-A  | 98  | GLN  |
| 1   | 38-A  | 100 | ILE  |
| 1   | 38-A  | 116 | TYR  |
| 1   | 38-A  | 138 | LYS  |
| 1   | 38-A  | 142 | PRO  |
| 1   | 38-A  | 143 | THR  |
| 1   | 38-A  | 150 | ASP  |
| 1   | 38-A  | 154 | LYS  |
| 1   | 38-A  | 156 | ASP  |
| 1   | 38-A  | 161 | LEU  |
| 1   | 38-A  | 178 | LYS  |
| 1   | 38-A  | 185 | LEU  |
| 1   | 38-A  | 187 | ASP  |
| 1   | 38-A  | 202 | LYS  |
| 1   | 38-A  | 216 | ARG  |
| 1   | 39-A  | 2   | SER  |
| 1   | 39-A  | 3   | VAL  |
| 1   | 39-A  | 5   | LYS  |
| 1   | 39-A  | 28  | GLU  |
| 1   | 39-A  | 35  | GLU  |
| 1   | 39-A  | 41  | ASP  |
| 1   | 39-A  | 50  | LEU  |
| 1   | 39-A  | 70  | LYS  |
| 1   | 39-A  | 88  | SER  |
| 1   | 39-A  | 90  | GLU  |
| 1   | 39-A  | 98  | GLN  |
| 1   | 39-A  | 100 | ILE  |
| 1   | 39-A  | 106 | ASP  |
| 1   | 39-A  | 116 | TYR  |
| 1   | 39-A  | 143 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 39-A  | 148 | VAL  |
| 1   | 39-A  | 153 | LEU  |
| 1   | 39-A  | 154 | LYS  |
| 1   | 39-A  | 158 | GLU  |
| 1   | 39-A  | 161 | LEU  |
| 1   | 39-A  | 168 | HIS  |
| 1   | 39-A  | 185 | LEU  |
| 1   | 39-A  | 193 | HIS  |
| 1   | 39-A  | 203 | ASP  |
| 1   | 39-A  | 206 | LYS  |
| 1   | 40-A  | 2   | SER  |
| 1   | 40-A  | 5   | LYS  |
| 1   | 40-A  | 7   | GLU  |
| 1   | 40-A  | 21  | HIS  |
| 1   | 40-A  | 81  | GLN  |
| 1   | 40-A  | 90  | GLU  |
| 1   | 40-A  | 100 | ILE  |
| 1   | 40-A  | 116 | TYR  |
| 1   | 40-A  | 149 | GLU  |
| 1   | 40-A  | 153 | LEU  |
| 1   | 40-A  | 158 | GLU  |
| 1   | 40-A  | 174 | LYS  |
| 1   | 40-A  | 178 | LYS  |
| 1   | 40-A  | 180 | LYS  |
| 1   | 40-A  | 181 | LYS  |
| 1   | 40-A  | 185 | LEU  |
| 1   | 40-A  | 196 | GLU  |
| 1   | 40-A  | 203 | ASP  |
| 1   | 40-A  | 216 | ARG  |
| 1   | 40-A  | 217 | TYR  |
| 1   | 41-A  | 5   | LYS  |
| 1   | 41-A  | 21  | HIS  |
| 1   | 41-A  | 39  | THR  |
| 1   | 41-A  | 73  | GLU  |
| 1   | 41-A  | 78  | TYR  |
| 1   | 41-A  | 81  | GLN  |
| 1   | 41-A  | 116 | TYR  |
| 1   | 41-A  | 117 | GLU  |
| 1   | 41-A  | 124 | ASN  |
| 1   | 41-A  | 134 | LYS  |
| 1   | 41-A  | 143 | THR  |
| 1   | 41-A  | 153 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 41-A  | 174 | LYS  |
| 1   | 41-A  | 185 | LEU  |
| 1   | 41-A  | 194 | ARG  |
| 1   | 41-A  | 196 | GLU  |
| 1   | 41-A  | 203 | ASP  |
| 1   | 42-A  | 2   | SER  |
| 1   | 42-A  | 13  | ARG  |
| 1   | 42-A  | 28  | GLU  |
| 1   | 42-A  | 30  | ILE  |
| 1   | 42-A  | 41  | ASP  |
| 1   | 42-A  | 50  | LEU  |
| 1   | 42-A  | 81  | GLN  |
| 1   | 42-A  | 90  | GLU  |
| 1   | 42-A  | 100 | ILE  |
| 1   | 42-A  | 102 | ILE  |
| 1   | 42-A  | 106 | ASP  |
| 1   | 42-A  | 116 | TYR  |
| 1   | 42-A  | 117 | GLU  |
| 1   | 42-A  | 124 | ASN  |
| 1   | 42-A  | 128 | ASN  |
| 1   | 42-A  | 138 | LYS  |
| 1   | 42-A  | 143 | THR  |
| 1   | 42-A  | 148 | VAL  |
| 1   | 42-A  | 149 | GLU  |
| 1   | 42-A  | 150 | ASP  |
| 1   | 42-A  | 153 | LEU  |
| 1   | 42-A  | 154 | LYS  |
| 1   | 42-A  | 156 | ASP  |
| 1   | 42-A  | 161 | LEU  |
| 1   | 42-A  | 185 | LEU  |
| 1   | 42-A  | 193 | HIS  |
| 1   | 42-A  | 206 | LYS  |
| 1   | 43-A  | 8   | MET  |
| 1   | 43-A  | 11  | LYS  |
| 1   | 43-A  | 41  | ASP  |
| 1   | 43-A  | 74  | ASP  |
| 1   | 43-A  | 98  | GLN  |
| 1   | 43-A  | 109 | MET  |
| 1   | 43-A  | 116 | TYR  |
| 1   | 43-A  | 142 | PRO  |
| 1   | 43-A  | 148 | VAL  |
| 1   | 43-A  | 149 | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 43-A  | 150 | ASP  |
| 1   | 43-A  | 161 | LEU  |
| 1   | 43-A  | 185 | LEU  |
| 1   | 43-A  | 190 | GLU  |
| 1   | 43-A  | 192 | ASP  |
| 1   | 43-A  | 193 | HIS  |
| 1   | 43-A  | 194 | ARG  |
| 1   | 43-A  | 206 | LYS  |
| 1   | 43-A  | 211 | GLU  |
| 1   | 43-A  | 212 | HIS  |
| 1   | 44-A  | 2   | SER  |
| 1   | 44-A  | 3   | VAL  |
| 1   | 44-A  | 11  | LYS  |
| 1   | 44-A  | 13  | ARG  |
| 1   | 44-A  | 30  | ILE  |
| 1   | 44-A  | 39  | THR  |
| 1   | 44-A  | 41  | ASP  |
| 1   | 44-A  | 50  | LEU  |
| 1   | 44-A  | 55  | ASP  |
| 1   | 44-A  | 73  | GLU  |
| 1   | 44-A  | 98  | GLN  |
| 1   | 44-A  | 110 | GLU  |
| 1   | 44-A  | 112 | ASP  |
| 1   | 44-A  | 116 | TYR  |
| 1   | 44-A  | 128 | ASN  |
| 1   | 44-A  | 134 | LYS  |
| 1   | 44-A  | 141 | SER  |
| 1   | 44-A  | 150 | ASP  |
| 1   | 44-A  | 153 | LEU  |
| 1   | 44-A  | 154 | LYS  |
| 1   | 44-A  | 156 | ASP  |
| 1   | 44-A  | 177 | TYR  |
| 1   | 44-A  | 178 | LYS  |
| 1   | 44-A  | 185 | LEU  |
| 1   | 44-A  | 190 | GLU  |
| 1   | 44-A  | 212 | HIS  |
| 1   | 44-A  | 217 | TYR  |
| 1   | 45-A  | 7   | GLU  |
| 1   | 45-A  | 11  | LYS  |
| 1   | 45-A  | 50  | LEU  |
| 1   | 45-A  | 81  | GLN  |
| 1   | 45-A  | 110 | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 45-A  | 112 | ASP  |
| 1   | 45-A  | 116 | TYR  |
| 1   | 45-A  | 134 | LYS  |
| 1   | 45-A  | 143 | THR  |
| 1   | 45-A  | 181 | LYS  |
| 1   | 45-A  | 202 | LYS  |
| 1   | 45-A  | 216 | ARG  |
| 1   | 46-A  | 3   | VAL  |
| 1   | 46-A  | 11  | LYS  |
| 1   | 46-A  | 19  | ASN  |
| 1   | 46-A  | 35  | GLU  |
| 1   | 46-A  | 53  | SER  |
| 1   | 46-A  | 81  | GLN  |
| 1   | 46-A  | 123 | THR  |
| 1   | 46-A  | 128 | ASN  |
| 1   | 46-A  | 132 | MET  |
| 1   | 46-A  | 143 | THR  |
| 1   | 46-A  | 146 | MET  |
| 1   | 46-A  | 150 | ASP  |
| 1   | 46-A  | 161 | LEU  |
| 1   | 46-A  | 168 | HIS  |
| 1   | 46-A  | 170 | ARG  |
| 1   | 46-A  | 181 | LYS  |
| 1   | 46-A  | 185 | LEU  |
| 1   | 46-A  | 187 | ASP  |
| 1   | 46-A  | 192 | ASP  |
| 1   | 46-A  | 193 | HIS  |
| 1   | 46-A  | 194 | ARG  |
| 1   | 46-A  | 216 | ARG  |
| 1   | 46-A  | 217 | TYR  |
| 1   | 47-A  | 11  | LYS  |
| 1   | 47-A  | 19  | ASN  |
| 1   | 47-A  | 35  | GLU  |
| 1   | 47-A  | 53  | SER  |
| 1   | 47-A  | 116 | TYR  |
| 1   | 47-A  | 124 | ASN  |
| 1   | 47-A  | 132 | MET  |
| 1   | 47-A  | 141 | SER  |
| 1   | 47-A  | 145 | LYS  |
| 1   | 47-A  | 150 | ASP  |
| 1   | 47-A  | 152 | VAL  |
| 1   | 47-A  | 154 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 47-A  | 156 | ASP  |
| 1   | 47-A  | 161 | LEU  |
| 1   | 47-A  | 178 | LYS  |
| 1   | 47-A  | 181 | LYS  |
| 1   | 47-A  | 185 | LEU  |
| 1   | 47-A  | 194 | ARG  |
| 1   | 47-A  | 196 | GLU  |
| 1   | 47-A  | 214 | GLU  |
| 1   | 47-A  | 216 | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (142) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-A   | 19  | ASN  |
| 1   | 1-A   | 81  | GLN  |
| 1   | 1-A   | 193 | HIS  |
| 1   | 2-A   | 19  | ASN  |
| 1   | 2-A   | 81  | GLN  |
| 1   | 2-A   | 133 | GLN  |
| 1   | 2-A   | 193 | HIS  |
| 1   | 3-A   | 19  | ASN  |
| 1   | 3-A   | 81  | GLN  |
| 1   | 3-A   | 133 | GLN  |
| 1   | 4-A   | 19  | ASN  |
| 1   | 4-A   | 168 | HIS  |
| 1   | 5-A   | 19  | ASN  |
| 1   | 6-A   | 19  | ASN  |
| 1   | 6-A   | 81  | GLN  |
| 1   | 6-A   | 212 | HIS  |
| 1   | 7-A   | 19  | ASN  |
| 1   | 7-A   | 128 | ASN  |
| 1   | 7-A   | 205 | ASN  |
| 1   | 8-A   | 19  | ASN  |
| 1   | 8-A   | 81  | GLN  |
| 1   | 8-A   | 98  | GLN  |
| 1   | 8-A   | 128 | ASN  |
| 1   | 8-A   | 168 | HIS  |
| 1   | 8-A   | 193 | HIS  |
| 1   | 8-A   | 205 | ASN  |
| 1   | 9-A   | 19  | ASN  |
| 1   | 9-A   | 81  | GLN  |
| 1   | 9-A   | 128 | ASN  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 9-A   | 205 | ASN  |
| 1   | 10-A  | 19  | ASN  |
| 1   | 10-A  | 21  | HIS  |
| 1   | 10-A  | 128 | ASN  |
| 1   | 10-A  | 205 | ASN  |
| 1   | 11-A  | 19  | ASN  |
| 1   | 11-A  | 193 | HIS  |
| 1   | 11-A  | 205 | ASN  |
| 1   | 11-A  | 212 | HIS  |
| 1   | 12-A  | 19  | ASN  |
| 1   | 12-A  | 21  | HIS  |
| 1   | 12-A  | 81  | GLN  |
| 1   | 12-A  | 205 | ASN  |
| 1   | 13-A  | 19  | ASN  |
| 1   | 13-A  | 128 | ASN  |
| 1   | 13-A  | 133 | GLN  |
| 1   | 13-A  | 205 | ASN  |
| 1   | 13-A  | 212 | HIS  |
| 1   | 14-A  | 19  | ASN  |
| 1   | 14-A  | 124 | ASN  |
| 1   | 14-A  | 128 | ASN  |
| 1   | 15-A  | 19  | ASN  |
| 1   | 15-A  | 81  | GLN  |
| 1   | 15-A  | 98  | GLN  |
| 1   | 16-A  | 19  | ASN  |
| 1   | 16-A  | 81  | GLN  |
| 1   | 16-A  | 98  | GLN  |
| 1   | 16-A  | 212 | HIS  |
| 1   | 17-A  | 19  | ASN  |
| 1   | 17-A  | 81  | GLN  |
| 1   | 18-A  | 19  | ASN  |
| 1   | 18-A  | 212 | HIS  |
| 1   | 19-A  | 19  | ASN  |
| 1   | 19-A  | 81  | GLN  |
| 1   | 19-A  | 205 | ASN  |
| 1   | 20-A  | 19  | ASN  |
| 1   | 20-A  | 38  | GLN  |
| 1   | 20-A  | 81  | GLN  |
| 1   | 20-A  | 193 | HIS  |
| 1   | 21-A  | 19  | ASN  |
| 1   | 21-A  | 128 | ASN  |
| 1   | 21-A  | 193 | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 21-A  | 212 | HIS  |
| 1   | 22-A  | 193 | HIS  |
| 1   | 23-A  | 81  | GLN  |
| 1   | 23-A  | 168 | HIS  |
| 1   | 24-A  | 81  | GLN  |
| 1   | 26-A  | 98  | GLN  |
| 1   | 26-A  | 124 | ASN  |
| 1   | 26-A  | 168 | HIS  |
| 1   | 26-A  | 205 | ASN  |
| 1   | 27-A  | 21  | HIS  |
| 1   | 27-A  | 124 | ASN  |
| 1   | 27-A  | 205 | ASN  |
| 1   | 28-A  | 21  | HIS  |
| 1   | 28-A  | 124 | ASN  |
| 1   | 28-A  | 128 | ASN  |
| 1   | 28-A  | 133 | GLN  |
| 1   | 29-A  | 124 | ASN  |
| 1   | 29-A  | 128 | ASN  |
| 1   | 29-A  | 205 | ASN  |
| 1   | 29-A  | 212 | HIS  |
| 1   | 30-A  | 21  | HIS  |
| 1   | 30-A  | 81  | GLN  |
| 1   | 30-A  | 205 | ASN  |
| 1   | 31-A  | 21  | HIS  |
| 1   | 31-A  | 81  | GLN  |
| 1   | 31-A  | 128 | ASN  |
| 1   | 31-A  | 133 | GLN  |
| 1   | 31-A  | 212 | HIS  |
| 1   | 32-A  | 133 | GLN  |
| 1   | 33-A  | 212 | HIS  |
| 1   | 34-A  | 21  | HIS  |
| 1   | 34-A  | 133 | GLN  |
| 1   | 35-A  | 21  | HIS  |
| 1   | 35-A  | 98  | GLN  |
| 1   | 35-A  | 133 | GLN  |
| 1   | 35-A  | 193 | HIS  |
| 1   | 36-A  | 98  | GLN  |
| 1   | 36-A  | 124 | ASN  |
| 1   | 37-A  | 21  | HIS  |
| 1   | 37-A  | 124 | ASN  |
| 1   | 37-A  | 128 | ASN  |
| 1   | 37-A  | 193 | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 39-A  | 21  | HIS  |
| 1   | 39-A  | 133 | GLN  |
| 1   | 40-A  | 81  | GLN  |
| 1   | 40-A  | 193 | HIS  |
| 1   | 40-A  | 205 | ASN  |
| 1   | 41-A  | 81  | GLN  |
| 1   | 41-A  | 124 | ASN  |
| 1   | 42-A  | 98  | GLN  |
| 1   | 42-A  | 124 | ASN  |
| 1   | 42-A  | 193 | HIS  |
| 1   | 43-A  | 38  | GLN  |
| 1   | 43-A  | 124 | ASN  |
| 1   | 43-A  | 128 | ASN  |
| 1   | 43-A  | 133 | GLN  |
| 1   | 43-A  | 212 | HIS  |
| 1   | 44-A  | 133 | GLN  |
| 1   | 45-A  | 19  | ASN  |
| 1   | 45-A  | 133 | GLN  |
| 1   | 45-A  | 193 | HIS  |
| 1   | 45-A  | 212 | HIS  |
| 1   | 46-A  | 19  | ASN  |
| 1   | 46-A  | 81  | GLN  |
| 1   | 46-A  | 133 | GLN  |
| 1   | 46-A  | 168 | HIS  |
| 1   | 47-A  | 19  | ASN  |
| 1   | 47-A  | 38  | GLN  |
| 1   | 47-A  | 81  | GLN  |
| 1   | 47-A  | 98  | GLN  |
| 1   | 47-A  | 212 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | CRQ  | 29-A  | 62  | 1    | 24,25,26     | 2.02 | 5 (20%)  | 27,34,36    | 2.16 | 11 (40%) |
| 1   | CRQ  | 16-A  | 62  | 1    | 24,25,26     | 1.98 | 7 (29%)  | 27,34,36    | 1.58 | 3 (11%)  |
| 1   | CRQ  | 25-A  | 62  | 1    | 24,25,26     | 2.04 | 7 (29%)  | 27,34,36    | 1.68 | 6 (22%)  |
| 1   | CRQ  | 31-A  | 62  | 1    | 24,25,26     | 1.95 | 6 (25%)  | 27,34,36    | 1.37 | 4 (14%)  |
| 1   | CRQ  | 30-A  | 62  | 1    | 24,25,26     | 1.93 | 7 (29%)  | 27,34,36    | 1.54 | 6 (22%)  |
| 1   | CRQ  | 35-A  | 62  | 1    | 24,25,26     | 2.10 | 6 (25%)  | 27,34,36    | 2.26 | 10 (37%) |
| 1   | CRQ  | 24-A  | 62  | 1    | 24,25,26     | 1.81 | 6 (25%)  | 27,34,36    | 1.41 | 5 (18%)  |
| 1   | CRQ  | 3-A   | 62  | 1    | 24,25,26     | 1.95 | 7 (29%)  | 27,34,36    | 1.69 | 5 (18%)  |
| 1   | CRQ  | 2-A   | 62  | 1    | 24,25,26     | 2.09 | 8 (33%)  | 27,34,36    | 1.35 | 4 (14%)  |
| 1   | CRQ  | 7-A   | 62  | 1    | 24,25,26     | 2.32 | 8 (33%)  | 27,34,36    | 1.58 | 4 (14%)  |
| 1   | CRQ  | 18-A  | 62  | 1    | 24,25,26     | 2.17 | 6 (25%)  | 27,34,36    | 1.55 | 5 (18%)  |
| 1   | CRQ  | 4-A   | 62  | 1    | 24,25,26     | 2.21 | 6 (25%)  | 27,34,36    | 1.80 | 7 (25%)  |
| 1   | CRQ  | 13-A  | 62  | 1    | 24,25,26     | 2.16 | 7 (29%)  | 27,34,36    | 1.48 | 3 (11%)  |
| 1   | CRQ  | 27-A  | 62  | 1    | 24,25,26     | 1.96 | 7 (29%)  | 27,34,36    | 1.29 | 3 (11%)  |
| 1   | CRQ  | 22-A  | 62  | 1    | 24,25,26     | 2.04 | 6 (25%)  | 27,34,36    | 1.61 | 8 (29%)  |
| 1   | CRQ  | 21-A  | 62  | 1    | 24,25,26     | 2.10 | 7 (29%)  | 27,34,36    | 1.58 | 4 (14%)  |
| 1   | CRQ  | 41-A  | 62  | 1    | 24,25,26     | 2.12 | 7 (29%)  | 27,34,36    | 1.51 | 6 (22%)  |
| 1   | CRQ  | 47-A  | 62  | 1    | 24,25,26     | 2.04 | 6 (25%)  | 27,34,36    | 1.83 | 7 (25%)  |
| 1   | CRQ  | 20-A  | 62  | 1    | 24,25,26     | 1.81 | 6 (25%)  | 27,34,36    | 1.24 | 3 (11%)  |
| 1   | CRQ  | 36-A  | 62  | 1    | 24,25,26     | 2.04 | 8 (33%)  | 27,34,36    | 1.73 | 4 (14%)  |
| 1   | CRQ  | 6-A   | 62  | 1    | 24,25,26     | 2.06 | 6 (25%)  | 27,34,36    | 2.09 | 9 (33%)  |
| 1   | CRQ  | 33-A  | 62  | 1    | 24,25,26     | 1.88 | 5 (20%)  | 27,34,36    | 1.98 | 10 (37%) |
| 1   | CRQ  | 37-A  | 62  | 1    | 24,25,26     | 2.13 | 7 (29%)  | 27,34,36    | 1.56 | 6 (22%)  |
| 1   | CRQ  | 1-A   | 62  | 1    | 24,25,26     | 1.94 | 5 (20%)  | 27,34,36    | 2.07 | 10 (37%) |
| 1   | CRQ  | 39-A  | 62  | 1    | 24,25,26     | 2.07 | 7 (29%)  | 27,34,36    | 1.36 | 4 (14%)  |
| 1   | CRQ  | 23-A  | 62  | 1    | 24,25,26     | 2.00 | 7 (29%)  | 27,34,36    | 1.53 | 3 (11%)  |
| 1   | CRQ  | 10-A  | 62  | 1    | 24,25,26     | 1.98 | 6 (25%)  | 27,34,36    | 1.48 | 5 (18%)  |
| 1   | CRQ  | 44-A  | 62  | 1    | 24,25,26     | 1.84 | 6 (25%)  | 27,34,36    | 1.43 | 4 (14%)  |
| 1   | CRQ  | 45-A  | 62  | 1    | 24,25,26     | 2.10 | 7 (29%)  | 27,34,36    | 1.49 | 3 (11%)  |
| 1   | CRQ  | 40-A  | 62  | 1    | 24,25,26     | 1.92 | 7 (29%)  | 27,34,36    | 1.54 | 7 (25%)  |
| 1   | CRQ  | 11-A  | 62  | 1    | 24,25,26     | 2.03 | 7 (29%)  | 27,34,36    | 1.65 | 5 (18%)  |
| 1   | CRQ  | 28-A  | 62  | 1    | 24,25,26     | 2.02 | 6 (25%)  | 27,34,36    | 1.58 | 5 (18%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | CRQ  | 8-A   | 62  | 1    | 24,25,26     | 1.91 | 6 (25%)  | 27,34,36    | 1.51 | 5 (18%)  |
| 1   | CRQ  | 26-A  | 62  | 1    | 24,25,26     | 1.74 | 6 (25%)  | 27,34,36    | 1.70 | 6 (22%)  |
| 1   | CRQ  | 38-A  | 62  | 1    | 24,25,26     | 1.92 | 6 (25%)  | 27,34,36    | 1.94 | 6 (22%)  |
| 1   | CRQ  | 5-A   | 62  | 1    | 24,25,26     | 1.97 | 6 (25%)  | 27,34,36    | 1.62 | 5 (18%)  |
| 1   | CRQ  | 17-A  | 62  | 1    | 24,25,26     | 1.80 | 6 (25%)  | 27,34,36    | 1.54 | 4 (14%)  |
| 1   | CRQ  | 12-A  | 62  | 1    | 24,25,26     | 2.13 | 6 (25%)  | 27,34,36    | 1.91 | 8 (29%)  |
| 1   | CRQ  | 9-A   | 62  | 1    | 24,25,26     | 1.80 | 5 (20%)  | 27,34,36    | 1.93 | 7 (25%)  |
| 1   | CRQ  | 19-A  | 62  | 1    | 24,25,26     | 2.11 | 5 (20%)  | 27,34,36    | 2.44 | 9 (33%)  |
| 1   | CRQ  | 14-A  | 62  | 1    | 24,25,26     | 2.10 | 6 (25%)  | 27,34,36    | 1.87 | 7 (25%)  |
| 1   | CRQ  | 34-A  | 62  | 1    | 24,25,26     | 1.98 | 6 (25%)  | 27,34,36    | 1.38 | 4 (14%)  |
| 1   | CRQ  | 32-A  | 62  | 1    | 24,25,26     | 2.24 | 6 (25%)  | 27,34,36    | 2.45 | 10 (37%) |
| 1   | CRQ  | 15-A  | 62  | 1    | 24,25,26     | 2.11 | 6 (25%)  | 27,34,36    | 2.03 | 11 (40%) |
| 1   | CRQ  | 43-A  | 62  | 1    | 24,25,26     | 2.06 | 8 (33%)  | 27,34,36    | 1.58 | 4 (14%)  |
| 1   | CRQ  | 46-A  | 62  | 1    | 24,25,26     | 2.22 | 6 (25%)  | 27,34,36    | 1.54 | 4 (14%)  |
| 1   | CRQ  | 42-A  | 62  | 1    | 24,25,26     | 2.06 | 7 (29%)  | 27,34,36    | 1.70 | 4 (14%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 1   | CRQ  | 29-A  | 62  | 1    | -       | 3/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 16-A  | 62  | 1    | -       | 0/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 25-A  | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 31-A  | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 30-A  | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 35-A  | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 24-A  | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 3-A   | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 2-A   | 62  | 1    | -       | 1/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 7-A   | 62  | 1    | -       | 1/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 18-A  | 62  | 1    | -       | 1/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 4-A   | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 13-A  | 62  | 1    | -       | 1/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 27-A  | 62  | 1    | -       | 1/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 22-A  | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |

Continued on next page...

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 1   | CRQ  | 21-A  | 62  | 1    | -       | 0/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 41-A  | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 47-A  | 62  | 1    | -       | 4/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 20-A  | 62  | 1    | -       | 3/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 36-A  | 62  | 1    | -       | 5/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 6-A   | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 33-A  | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 37-A  | 62  | 1    | -       | 1/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 1-A   | 62  | 1    | -       | 0/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 39-A  | 62  | 1    | -       | 0/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 23-A  | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 10-A  | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 44-A  | 62  | 1    | -       | 1/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 45-A  | 62  | 1    | -       | 1/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 40-A  | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 11-A  | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 28-A  | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 8-A   | 62  | 1    | -       | 1/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 26-A  | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 38-A  | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 5-A   | 62  | 1    | -       | 1/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 17-A  | 62  | 1    | -       | 3/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 12-A  | 62  | 1    | -       | 1/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 9-A   | 62  | 1    | -       | 1/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 19-A  | 62  | 1    | -       | 0/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 14-A  | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 34-A  | 62  | 1    | -       | 1/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 32-A  | 62  | 1    | -       | 0/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 15-A  | 62  | 1    | -       | 2/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 43-A  | 62  | 1    | -       | 1/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 46-A  | 62  | 1    | -       | 0/10/32/33 | 0/2/2/2 |
| 1   | CRQ  | 42-A  | 62  | 1    | -       | 0/10/32/33 | 0/2/2/2 |

All (300) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | 4-A   | 62  | CRQ  | CB2-CA2 | 6.28  | 1.40        | 1.35     |
| 1   | 19-A  | 62  | CRQ  | C1-N3   | 6.14  | 1.48        | 1.38     |
| 1   | 32-A  | 62  | CRQ  | CA2-C2  | -6.00 | 1.42        | 1.48     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | 37-A  | 62  | CRQ  | C1-N3   | 5.94  | 1.48        | 1.38     |
| 1   | 1-A   | 62  | CRQ  | C1-N3   | 5.84  | 1.48        | 1.38     |
| 1   | 32-A  | 62  | CRQ  | C1-N3   | 5.79  | 1.47        | 1.38     |
| 1   | 15-A  | 62  | CRQ  | C1-N3   | 5.78  | 1.47        | 1.38     |
| 1   | 47-A  | 62  | CRQ  | CA2-C2  | -5.68 | 1.43        | 1.48     |
| 1   | 7-A   | 62  | CRQ  | CB2-CA2 | 5.62  | 1.39        | 1.35     |
| 1   | 2-A   | 62  | CRQ  | CB2-CA2 | 5.61  | 1.39        | 1.35     |
| 1   | 36-A  | 62  | CRQ  | CB2-CA2 | 5.59  | 1.39        | 1.35     |
| 1   | 22-A  | 62  | CRQ  | C1-N3   | 5.45  | 1.47        | 1.38     |
| 1   | 6-A   | 62  | CRQ  | C1-N3   | 5.44  | 1.47        | 1.38     |
| 1   | 10-A  | 62  | CRQ  | C1-N3   | 5.43  | 1.47        | 1.38     |
| 1   | 19-A  | 62  | CRQ  | CA2-C2  | -5.40 | 1.43        | 1.48     |
| 1   | 41-A  | 62  | CRQ  | C1-N3   | 5.37  | 1.47        | 1.38     |
| 1   | 21-A  | 62  | CRQ  | C1-N3   | 5.17  | 1.46        | 1.38     |
| 1   | 46-A  | 62  | CRQ  | CA2-C2  | -5.17 | 1.43        | 1.48     |
| 1   | 39-A  | 62  | CRQ  | C1-N3   | 5.15  | 1.46        | 1.38     |
| 1   | 43-A  | 62  | CRQ  | CB2-CA2 | 5.11  | 1.39        | 1.35     |
| 1   | 7-A   | 62  | CRQ  | C1-N3   | 5.10  | 1.46        | 1.38     |
| 1   | 29-A  | 62  | CRQ  | CB2-CA2 | 5.08  | 1.39        | 1.35     |
| 1   | 42-A  | 62  | CRQ  | C1-N3   | 5.07  | 1.46        | 1.38     |
| 1   | 23-A  | 62  | CRQ  | C1-N3   | 5.07  | 1.46        | 1.38     |
| 1   | 11-A  | 62  | CRQ  | CB2-CA2 | 5.01  | 1.39        | 1.35     |
| 1   | 8-A   | 62  | CRQ  | C1-N3   | 5.00  | 1.46        | 1.38     |
| 1   | 5-A   | 62  | CRQ  | C1-N3   | 4.97  | 1.46        | 1.38     |
| 1   | 13-A  | 62  | CRQ  | CB2-CA2 | 4.94  | 1.39        | 1.35     |
| 1   | 47-A  | 62  | CRQ  | C1-N3   | 4.90  | 1.46        | 1.38     |
| 1   | 45-A  | 62  | CRQ  | C1-N3   | 4.86  | 1.46        | 1.38     |
| 1   | 20-A  | 62  | CRQ  | C1-N3   | 4.84  | 1.46        | 1.38     |
| 1   | 46-A  | 62  | CRQ  | C1-N3   | 4.82  | 1.46        | 1.38     |
| 1   | 21-A  | 62  | CRQ  | CB2-CA2 | 4.82  | 1.39        | 1.35     |
| 1   | 18-A  | 62  | CRQ  | C1-N3   | 4.81  | 1.46        | 1.38     |
| 1   | 35-A  | 62  | CRQ  | C1-N3   | 4.79  | 1.46        | 1.38     |
| 1   | 31-A  | 62  | CRQ  | CB2-CA2 | 4.74  | 1.39        | 1.35     |
| 1   | 16-A  | 62  | CRQ  | CB2-CA2 | 4.73  | 1.39        | 1.35     |
| 1   | 15-A  | 62  | CRQ  | CA2-C2  | -4.73 | 1.44        | 1.48     |
| 1   | 14-A  | 62  | CRQ  | C1-N3   | 4.70  | 1.46        | 1.38     |
| 1   | 18-A  | 62  | CRQ  | CA2-C2  | -4.69 | 1.44        | 1.48     |
| 1   | 11-A  | 62  | CRQ  | C1-N3   | 4.66  | 1.46        | 1.38     |
| 1   | 28-A  | 62  | CRQ  | C1-N3   | 4.65  | 1.46        | 1.38     |
| 1   | 45-A  | 62  | CRQ  | CA2-C2  | -4.60 | 1.44        | 1.48     |
| 1   | 33-A  | 62  | CRQ  | CA3-N3  | -4.60 | 1.38        | 1.47     |
| 1   | 4-A   | 62  | CRQ  | C1-N3   | 4.59  | 1.45        | 1.38     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | 14-A  | 62  | CRQ  | CA2-C2  | -4.58 | 1.44        | 1.48     |
| 1   | 12-A  | 62  | CRQ  | CB2-CA2 | 4.57  | 1.38        | 1.35     |
| 1   | 12-A  | 62  | CRQ  | C1-N3   | 4.57  | 1.45        | 1.38     |
| 1   | 46-A  | 62  | CRQ  | CB2-CA2 | 4.56  | 1.38        | 1.35     |
| 1   | 38-A  | 62  | CRQ  | C1-N3   | 4.54  | 1.45        | 1.38     |
| 1   | 3-A   | 62  | CRQ  | C1-N3   | 4.50  | 1.45        | 1.38     |
| 1   | 25-A  | 62  | CRQ  | C1-N3   | 4.48  | 1.45        | 1.38     |
| 1   | 13-A  | 62  | CRQ  | C1-N3   | 4.47  | 1.45        | 1.38     |
| 1   | 25-A  | 62  | CRQ  | CA3-N3  | -4.46 | 1.38        | 1.47     |
| 1   | 14-A  | 62  | CRQ  | CB2-CA2 | 4.42  | 1.38        | 1.35     |
| 1   | 12-A  | 62  | CRQ  | CA3-N3  | -4.42 | 1.38        | 1.47     |
| 1   | 37-A  | 62  | CRQ  | CA2-C2  | -4.41 | 1.44        | 1.48     |
| 1   | 10-A  | 62  | CRQ  | CA2-C2  | -4.39 | 1.44        | 1.48     |
| 1   | 18-A  | 62  | CRQ  | CB2-CA2 | 4.39  | 1.38        | 1.35     |
| 1   | 30-A  | 62  | CRQ  | CB2-CA2 | 4.38  | 1.38        | 1.35     |
| 1   | 42-A  | 62  | CRQ  | CB2-CA2 | 4.37  | 1.38        | 1.35     |
| 1   | 28-A  | 62  | CRQ  | CB2-CA2 | 4.35  | 1.38        | 1.35     |
| 1   | 35-A  | 62  | CRQ  | CA2-C2  | -4.34 | 1.44        | 1.48     |
| 1   | 41-A  | 62  | CRQ  | CB2-CA2 | 4.33  | 1.38        | 1.35     |
| 1   | 17-A  | 62  | CRQ  | CA2-C2  | -4.32 | 1.44        | 1.48     |
| 1   | 40-A  | 62  | CRQ  | CA2-C2  | -4.29 | 1.44        | 1.48     |
| 1   | 38-A  | 62  | CRQ  | CB2-CA2 | 4.24  | 1.38        | 1.35     |
| 1   | 25-A  | 62  | CRQ  | CA2-C2  | -4.20 | 1.44        | 1.48     |
| 1   | 30-A  | 62  | CRQ  | C1-N3   | 4.17  | 1.45        | 1.38     |
| 1   | 35-A  | 62  | CRQ  | CA3-N3  | -4.17 | 1.39        | 1.47     |
| 1   | 34-A  | 62  | CRQ  | C1-N3   | 4.16  | 1.45        | 1.38     |
| 1   | 7-A   | 62  | CRQ  | CA2-C2  | -4.15 | 1.44        | 1.48     |
| 1   | 3-A   | 62  | CRQ  | CA2-C2  | -4.14 | 1.44        | 1.48     |
| 1   | 27-A  | 62  | CRQ  | CA2-C2  | -4.14 | 1.44        | 1.48     |
| 1   | 27-A  | 62  | CRQ  | C1-N3   | 4.14  | 1.45        | 1.38     |
| 1   | 43-A  | 62  | CRQ  | C1-N3   | 4.13  | 1.45        | 1.38     |
| 1   | 42-A  | 62  | CRQ  | CA2-C2  | -4.12 | 1.44        | 1.48     |
| 1   | 35-A  | 62  | CRQ  | CB2-CA2 | 4.11  | 1.38        | 1.35     |
| 1   | 22-A  | 62  | CRQ  | CA2-C2  | -4.08 | 1.44        | 1.48     |
| 1   | 44-A  | 62  | CRQ  | C1-N3   | 4.07  | 1.45        | 1.38     |
| 1   | 33-A  | 62  | CRQ  | CA2-C2  | -4.04 | 1.44        | 1.48     |
| 1   | 13-A  | 62  | CRQ  | CA2-C2  | -4.04 | 1.44        | 1.48     |
| 1   | 18-A  | 62  | CRQ  | CA3-N3  | -4.04 | 1.39        | 1.47     |
| 1   | 4-A   | 62  | CRQ  | CA1-N   | 4.03  | 1.37        | 1.27     |
| 1   | 26-A  | 62  | CRQ  | C1-N3   | 4.01  | 1.45        | 1.38     |
| 1   | 6-A   | 62  | CRQ  | CA3-N3  | -4.01 | 1.39        | 1.47     |
| 1   | 45-A  | 62  | CRQ  | CA3-N3  | -4.00 | 1.39        | 1.47     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | 29-A  | 62  | CRQ  | C1-N3   | 4.00  | 1.45        | 1.38     |
| 1   | 31-A  | 62  | CRQ  | CA3-N3  | -3.99 | 1.39        | 1.47     |
| 1   | 34-A  | 62  | CRQ  | CB2-CA2 | 3.99  | 1.38        | 1.35     |
| 1   | 34-A  | 62  | CRQ  | CA2-C2  | -3.97 | 1.44        | 1.48     |
| 1   | 9-A   | 62  | CRQ  | CA2-C2  | -3.97 | 1.44        | 1.48     |
| 1   | 46-A  | 62  | CRQ  | CA3-N3  | -3.94 | 1.39        | 1.47     |
| 1   | 44-A  | 62  | CRQ  | CA2-C2  | -3.93 | 1.44        | 1.48     |
| 1   | 29-A  | 62  | CRQ  | CA3-N3  | -3.92 | 1.39        | 1.47     |
| 1   | 31-A  | 62  | CRQ  | C1-N3   | 3.92  | 1.44        | 1.38     |
| 1   | 23-A  | 62  | CRQ  | CB2-CA2 | 3.92  | 1.38        | 1.35     |
| 1   | 13-A  | 62  | CRQ  | CA3-N3  | -3.91 | 1.39        | 1.47     |
| 1   | 39-A  | 62  | CRQ  | CA2-C2  | -3.90 | 1.44        | 1.48     |
| 1   | 16-A  | 62  | CRQ  | C1-N3   | 3.89  | 1.44        | 1.38     |
| 1   | 27-A  | 62  | CRQ  | CB2-CA2 | 3.89  | 1.38        | 1.35     |
| 1   | 28-A  | 62  | CRQ  | CA2-C2  | -3.88 | 1.44        | 1.48     |
| 1   | 12-A  | 62  | CRQ  | CA2-C2  | -3.86 | 1.44        | 1.48     |
| 1   | 3-A   | 62  | CRQ  | CA1-N   | 3.84  | 1.36        | 1.27     |
| 1   | 26-A  | 62  | CRQ  | CA3-N3  | -3.84 | 1.39        | 1.47     |
| 1   | 28-A  | 62  | CRQ  | CA1-N   | 3.82  | 1.36        | 1.27     |
| 1   | 21-A  | 62  | CRQ  | CA1-N   | 3.80  | 1.36        | 1.27     |
| 1   | 8-A   | 62  | CRQ  | CB2-CA2 | 3.80  | 1.38        | 1.35     |
| 1   | 7-A   | 62  | CRQ  | CA3-N3  | -3.80 | 1.39        | 1.47     |
| 1   | 22-A  | 62  | CRQ  | CB2-CA2 | 3.78  | 1.38        | 1.35     |
| 1   | 1-A   | 62  | CRQ  | CA2-C2  | -3.78 | 1.44        | 1.48     |
| 1   | 6-A   | 62  | CRQ  | CA1-N   | 3.78  | 1.36        | 1.27     |
| 1   | 33-A  | 62  | CRQ  | C1-N3   | 3.77  | 1.44        | 1.38     |
| 1   | 17-A  | 62  | CRQ  | C1-N3   | 3.76  | 1.44        | 1.38     |
| 1   | 15-A  | 62  | CRQ  | CA1-N   | 3.75  | 1.36        | 1.27     |
| 1   | 21-A  | 62  | CRQ  | CA2-C2  | -3.75 | 1.44        | 1.48     |
| 1   | 5-A   | 62  | CRQ  | CA1-N   | 3.73  | 1.36        | 1.27     |
| 1   | 41-A  | 62  | CRQ  | CA2-C2  | -3.72 | 1.44        | 1.48     |
| 1   | 32-A  | 62  | CRQ  | CA1-N   | 3.69  | 1.36        | 1.27     |
| 1   | 47-A  | 62  | CRQ  | CA3-N3  | -3.68 | 1.39        | 1.47     |
| 1   | 40-A  | 62  | CRQ  | CA3-N3  | -3.68 | 1.40        | 1.47     |
| 1   | 24-A  | 62  | CRQ  | CA2-C2  | -3.67 | 1.45        | 1.48     |
| 1   | 16-A  | 62  | CRQ  | CA1-N   | 3.66  | 1.36        | 1.27     |
| 1   | 24-A  | 62  | CRQ  | C1-N3   | 3.66  | 1.44        | 1.38     |
| 1   | 41-A  | 62  | CRQ  | CA1-N   | 3.66  | 1.36        | 1.27     |
| 1   | 23-A  | 62  | CRQ  | CA2-C2  | -3.65 | 1.45        | 1.48     |
| 1   | 39-A  | 62  | CRQ  | CB2-CA2 | 3.65  | 1.38        | 1.35     |
| 1   | 38-A  | 62  | CRQ  | CA1-N   | 3.64  | 1.36        | 1.27     |
| 1   | 45-A  | 62  | CRQ  | CB2-CA2 | 3.63  | 1.38        | 1.35     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | 32-A  | 62  | CRQ  | CB2-CA2 | 3.62  | 1.38        | 1.35     |
| 1   | 33-A  | 62  | CRQ  | CA1-N   | 3.61  | 1.36        | 1.27     |
| 1   | 40-A  | 62  | CRQ  | C1-N3   | 3.61  | 1.44        | 1.38     |
| 1   | 36-A  | 62  | CRQ  | CA2-C2  | -3.61 | 1.45        | 1.48     |
| 1   | 9-A   | 62  | CRQ  | C1-N3   | 3.61  | 1.44        | 1.38     |
| 1   | 13-A  | 62  | CRQ  | CA1-N   | 3.61  | 1.36        | 1.27     |
| 1   | 39-A  | 62  | CRQ  | CA3-N3  | -3.58 | 1.40        | 1.47     |
| 1   | 2-A   | 62  | CRQ  | CA3-N3  | -3.56 | 1.40        | 1.47     |
| 1   | 5-A   | 62  | CRQ  | CA3-N3  | -3.54 | 1.40        | 1.47     |
| 1   | 41-A  | 62  | CRQ  | CA3-N3  | -3.53 | 1.40        | 1.47     |
| 1   | 24-A  | 62  | CRQ  | CB2-CA2 | 3.52  | 1.38        | 1.35     |
| 1   | 34-A  | 62  | CRQ  | CA3-N3  | -3.52 | 1.40        | 1.47     |
| 1   | 34-A  | 62  | CRQ  | CA1-N   | 3.51  | 1.36        | 1.27     |
| 1   | 22-A  | 62  | CRQ  | CA1-N   | 3.50  | 1.36        | 1.27     |
| 1   | 2-A   | 62  | CRQ  | C1-N3   | 3.50  | 1.44        | 1.38     |
| 1   | 25-A  | 62  | CRQ  | CA1-N   | 3.49  | 1.35        | 1.27     |
| 1   | 40-A  | 62  | CRQ  | CA1-N   | 3.49  | 1.35        | 1.27     |
| 1   | 17-A  | 62  | CRQ  | CA3-N3  | -3.49 | 1.40        | 1.47     |
| 1   | 45-A  | 62  | CRQ  | CA1-N   | 3.48  | 1.35        | 1.27     |
| 1   | 36-A  | 62  | CRQ  | C1-N3   | 3.48  | 1.44        | 1.38     |
| 1   | 5-A   | 62  | CRQ  | CA2-C2  | -3.48 | 1.45        | 1.48     |
| 1   | 9-A   | 62  | CRQ  | CA1-N   | 3.47  | 1.35        | 1.27     |
| 1   | 29-A  | 62  | CRQ  | CA1-N   | 3.45  | 1.35        | 1.27     |
| 1   | 20-A  | 62  | CRQ  | CA1-N   | 3.44  | 1.35        | 1.27     |
| 1   | 12-A  | 62  | CRQ  | CA1-N   | 3.44  | 1.35        | 1.27     |
| 1   | 30-A  | 62  | CRQ  | CA1-N   | 3.43  | 1.35        | 1.27     |
| 1   | 20-A  | 62  | CRQ  | CB2-CA2 | 3.43  | 1.38        | 1.35     |
| 1   | 46-A  | 62  | CRQ  | CA1-N   | 3.42  | 1.35        | 1.27     |
| 1   | 11-A  | 62  | CRQ  | CA2-C2  | -3.41 | 1.45        | 1.48     |
| 1   | 23-A  | 62  | CRQ  | CA1-N   | 3.39  | 1.35        | 1.27     |
| 1   | 30-A  | 62  | CRQ  | CA2-C2  | -3.39 | 1.45        | 1.48     |
| 1   | 44-A  | 62  | CRQ  | CA3-N3  | -3.39 | 1.40        | 1.47     |
| 1   | 39-A  | 62  | CRQ  | CA1-N   | 3.38  | 1.35        | 1.27     |
| 1   | 6-A   | 62  | CRQ  | CA2-C2  | -3.37 | 1.45        | 1.48     |
| 1   | 27-A  | 62  | CRQ  | CA3-N3  | -3.36 | 1.40        | 1.47     |
| 1   | 14-A  | 62  | CRQ  | CA1-N   | 3.34  | 1.35        | 1.27     |
| 1   | 40-A  | 62  | CRQ  | CB2-CA2 | 3.34  | 1.37        | 1.35     |
| 1   | 5-A   | 62  | CRQ  | CB2-CA2 | 3.33  | 1.37        | 1.35     |
| 1   | 17-A  | 62  | CRQ  | CA1-N   | 3.31  | 1.35        | 1.27     |
| 1   | 1-A   | 62  | CRQ  | CA1-N   | 3.30  | 1.35        | 1.27     |
| 1   | 27-A  | 62  | CRQ  | CA1-N   | 3.29  | 1.35        | 1.27     |
| 1   | 24-A  | 62  | CRQ  | CA1-N   | 3.29  | 1.35        | 1.27     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | 37-A  | 62  | CRQ  | CA3-N3  | -3.28 | 1.40        | 1.47     |
| 1   | 31-A  | 62  | CRQ  | CA1-N   | 3.27  | 1.35        | 1.27     |
| 1   | 24-A  | 62  | CRQ  | CA3-N3  | -3.25 | 1.40        | 1.47     |
| 1   | 43-A  | 62  | CRQ  | CA3-N3  | -3.25 | 1.40        | 1.47     |
| 1   | 8-A   | 62  | CRQ  | CA1-N   | 3.25  | 1.35        | 1.27     |
| 1   | 44-A  | 62  | CRQ  | CA1-N   | 3.25  | 1.35        | 1.27     |
| 1   | 29-A  | 62  | CRQ  | CD3-NE1 | 3.24  | 1.43        | 1.32     |
| 1   | 19-A  | 62  | CRQ  | CA1-N   | 3.21  | 1.35        | 1.27     |
| 1   | 3-A   | 62  | CRQ  | CB2-CA2 | 3.21  | 1.37        | 1.35     |
| 1   | 44-A  | 62  | CRQ  | CB2-CA2 | 3.19  | 1.37        | 1.35     |
| 1   | 9-A   | 62  | CRQ  | CD3-NE1 | 3.19  | 1.43        | 1.32     |
| 1   | 10-A  | 62  | CRQ  | CA1-N   | 3.18  | 1.35        | 1.27     |
| 1   | 7-A   | 62  | CRQ  | CA1-N   | 3.18  | 1.35        | 1.27     |
| 1   | 14-A  | 62  | CRQ  | CA3-N3  | -3.17 | 1.41        | 1.47     |
| 1   | 2-A   | 62  | CRQ  | CA1-N   | 3.17  | 1.35        | 1.27     |
| 1   | 8-A   | 62  | CRQ  | CA2-C2  | -3.17 | 1.45        | 1.48     |
| 1   | 42-A  | 62  | CRQ  | CA1-N   | 3.16  | 1.35        | 1.27     |
| 1   | 38-A  | 62  | CRQ  | CD3-NE1 | 3.14  | 1.43        | 1.32     |
| 1   | 25-A  | 62  | CRQ  | CB2-CA2 | 3.14  | 1.37        | 1.35     |
| 1   | 16-A  | 62  | CRQ  | CA3-N3  | -3.11 | 1.41        | 1.47     |
| 1   | 9-A   | 62  | CRQ  | CA3-N3  | -3.11 | 1.41        | 1.47     |
| 1   | 43-A  | 62  | CRQ  | CA1-N   | 3.11  | 1.35        | 1.27     |
| 1   | 37-A  | 62  | CRQ  | CB2-CA2 | 3.10  | 1.37        | 1.35     |
| 1   | 14-A  | 62  | CRQ  | CD3-NE1 | 3.10  | 1.42        | 1.32     |
| 1   | 6-A   | 62  | CRQ  | CB2-CA2 | 3.09  | 1.37        | 1.35     |
| 1   | 42-A  | 62  | CRQ  | CA3-N3  | -3.09 | 1.41        | 1.47     |
| 1   | 26-A  | 62  | CRQ  | CA1-N   | 3.09  | 1.35        | 1.27     |
| 1   | 15-A  | 62  | CRQ  | CD3-NE1 | 3.07  | 1.42        | 1.32     |
| 1   | 30-A  | 62  | CRQ  | CA3-N3  | -3.07 | 1.41        | 1.47     |
| 1   | 42-A  | 62  | CRQ  | CD3-NE1 | 3.06  | 1.42        | 1.32     |
| 1   | 31-A  | 62  | CRQ  | CD3-NE1 | 3.06  | 1.42        | 1.32     |
| 1   | 47-A  | 62  | CRQ  | CA1-N   | 3.06  | 1.34        | 1.27     |
| 1   | 6-A   | 62  | CRQ  | CD3-NE1 | 3.05  | 1.42        | 1.32     |
| 1   | 2-A   | 62  | CRQ  | CD3-NE1 | 3.04  | 1.42        | 1.32     |
| 1   | 10-A  | 62  | CRQ  | CD3-NE1 | 3.04  | 1.42        | 1.32     |
| 1   | 35-A  | 62  | CRQ  | CA1-N   | 3.04  | 1.34        | 1.27     |
| 1   | 16-A  | 62  | CRQ  | CD3-NE1 | 3.04  | 1.42        | 1.32     |
| 1   | 43-A  | 62  | CRQ  | CA2-C2  | -3.03 | 1.45        | 1.48     |
| 1   | 25-A  | 62  | CRQ  | CD3-NE1 | 3.01  | 1.42        | 1.32     |
| 1   | 43-A  | 62  | CRQ  | CD3-NE1 | 3.01  | 1.42        | 1.32     |
| 1   | 19-A  | 62  | CRQ  | CD3-NE1 | 3.00  | 1.42        | 1.32     |
| 1   | 11-A  | 62  | CRQ  | CA1-N   | 3.00  | 1.34        | 1.27     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | 26-A  | 62  | CRQ  | CA2-C2  | -3.00 | 1.45        | 1.48     |
| 1   | 39-A  | 62  | CRQ  | CD3-NE1 | 2.99  | 1.42        | 1.32     |
| 1   | 3-A   | 62  | CRQ  | CA3-N3  | -2.99 | 1.41        | 1.47     |
| 1   | 37-A  | 62  | CRQ  | CA1-N   | 2.98  | 1.34        | 1.27     |
| 1   | 15-A  | 62  | CRQ  | CB2-CA2 | 2.98  | 1.37        | 1.35     |
| 1   | 1-A   | 62  | CRQ  | CA3-N3  | -2.97 | 1.41        | 1.47     |
| 1   | 36-A  | 62  | CRQ  | CA1-N   | 2.97  | 1.34        | 1.27     |
| 1   | 28-A  | 62  | CRQ  | CD3-NE1 | 2.96  | 1.42        | 1.32     |
| 1   | 10-A  | 62  | CRQ  | CB2-CA2 | 2.96  | 1.37        | 1.35     |
| 1   | 2-A   | 62  | CRQ  | CA2-C2  | -2.96 | 1.45        | 1.48     |
| 1   | 45-A  | 62  | CRQ  | CD3-NE1 | 2.96  | 1.42        | 1.32     |
| 1   | 16-A  | 62  | CRQ  | CA2-C2  | -2.95 | 1.45        | 1.48     |
| 1   | 32-A  | 62  | CRQ  | CD3-NE1 | 2.95  | 1.42        | 1.32     |
| 1   | 37-A  | 62  | CRQ  | CD3-NE1 | 2.94  | 1.42        | 1.32     |
| 1   | 19-A  | 62  | CRQ  | CA3-N3  | -2.94 | 1.41        | 1.47     |
| 1   | 46-A  | 62  | CRQ  | CD3-NE1 | 2.93  | 1.42        | 1.32     |
| 1   | 8-A   | 62  | CRQ  | CD3-NE1 | 2.92  | 1.42        | 1.32     |
| 1   | 7-A   | 62  | CRQ  | CD3-NE1 | 2.92  | 1.42        | 1.32     |
| 1   | 2-A   | 62  | CRQ  | CG2-CB2 | 2.92  | 1.52        | 1.46     |
| 1   | 11-A  | 62  | CRQ  | CD3-NE1 | 2.91  | 1.42        | 1.32     |
| 1   | 18-A  | 62  | CRQ  | CD3-NE1 | 2.90  | 1.42        | 1.32     |
| 1   | 40-A  | 62  | CRQ  | CD3-NE1 | 2.90  | 1.42        | 1.32     |
| 1   | 8-A   | 62  | CRQ  | CA3-N3  | -2.90 | 1.41        | 1.47     |
| 1   | 34-A  | 62  | CRQ  | CD3-NE1 | 2.90  | 1.42        | 1.32     |
| 1   | 44-A  | 62  | CRQ  | CD3-NE1 | 2.89  | 1.42        | 1.32     |
| 1   | 27-A  | 62  | CRQ  | CD3-NE1 | 2.88  | 1.42        | 1.32     |
| 1   | 35-A  | 62  | CRQ  | CD3-NE1 | 2.85  | 1.42        | 1.32     |
| 1   | 41-A  | 62  | CRQ  | CD3-NE1 | 2.85  | 1.42        | 1.32     |
| 1   | 13-A  | 62  | CRQ  | CD3-NE1 | 2.84  | 1.42        | 1.32     |
| 1   | 47-A  | 62  | CRQ  | CD3-NE1 | 2.83  | 1.42        | 1.32     |
| 1   | 5-A   | 62  | CRQ  | CD3-NE1 | 2.83  | 1.42        | 1.32     |
| 1   | 26-A  | 62  | CRQ  | CD3-NE1 | 2.81  | 1.41        | 1.32     |
| 1   | 22-A  | 62  | CRQ  | CA3-N3  | -2.80 | 1.41        | 1.47     |
| 1   | 21-A  | 62  | CRQ  | CD3-NE1 | 2.80  | 1.41        | 1.32     |
| 1   | 23-A  | 62  | CRQ  | CA3-N3  | -2.80 | 1.41        | 1.47     |
| 1   | 33-A  | 62  | CRQ  | CD3-NE1 | 2.78  | 1.41        | 1.32     |
| 1   | 21-A  | 62  | CRQ  | CA3-N3  | -2.75 | 1.41        | 1.47     |
| 1   | 20-A  | 62  | CRQ  | CD3-NE1 | 2.75  | 1.41        | 1.32     |
| 1   | 22-A  | 62  | CRQ  | CD3-NE1 | 2.74  | 1.41        | 1.32     |
| 1   | 12-A  | 62  | CRQ  | CD3-NE1 | 2.74  | 1.41        | 1.32     |
| 1   | 43-A  | 62  | CRQ  | CA2-N2  | 2.73  | 1.44        | 1.38     |
| 1   | 10-A  | 62  | CRQ  | CA3-N3  | -2.73 | 1.41        | 1.47     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | 23-A  | 62  | CRQ  | CD3-NE1 | 2.72  | 1.41        | 1.32     |
| 1   | 36-A  | 62  | CRQ  | CD3-NE1 | 2.72  | 1.41        | 1.32     |
| 1   | 11-A  | 62  | CRQ  | CG2-CB2 | 2.72  | 1.52        | 1.46     |
| 1   | 18-A  | 62  | CRQ  | CA1-N   | 2.71  | 1.34        | 1.27     |
| 1   | 3-A   | 62  | CRQ  | CD3-NE1 | 2.71  | 1.41        | 1.32     |
| 1   | 32-A  | 62  | CRQ  | CA3-N3  | -2.69 | 1.41        | 1.47     |
| 1   | 1-A   | 62  | CRQ  | CD3-NE1 | 2.68  | 1.41        | 1.32     |
| 1   | 17-A  | 62  | CRQ  | CB2-CA2 | 2.68  | 1.37        | 1.35     |
| 1   | 30-A  | 62  | CRQ  | CD3-NE1 | 2.67  | 1.41        | 1.32     |
| 1   | 4-A   | 62  | CRQ  | CA3-N3  | -2.66 | 1.42        | 1.47     |
| 1   | 24-A  | 62  | CRQ  | CD3-NE1 | 2.65  | 1.41        | 1.32     |
| 1   | 36-A  | 62  | CRQ  | CA3-N3  | -2.64 | 1.42        | 1.47     |
| 1   | 17-A  | 62  | CRQ  | CD3-NE1 | 2.62  | 1.41        | 1.32     |
| 1   | 4-A   | 62  | CRQ  | CD3-NE1 | 2.59  | 1.41        | 1.32     |
| 1   | 36-A  | 62  | CRQ  | CA2-N2  | 2.58  | 1.44        | 1.38     |
| 1   | 28-A  | 62  | CRQ  | CA3-N3  | -2.52 | 1.42        | 1.47     |
| 1   | 40-A  | 62  | CRQ  | CA2-N2  | 2.51  | 1.43        | 1.38     |
| 1   | 7-A   | 62  | CRQ  | CA2-N2  | 2.50  | 1.43        | 1.38     |
| 1   | 39-A  | 62  | CRQ  | CA2-N2  | 2.47  | 1.43        | 1.38     |
| 1   | 11-A  | 62  | CRQ  | CA3-N3  | -2.47 | 1.42        | 1.47     |
| 1   | 20-A  | 62  | CRQ  | CA3-N3  | -2.43 | 1.42        | 1.47     |
| 1   | 38-A  | 62  | CRQ  | CA2-C2  | -2.42 | 1.46        | 1.48     |
| 1   | 20-A  | 62  | CRQ  | CA2-C2  | -2.39 | 1.46        | 1.48     |
| 1   | 30-A  | 62  | CRQ  | CG2-CB2 | 2.35  | 1.51        | 1.46     |
| 1   | 7-A   | 62  | CRQ  | CG2-CB2 | 2.35  | 1.51        | 1.46     |
| 1   | 3-A   | 62  | CRQ  | CA2-N2  | 2.29  | 1.43        | 1.38     |
| 1   | 26-A  | 62  | CRQ  | CB2-CA2 | 2.28  | 1.37        | 1.35     |
| 1   | 15-A  | 62  | CRQ  | CA3-N3  | -2.23 | 1.42        | 1.47     |
| 1   | 37-A  | 62  | CRQ  | CA2-N2  | 2.23  | 1.43        | 1.38     |
| 1   | 4-A   | 62  | CRQ  | CG2-CB2 | 2.22  | 1.51        | 1.46     |
| 1   | 27-A  | 62  | CRQ  | CA2-N2  | 2.22  | 1.43        | 1.38     |
| 1   | 21-A  | 62  | CRQ  | CA2-N2  | 2.22  | 1.43        | 1.38     |
| 1   | 41-A  | 62  | CRQ  | CA2-N2  | 2.20  | 1.43        | 1.38     |
| 1   | 38-A  | 62  | CRQ  | CG2-CB2 | 2.16  | 1.51        | 1.46     |
| 1   | 42-A  | 62  | CRQ  | CA2-N2  | 2.14  | 1.43        | 1.38     |
| 1   | 45-A  | 62  | CRQ  | CA2-N2  | 2.13  | 1.43        | 1.38     |
| 1   | 36-A  | 62  | CRQ  | CG2-CB2 | 2.10  | 1.50        | 1.46     |
| 1   | 31-A  | 62  | CRQ  | CA2-C2  | -2.10 | 1.46        | 1.48     |
| 1   | 25-A  | 62  | CRQ  | CA2-N2  | 2.07  | 1.43        | 1.38     |
| 1   | 13-A  | 62  | CRQ  | CA2-N2  | 2.04  | 1.42        | 1.38     |
| 1   | 47-A  | 62  | CRQ  | CA2-N2  | 2.04  | 1.42        | 1.38     |
| 1   | 43-A  | 62  | CRQ  | CG2-CB2 | 2.03  | 1.50        | 1.46     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | 2-A   | 62  | CRQ  | CA2-N2 | 2.03 | 1.42        | 1.38     |
| 1   | 16-A  | 62  | CRQ  | CA2-N2 | 2.03 | 1.42        | 1.38     |
| 1   | 23-A  | 62  | CRQ  | CA2-N2 | 2.00 | 1.42        | 1.38     |

All (273) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | 32-A  | 62  | CRQ  | CA2-C2-N3   | 8.19  | 107.24      | 103.37   |
| 1   | 19-A  | 62  | CRQ  | O2-C2-CA2   | -8.00 | 126.47      | 130.96   |
| 1   | 35-A  | 62  | CRQ  | CG2-CB2-CA2 | -6.16 | 122.40      | 129.94   |
| 1   | 1-A   | 62  | CRQ  | O2-C2-CA2   | -5.65 | 127.79      | 130.96   |
| 1   | 42-A  | 62  | CRQ  | CA2-C2-N3   | 5.52  | 105.98      | 103.37   |
| 1   | 9-A   | 62  | CRQ  | CG2-CB2-CA2 | 5.45  | 136.62      | 129.94   |
| 1   | 38-A  | 62  | CRQ  | CA2-C2-N3   | 5.08  | 105.77      | 103.37   |
| 1   | 38-A  | 62  | CRQ  | O2-C2-CA2   | -4.94 | 128.19      | 130.96   |
| 1   | 6-A   | 62  | CRQ  | C2-CA2-N2   | 4.75  | 112.26      | 108.93   |
| 1   | 21-A  | 62  | CRQ  | CA2-C2-N3   | 4.74  | 105.61      | 103.37   |
| 1   | 43-A  | 62  | CRQ  | CA2-C2-N3   | 4.70  | 105.59      | 103.37   |
| 1   | 12-A  | 62  | CRQ  | O-C-CA3     | -4.59 | 112.53      | 126.39   |
| 1   | 36-A  | 62  | CRQ  | CA2-C2-N3   | 4.53  | 105.52      | 103.37   |
| 1   | 16-A  | 62  | CRQ  | O2-C2-CA2   | 4.48  | 133.47      | 130.96   |
| 1   | 36-A  | 62  | CRQ  | CG2-CB2-CA2 | -4.46 | 124.47      | 129.94   |
| 1   | 16-A  | 62  | CRQ  | O-C-CA3     | -4.45 | 112.95      | 126.39   |
| 1   | 30-A  | 62  | CRQ  | O-C-CA3     | -4.44 | 113.00      | 126.39   |
| 1   | 6-A   | 62  | CRQ  | O-C-CA3     | -4.43 | 113.01      | 126.39   |
| 1   | 29-A  | 62  | CRQ  | CG2-CB2-CA2 | -4.41 | 124.54      | 129.94   |
| 1   | 17-A  | 62  | CRQ  | O-C-CA3     | -4.38 | 113.17      | 126.39   |
| 1   | 47-A  | 62  | CRQ  | C2-CA2-N2   | 4.35  | 111.98      | 108.93   |
| 1   | 5-A   | 62  | CRQ  | O-C-CA3     | -4.35 | 113.26      | 126.39   |
| 1   | 29-A  | 62  | CRQ  | CA3-N3-C1   | -4.33 | 119.74      | 128.22   |
| 1   | 14-A  | 62  | CRQ  | O2-C2-CA2   | -4.33 | 128.53      | 130.96   |
| 1   | 47-A  | 62  | CRQ  | O-C-CA3     | -4.31 | 113.37      | 126.39   |
| 1   | 25-A  | 62  | CRQ  | O-C-CA3     | -4.28 | 113.47      | 126.39   |
| 1   | 15-A  | 62  | CRQ  | O2-C2-CA2   | -4.25 | 128.57      | 130.96   |
| 1   | 4-A   | 62  | CRQ  | CA2-C2-N3   | 4.19  | 105.35      | 103.37   |
| 1   | 14-A  | 62  | CRQ  | O-C-CA3     | -4.17 | 113.79      | 126.39   |
| 1   | 39-A  | 62  | CRQ  | O-C-CA3     | -4.17 | 113.81      | 126.39   |
| 1   | 7-A   | 62  | CRQ  | O2-C2-CA2   | -4.14 | 128.63      | 130.96   |
| 1   | 44-A  | 62  | CRQ  | O-C-CA3     | -4.12 | 113.96      | 126.39   |
| 1   | 28-A  | 62  | CRQ  | CG2-CB2-CA2 | 4.10  | 134.97      | 129.94   |
| 1   | 12-A  | 62  | CRQ  | C2-CA2-N2   | 4.10  | 111.81      | 108.93   |
| 1   | 45-A  | 62  | CRQ  | O-C-CA3     | -4.07 | 114.10      | 126.39   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | 18-A  | 62  | CRQ  | O-C-CA3     | -4.05 | 114.16      | 126.39   |
| 1   | 11-A  | 62  | CRQ  | O-C-CA3     | -4.05 | 114.17      | 126.39   |
| 1   | 15-A  | 62  | CRQ  | CB2-CA2-C2  | -4.03 | 117.47      | 122.28   |
| 1   | 42-A  | 62  | CRQ  | O-C-CA3     | -4.03 | 114.22      | 126.39   |
| 1   | 13-A  | 62  | CRQ  | O-C-CA3     | -4.02 | 114.25      | 126.39   |
| 1   | 30-A  | 62  | CRQ  | CA2-C2-N3   | 4.00  | 105.26      | 103.37   |
| 1   | 26-A  | 62  | CRQ  | O-C-CA3     | -3.99 | 114.35      | 126.39   |
| 1   | 19-A  | 62  | CRQ  | O-C-CA3     | -3.97 | 114.41      | 126.39   |
| 1   | 18-A  | 62  | CRQ  | CA2-C2-N3   | 3.97  | 105.25      | 103.37   |
| 1   | 41-A  | 62  | CRQ  | O-C-CA3     | -3.97 | 114.41      | 126.39   |
| 1   | 3-A   | 62  | CRQ  | CA2-C2-N3   | 3.95  | 105.24      | 103.37   |
| 1   | 9-A   | 62  | CRQ  | O-C-CA3     | -3.91 | 114.57      | 126.39   |
| 1   | 33-A  | 62  | CRQ  | O-C-CA3     | -3.91 | 114.59      | 126.39   |
| 1   | 4-A   | 62  | CRQ  | O-C-CA3     | -3.90 | 114.62      | 126.39   |
| 1   | 46-A  | 62  | CRQ  | O-C-CA3     | -3.90 | 114.62      | 126.39   |
| 1   | 46-A  | 62  | CRQ  | CA2-C2-N3   | 3.88  | 105.20      | 103.37   |
| 1   | 34-A  | 62  | CRQ  | O-C-CA3     | -3.87 | 114.71      | 126.39   |
| 1   | 8-A   | 62  | CRQ  | O-C-CA3     | -3.85 | 114.76      | 126.39   |
| 1   | 4-A   | 62  | CRQ  | CD1-CE1-CZ  | 3.85  | 124.09      | 119.88   |
| 1   | 19-A  | 62  | CRQ  | C2-CA2-N2   | 3.84  | 111.63      | 108.93   |
| 1   | 32-A  | 62  | CRQ  | O-C-CA3     | -3.81 | 114.88      | 126.39   |
| 1   | 19-A  | 62  | CRQ  | CB2-CA2-C2  | -3.80 | 117.74      | 122.28   |
| 1   | 45-A  | 62  | CRQ  | CA2-C2-N3   | 3.79  | 105.16      | 103.37   |
| 1   | 35-A  | 62  | CRQ  | O2-C2-CA2   | -3.77 | 128.84      | 130.96   |
| 1   | 31-A  | 62  | CRQ  | O-C-CA3     | -3.71 | 115.20      | 126.39   |
| 1   | 3-A   | 62  | CRQ  | O-C-CA3     | -3.70 | 115.20      | 126.39   |
| 1   | 2-A   | 62  | CRQ  | O-C-CA3     | -3.69 | 115.25      | 126.39   |
| 1   | 10-A  | 62  | CRQ  | O-C-CA3     | -3.63 | 115.42      | 126.39   |
| 1   | 8-A   | 62  | CRQ  | O2-C2-CA2   | 3.62  | 132.99      | 130.96   |
| 1   | 22-A  | 62  | CRQ  | O-C-CA3     | -3.61 | 115.50      | 126.39   |
| 1   | 6-A   | 62  | CRQ  | CE1-CD1-CG2 | -3.60 | 116.55      | 121.25   |
| 1   | 29-A  | 62  | CRQ  | CA3-N3-C2   | 3.58  | 132.00      | 123.80   |
| 1   | 23-A  | 62  | CRQ  | O-C-CA3     | -3.56 | 115.63      | 126.39   |
| 1   | 35-A  | 62  | CRQ  | O-C-CA3     | -3.56 | 115.64      | 126.39   |
| 1   | 28-A  | 62  | CRQ  | O-C-CA3     | -3.56 | 115.64      | 126.39   |
| 1   | 32-A  | 62  | CRQ  | O2-C2-CA2   | -3.56 | 128.96      | 130.96   |
| 1   | 7-A   | 62  | CRQ  | O-C-CA3     | -3.55 | 115.67      | 126.39   |
| 1   | 23-A  | 62  | CRQ  | CG2-CB2-CA2 | 3.52  | 134.26      | 129.94   |
| 1   | 11-A  | 62  | CRQ  | O2-C2-CA2   | 3.52  | 132.94      | 130.96   |
| 1   | 25-A  | 62  | CRQ  | C2-CA2-N2   | 3.47  | 111.36      | 108.93   |
| 1   | 35-A  | 62  | CRQ  | C2-CA2-N2   | 3.47  | 111.36      | 108.93   |
| 1   | 5-A   | 62  | CRQ  | C2-CA2-N2   | 3.46  | 111.36      | 108.93   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | 15-A  | 62  | CRQ  | O-C-CA3     | -3.46 | 115.94      | 126.39   |
| 1   | 43-A  | 62  | CRQ  | O-C-CA3     | -3.45 | 115.96      | 126.39   |
| 1   | 22-A  | 62  | CRQ  | O2-C2-CA2   | -3.45 | 129.02      | 130.96   |
| 1   | 29-A  | 62  | CRQ  | O-C-CA3     | -3.45 | 115.97      | 126.39   |
| 1   | 33-A  | 62  | CRQ  | C2-CA2-N2   | 3.44  | 111.34      | 108.93   |
| 1   | 28-A  | 62  | CRQ  | CA2-C2-N3   | 3.41  | 104.98      | 103.37   |
| 1   | 1-A   | 62  | CRQ  | C2-CA2-N2   | 3.40  | 111.31      | 108.93   |
| 1   | 27-A  | 62  | CRQ  | O-C-CA3     | -3.40 | 116.13      | 126.39   |
| 1   | 37-A  | 62  | CRQ  | O-C-CA3     | -3.37 | 116.20      | 126.39   |
| 1   | 32-A  | 62  | CRQ  | CG2-CB2-CA2 | 3.33  | 134.02      | 129.94   |
| 1   | 1-A   | 62  | CRQ  | CE1-CD1-CG2 | -3.30 | 116.94      | 121.25   |
| 1   | 38-A  | 62  | CRQ  | O-C-CA3     | -3.30 | 116.43      | 126.39   |
| 1   | 3-A   | 62  | CRQ  | O2-C2-CA2   | 3.29  | 132.81      | 130.96   |
| 1   | 47-A  | 62  | CRQ  | CB2-CA2-C2  | -3.29 | 118.34      | 122.28   |
| 1   | 32-A  | 62  | CRQ  | N3-C1-N2    | -3.29 | 108.94      | 113.28   |
| 1   | 33-A  | 62  | CRQ  | CA3-N3-C1   | -3.27 | 121.81      | 128.22   |
| 1   | 35-A  | 62  | CRQ  | CD2-CG2-CD1 | 3.27  | 122.48      | 117.64   |
| 1   | 6-A   | 62  | CRQ  | CD1-CE1-CZ  | 3.26  | 123.45      | 119.88   |
| 1   | 29-A  | 62  | CRQ  | CB2-CA2-N2  | -3.25 | 124.32      | 128.83   |
| 1   | 21-A  | 62  | CRQ  | O-C-CA3     | -3.24 | 116.60      | 126.39   |
| 1   | 37-A  | 62  | CRQ  | C2-CA2-N2   | 3.22  | 111.19      | 108.93   |
| 1   | 6-A   | 62  | CRQ  | O2-C2-CA2   | -3.22 | 129.15      | 130.96   |
| 1   | 1-A   | 62  | CRQ  | O-C-CA3     | -3.21 | 116.70      | 126.39   |
| 1   | 29-A  | 62  | CRQ  | CD1-CE1-CZ  | 3.21  | 123.39      | 119.88   |
| 1   | 26-A  | 62  | CRQ  | C2-CA2-N2   | 3.18  | 111.16      | 108.93   |
| 1   | 47-A  | 62  | CRQ  | CD2-CG2-CD1 | 3.13  | 122.27      | 117.64   |
| 1   | 12-A  | 62  | CRQ  | CG2-CB2-CA2 | -3.12 | 126.12      | 129.94   |
| 1   | 36-A  | 62  | CRQ  | O-C-CA3     | -3.12 | 116.98      | 126.39   |
| 1   | 29-A  | 62  | CRQ  | CB2-CA2-C2  | 3.11  | 125.99      | 122.28   |
| 1   | 9-A   | 62  | CRQ  | CD2-CG2-CB2 | -3.11 | 110.64      | 121.22   |
| 1   | 26-A  | 62  | CRQ  | CG2-CB2-CA2 | 3.09  | 133.73      | 129.94   |
| 1   | 32-A  | 62  | CRQ  | CB2-CA2-C2  | -3.08 | 118.60      | 122.28   |
| 1   | 33-A  | 62  | CRQ  | CE1-CD1-CG2 | -3.05 | 117.27      | 121.25   |
| 1   | 33-A  | 62  | CRQ  | CG2-CB2-CA2 | -3.05 | 126.21      | 129.94   |
| 1   | 40-A  | 62  | CRQ  | O-C-CA3     | -3.04 | 117.22      | 126.39   |
| 1   | 2-A   | 62  | CRQ  | CA2-C2-N3   | 3.02  | 104.80      | 103.37   |
| 1   | 41-A  | 62  | CRQ  | C2-CA2-N2   | 3.02  | 111.05      | 108.93   |
| 1   | 20-A  | 62  | CRQ  | O-C-CA3     | -3.01 | 117.29      | 126.39   |
| 1   | 32-A  | 62  | CRQ  | CB2-CA2-N2  | 3.00  | 132.99      | 128.83   |
| 1   | 14-A  | 62  | CRQ  | N3-C1-N2    | -3.00 | 109.32      | 113.28   |
| 1   | 23-A  | 62  | CRQ  | CA2-C2-N3   | 2.99  | 104.79      | 103.37   |
| 1   | 19-A  | 62  | CRQ  | CD2-CG2-CD1 | 2.99  | 122.07      | 117.64   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | 40-A  | 62  | CRQ  | C2-CA2-N2   | 2.98  | 111.02      | 108.93   |
| 1   | 3-A   | 62  | CRQ  | CG1-CB1-CA1 | -2.98 | 104.29      | 113.53   |
| 1   | 1-A   | 62  | CRQ  | CD1-CE1-CZ  | 2.97  | 123.13      | 119.88   |
| 1   | 38-A  | 62  | CRQ  | CA2-N2-C1   | 2.97  | 109.75      | 104.33   |
| 1   | 33-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.96 | 104.35      | 113.53   |
| 1   | 15-A  | 62  | CRQ  | N3-C1-N2    | -2.96 | 109.38      | 113.28   |
| 1   | 14-A  | 62  | CRQ  | CG2-CB2-CA2 | 2.95  | 133.56      | 129.94   |
| 1   | 24-A  | 62  | CRQ  | O-C-CA3     | -2.94 | 117.52      | 126.39   |
| 1   | 39-A  | 62  | CRQ  | C2-CA2-N2   | 2.92  | 110.98      | 108.93   |
| 1   | 37-A  | 62  | CRQ  | CE1-CD1-CG2 | -2.91 | 117.45      | 121.25   |
| 1   | 47-A  | 62  | CRQ  | CE1-CD1-CG2 | -2.90 | 117.47      | 121.25   |
| 1   | 15-A  | 62  | CRQ  | CG2-CB2-CA2 | 2.89  | 133.49      | 129.94   |
| 1   | 15-A  | 62  | CRQ  | CD2-CG2-CD1 | 2.88  | 121.90      | 117.64   |
| 1   | 19-A  | 62  | CRQ  | N3-C1-N2    | -2.85 | 109.52      | 113.28   |
| 1   | 32-A  | 62  | CRQ  | CA2-N2-C1   | 2.82  | 109.48      | 104.33   |
| 1   | 40-A  | 62  | CRQ  | CE1-CD1-CG2 | -2.81 | 117.59      | 121.25   |
| 1   | 17-A  | 62  | CRQ  | C2-CA2-N2   | 2.80  | 110.89      | 108.93   |
| 1   | 13-A  | 62  | CRQ  | C2-CA2-N2   | 2.78  | 110.88      | 108.93   |
| 1   | 15-A  | 62  | CRQ  | CE2-CD2-CG2 | -2.77 | 117.63      | 121.25   |
| 1   | 33-A  | 62  | CRQ  | CD2-CG2-CD1 | 2.75  | 121.71      | 117.64   |
| 1   | 38-A  | 62  | CRQ  | CG2-CB2-CA2 | 2.74  | 133.31      | 129.94   |
| 1   | 44-A  | 62  | CRQ  | N3-C1-N2    | -2.72 | 109.69      | 113.28   |
| 1   | 10-A  | 62  | CRQ  | C2-CA2-N2   | 2.69  | 110.81      | 108.93   |
| 1   | 19-A  | 62  | CRQ  | O2-C2-N3    | 2.68  | 129.67      | 124.35   |
| 1   | 14-A  | 62  | CRQ  | CB2-CA2-C2  | -2.67 | 119.09      | 122.28   |
| 1   | 41-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.65 | 105.32      | 113.53   |
| 1   | 17-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.64 | 105.34      | 113.53   |
| 1   | 35-A  | 62  | CRQ  | N3-C1-N2    | -2.63 | 109.80      | 113.28   |
| 1   | 9-A   | 62  | CRQ  | C2-CA2-N2   | 2.61  | 110.76      | 108.93   |
| 1   | 9-A   | 62  | CRQ  | CG1-CB1-CA1 | -2.60 | 105.45      | 113.53   |
| 1   | 27-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.60 | 105.46      | 113.53   |
| 1   | 40-A  | 62  | CRQ  | CG2-CB2-CA2 | -2.59 | 126.77      | 129.94   |
| 1   | 25-A  | 62  | CRQ  | CB2-CA2-C2  | -2.59 | 119.19      | 122.28   |
| 1   | 46-A  | 62  | CRQ  | N3-C1-N2    | -2.59 | 109.86      | 113.28   |
| 1   | 24-A  | 62  | CRQ  | CG2-CB2-CA2 | -2.59 | 126.78      | 129.94   |
| 1   | 18-A  | 62  | CRQ  | N3-C1-N2    | -2.58 | 109.87      | 113.28   |
| 1   | 7-A   | 62  | CRQ  | N3-C1-N2    | -2.58 | 109.87      | 113.28   |
| 1   | 41-A  | 62  | CRQ  | CB2-CA2-C2  | -2.58 | 119.20      | 122.28   |
| 1   | 4-A   | 62  | CRQ  | OH-CZ-CE2   | 2.58  | 127.36      | 120.02   |
| 1   | 15-A  | 62  | CRQ  | C2-CA2-N2   | 2.52  | 110.70      | 108.93   |
| 1   | 13-A  | 62  | CRQ  | N3-C1-N2    | -2.52 | 109.95      | 113.28   |
| 1   | 32-A  | 62  | CRQ  | CA3-N3-C1   | 2.52  | 133.16      | 128.22   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | 1-A   | 62  | CRQ  | CB2-CA2-C2  | -2.51 | 119.28      | 122.28   |
| 1   | 22-A  | 62  | CRQ  | N3-C1-N2    | -2.50 | 109.97      | 113.28   |
| 1   | 45-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.49 | 105.80      | 113.53   |
| 1   | 12-A  | 62  | CRQ  | N3-C1-N2    | -2.49 | 109.99      | 113.28   |
| 1   | 12-A  | 62  | CRQ  | CA2-C2-N3   | -2.49 | 102.19      | 103.37   |
| 1   | 29-A  | 62  | CRQ  | CA2-N2-C1   | 2.48  | 108.86      | 104.33   |
| 1   | 2-A   | 62  | CRQ  | N3-C1-N2    | -2.47 | 110.01      | 113.28   |
| 1   | 5-A   | 62  | CRQ  | CE1-CD1-CG2 | -2.47 | 118.03      | 121.25   |
| 1   | 17-A  | 62  | CRQ  | CD2-CG2-CD1 | 2.47  | 121.29      | 117.64   |
| 1   | 27-A  | 62  | CRQ  | C2-CA2-N2   | 2.46  | 110.66      | 108.93   |
| 1   | 18-A  | 62  | CRQ  | CA2-N2-C1   | 2.46  | 108.82      | 104.33   |
| 1   | 26-A  | 62  | CRQ  | CA3-N3-C1   | -2.45 | 123.42      | 128.22   |
| 1   | 2-A   | 62  | CRQ  | CA2-N2-C1   | 2.45  | 108.81      | 104.33   |
| 1   | 29-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.44 | 105.95      | 113.53   |
| 1   | 1-A   | 62  | CRQ  | CG1-CB1-CA1 | -2.44 | 105.96      | 113.53   |
| 1   | 24-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.43 | 105.98      | 113.53   |
| 1   | 47-A  | 62  | CRQ  | N3-C1-N2    | -2.43 | 110.06      | 113.28   |
| 1   | 10-A  | 62  | CRQ  | CA2-C2-N3   | 2.43  | 104.52      | 103.37   |
| 1   | 35-A  | 62  | CRQ  | CE1-CD1-CG2 | -2.42 | 118.09      | 121.25   |
| 1   | 22-A  | 62  | CRQ  | CD2-CG2-CD1 | 2.42  | 121.22      | 117.64   |
| 1   | 4-A   | 62  | CRQ  | CA2-N2-C1   | 2.42  | 108.76      | 104.33   |
| 1   | 22-A  | 62  | CRQ  | CB2-CA2-C2  | -2.42 | 119.39      | 122.28   |
| 1   | 24-A  | 62  | CRQ  | CD1-CE1-CZ  | 2.42  | 122.52      | 119.88   |
| 1   | 21-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.41 | 106.04      | 113.53   |
| 1   | 3-A   | 62  | CRQ  | N3-C1-N2    | -2.41 | 110.09      | 113.28   |
| 1   | 8-A   | 62  | CRQ  | N3-C1-N2    | -2.40 | 110.11      | 113.28   |
| 1   | 43-A  | 62  | CRQ  | O2-C2-CA2   | 2.40  | 132.31      | 130.96   |
| 1   | 38-A  | 62  | CRQ  | N3-C1-N2    | -2.36 | 110.16      | 113.28   |
| 1   | 47-A  | 62  | CRQ  | CD2-CE2-CZ  | -2.36 | 117.29      | 119.88   |
| 1   | 12-A  | 62  | CRQ  | O2-C2-CA2   | -2.35 | 129.64      | 130.96   |
| 1   | 42-A  | 62  | CRQ  | N3-C1-N2    | -2.34 | 110.19      | 113.28   |
| 1   | 1-A   | 62  | CRQ  | CG2-CB2-CA2 | 2.33  | 132.80      | 129.94   |
| 1   | 16-A  | 62  | CRQ  | N3-C1-N2    | -2.33 | 110.20      | 113.28   |
| 1   | 5-A   | 62  | CRQ  | CG1-CB1-CA1 | -2.32 | 106.33      | 113.53   |
| 1   | 37-A  | 62  | CRQ  | CB2-CA2-C2  | -2.30 | 119.53      | 122.28   |
| 1   | 1-A   | 62  | CRQ  | N3-C1-N2    | -2.30 | 110.25      | 113.28   |
| 1   | 35-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.29 | 106.41      | 113.53   |
| 1   | 25-A  | 62  | CRQ  | CA3-N3-C1   | -2.27 | 123.77      | 128.22   |
| 1   | 22-A  | 62  | CRQ  | C2-CA2-N2   | 2.26  | 110.52      | 108.93   |
| 1   | 33-A  | 62  | CRQ  | CA3-N3-C2   | 2.26  | 128.99      | 123.80   |
| 1   | 40-A  | 62  | CRQ  | CD2-CG2-CD1 | 2.26  | 120.99      | 117.64   |
| 1   | 31-A  | 62  | CRQ  | CG2-CB2-CA2 | -2.26 | 127.17      | 129.94   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | 11-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.26 | 106.53      | 113.53   |
| 1   | 34-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.26 | 106.53      | 113.53   |
| 1   | 19-A  | 62  | CRQ  | CE2-CD2-CG2 | -2.26 | 118.31      | 121.25   |
| 1   | 37-A  | 62  | CRQ  | N3-C1-N2    | -2.25 | 110.30      | 113.28   |
| 1   | 10-A  | 62  | CRQ  | CB2-CA2-C2  | -2.25 | 119.59      | 122.28   |
| 1   | 6-A   | 62  | CRQ  | CA2-C2-N3   | -2.25 | 102.31      | 103.37   |
| 1   | 8-A   | 62  | CRQ  | C2-CA2-N2   | 2.25  | 110.51      | 108.93   |
| 1   | 6-A   | 62  | CRQ  | CG1-CB1-CA1 | -2.25 | 106.56      | 113.53   |
| 1   | 29-A  | 62  | CRQ  | N3-C1-N2    | -2.24 | 110.32      | 113.28   |
| 1   | 33-A  | 62  | CRQ  | CA2-C2-N3   | -2.24 | 102.31      | 103.37   |
| 1   | 43-A  | 62  | CRQ  | CD1-CE1-CZ  | 2.24  | 122.33      | 119.88   |
| 1   | 4-A   | 62  | CRQ  | N3-C1-N2    | -2.24 | 110.32      | 113.28   |
| 1   | 24-A  | 62  | CRQ  | CE1-CD1-CG2 | -2.23 | 118.34      | 121.25   |
| 1   | 26-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.22 | 106.63      | 113.53   |
| 1   | 41-A  | 62  | CRQ  | CD2-CG2-CD1 | 2.22  | 120.92      | 117.64   |
| 1   | 11-A  | 62  | CRQ  | CA2-C2-N3   | 2.21  | 104.42      | 103.37   |
| 1   | 35-A  | 62  | CRQ  | CA3-N3-C1   | -2.21 | 123.88      | 128.22   |
| 1   | 8-A   | 62  | CRQ  | CG1-CB1-CA1 | -2.21 | 106.67      | 113.53   |
| 1   | 14-A  | 62  | CRQ  | CA2-N2-C1   | 2.21  | 108.37      | 104.33   |
| 1   | 9-A   | 62  | CRQ  | CD1-CG2-CB2 | 2.20  | 128.73      | 121.22   |
| 1   | 11-A  | 62  | CRQ  | N3-C1-N2    | -2.20 | 110.37      | 113.28   |
| 1   | 32-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.20 | 106.72      | 113.53   |
| 1   | 25-A  | 62  | CRQ  | N3-C1-N2    | -2.19 | 110.38      | 113.28   |
| 1   | 15-A  | 62  | CRQ  | CA2-N2-C1   | 2.19  | 108.33      | 104.33   |
| 1   | 20-A  | 62  | CRQ  | CA2-N2-C1   | 2.18  | 108.33      | 104.33   |
| 1   | 31-A  | 62  | CRQ  | CB2-CA2-N2  | -2.18 | 125.80      | 128.83   |
| 1   | 30-A  | 62  | CRQ  | N3-C1-N2    | -2.18 | 110.40      | 113.28   |
| 1   | 37-A  | 62  | CRQ  | CD1-CE1-CZ  | 2.18  | 122.27      | 119.88   |
| 1   | 42-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.17 | 106.81      | 113.53   |
| 1   | 33-A  | 62  | CRQ  | N3-C1-N2    | -2.16 | 110.42      | 113.28   |
| 1   | 28-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.16 | 106.84      | 113.53   |
| 1   | 25-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.15 | 106.86      | 113.53   |
| 1   | 10-A  | 62  | CRQ  | N3-C1-N2    | -2.15 | 110.44      | 113.28   |
| 1   | 12-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.15 | 106.87      | 113.53   |
| 1   | 29-A  | 62  | CRQ  | O2-C2-CA2   | -2.15 | 129.75      | 130.96   |
| 1   | 44-A  | 62  | CRQ  | CA2-N2-C1   | 2.15  | 108.26      | 104.33   |
| 1   | 44-A  | 62  | CRQ  | CG2-CB2-CA2 | 2.14  | 132.57      | 129.94   |
| 1   | 40-A  | 62  | CRQ  | CD2-CE2-CZ  | -2.13 | 117.54      | 119.88   |
| 1   | 31-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.12 | 106.95      | 113.53   |
| 1   | 9-A   | 62  | CRQ  | O2-C2-CA2   | 2.12  | 132.15      | 130.96   |
| 1   | 30-A  | 62  | CRQ  | CG2-CB2-CA2 | 2.12  | 132.54      | 129.94   |
| 1   | 6-A   | 62  | CRQ  | O2-C2-N3    | 2.11  | 128.54      | 124.35   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | 7-A   | 62  | CRQ  | C2-CA2-N2   | 2.10  | 110.40      | 108.93   |
| 1   | 22-A  | 62  | CRQ  | CA2-C2-N3   | 2.09  | 104.36      | 103.37   |
| 1   | 14-A  | 62  | CRQ  | CE2-CD2-CG2 | -2.09 | 118.52      | 121.25   |
| 1   | 35-A  | 62  | CRQ  | CD2-CE2-CZ  | -2.09 | 117.59      | 119.88   |
| 1   | 6-A   | 62  | CRQ  | N3-C1-N2    | -2.08 | 110.53      | 113.28   |
| 1   | 39-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.08 | 107.09      | 113.53   |
| 1   | 30-A  | 62  | CRQ  | CA2-N2-C1   | 2.07  | 108.13      | 104.33   |
| 1   | 40-A  | 62  | CRQ  | CA3-N3-C1   | -2.07 | 124.16      | 128.22   |
| 1   | 41-A  | 62  | CRQ  | N3-C1-N2    | -2.07 | 110.55      | 113.28   |
| 1   | 1-A   | 62  | CRQ  | O2-C2-N3    | 2.07  | 128.46      | 124.35   |
| 1   | 12-A  | 62  | CRQ  | CA3-N3-C1   | -2.07 | 124.17      | 128.22   |
| 1   | 15-A  | 62  | CRQ  | CA2-C2-N3   | 2.06  | 104.35      | 103.37   |
| 1   | 19-A  | 62  | CRQ  | CD2-CG2-CB2 | -2.06 | 114.20      | 121.22   |
| 1   | 36-A  | 62  | CRQ  | O2-C2-CA2   | 2.06  | 132.12      | 130.96   |
| 1   | 5-A   | 62  | CRQ  | N3-C1-N2    | -2.06 | 110.56      | 113.28   |
| 1   | 30-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.05 | 107.16      | 113.53   |
| 1   | 34-A  | 62  | CRQ  | N3-C1-N2    | -2.05 | 110.57      | 113.28   |
| 1   | 22-A  | 62  | CRQ  | CA2-N2-C1   | 2.05  | 108.07      | 104.33   |
| 1   | 26-A  | 62  | CRQ  | CA3-N3-C2   | 2.04  | 128.49      | 123.80   |
| 1   | 18-A  | 62  | CRQ  | O2-C2-CA2   | -2.04 | 129.81      | 130.96   |
| 1   | 21-A  | 62  | CRQ  | CD2-CG2-CD1 | 2.04  | 120.66      | 117.64   |
| 1   | 34-A  | 62  | CRQ  | C2-CA2-N2   | 2.04  | 110.36      | 108.93   |
| 1   | 20-A  | 62  | CRQ  | CG1-CB1-CA1 | -2.04 | 107.21      | 113.53   |
| 1   | 28-A  | 62  | CRQ  | CB2-CA2-C2  | -2.03 | 119.86      | 122.28   |
| 1   | 15-A  | 62  | CRQ  | CB2-CA2-N2  | 2.03  | 131.64      | 128.83   |
| 1   | 39-A  | 62  | CRQ  | CA2-C2-N3   | 2.02  | 104.33      | 103.37   |
| 1   | 4-A   | 62  | CRQ  | CE2-CZ-CE1  | -2.02 | 116.36      | 119.77   |
| 1   | 46-A  | 62  | CRQ  | CB2-CA2-C2  | -2.01 | 119.87      | 122.28   |

There are no chirality outliers.

All (72) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 1   | 29-A  | 62  | CRQ  | C-CA3-N3-C1    |
| 1   | 29-A  | 62  | CRQ  | C-CA3-N3-C2    |
| 1   | 25-A  | 62  | CRQ  | C-CA3-N3-C2    |
| 1   | 31-A  | 62  | CRQ  | C-CA3-N3-C1    |
| 1   | 31-A  | 62  | CRQ  | C-CA3-N3-C2    |
| 1   | 30-A  | 62  | CRQ  | C2-CA2-CB2-CG2 |
| 1   | 35-A  | 62  | CRQ  | C-CA3-N3-C2    |
| 1   | 24-A  | 62  | CRQ  | C-CA3-N3-C2    |
| 1   | 3-A   | 62  | CRQ  | C2-CA2-CB2-CG2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 1   | 4-A   | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 4-A   | 62  | CRQ  | C2-CA2-CB2-CG2  |
| 1   | 23-A  | 62  | CRQ  | C2-CA2-CB2-CG2  |
| 1   | 27-A  | 62  | CRQ  | C-CA3-N3-C2     |
| 1   | 22-A  | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 22-A  | 62  | CRQ  | C2-CA2-CB2-CG2  |
| 1   | 47-A  | 62  | CRQ  | C1-CA1-CB1-CG1  |
| 1   | 20-A  | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 20-A  | 62  | CRQ  | C2-CA2-CB2-CG2  |
| 1   | 36-A  | 62  | CRQ  | C2-CA2-CB2-CG2  |
| 1   | 6-A   | 62  | CRQ  | C-CA3-N3-C2     |
| 1   | 33-A  | 62  | CRQ  | C-CA3-N3-C2     |
| 1   | 10-A  | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 10-A  | 62  | CRQ  | C2-CA2-CB2-CG2  |
| 1   | 40-A  | 62  | CRQ  | C-CA3-N3-C2     |
| 1   | 28-A  | 62  | CRQ  | C2-CA2-CB2-CG2  |
| 1   | 26-A  | 62  | CRQ  | C-CA3-N3-C2     |
| 1   | 38-A  | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 38-A  | 62  | CRQ  | C2-CA2-CB2-CG2  |
| 1   | 17-A  | 62  | CRQ  | C1-CA1-CB1-CG1  |
| 1   | 12-A  | 62  | CRQ  | C-CA3-N3-C2     |
| 1   | 14-A  | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 14-A  | 62  | CRQ  | C2-CA2-CB2-CG2  |
| 1   | 34-A  | 62  | CRQ  | C-CA3-N3-C2     |
| 1   | 15-A  | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 15-A  | 62  | CRQ  | C2-CA2-CB2-CG2  |
| 1   | 43-A  | 62  | CRQ  | C-CA3-N3-C2     |
| 1   | 30-A  | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 3-A   | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 23-A  | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 41-A  | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 47-A  | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 36-A  | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 37-A  | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 11-A  | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 28-A  | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 17-A  | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 36-A  | 62  | CRQ  | CA2-CB2-CG2-CD2 |
| 1   | 2-A   | 62  | CRQ  | C-CA3-N3-C2     |
| 1   | 13-A  | 62  | CRQ  | C-CA3-N3-C2     |
| 1   | 5-A   | 62  | CRQ  | C-CA3-N3-C2     |
| 1   | 17-A  | 62  | CRQ  | C-CA3-N3-C2     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 1   | 9-A   | 62  | CRQ  | C-CA3-N3-C2     |
| 1   | 47-A  | 62  | CRQ  | C2-CA2-CB2-CG2  |
| 1   | 11-A  | 62  | CRQ  | C2-CA2-CB2-CG2  |
| 1   | 24-A  | 62  | CRQ  | C-CA3-N3-C1     |
| 1   | 33-A  | 62  | CRQ  | C-CA3-N3-C1     |
| 1   | 40-A  | 62  | CRQ  | C-CA3-N3-C1     |
| 1   | 36-A  | 62  | CRQ  | CA2-CB2-CG2-CD1 |
| 1   | 7-A   | 62  | CRQ  | C-CA3-N3-C2     |
| 1   | 36-A  | 62  | CRQ  | C-CA3-N3-C2     |
| 1   | 8-A   | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 41-A  | 62  | CRQ  | C2-CA2-CB2-CG2  |
| 1   | 18-A  | 62  | CRQ  | C-CA3-N3-C2     |
| 1   | 35-A  | 62  | CRQ  | C-CA3-N3-C1     |
| 1   | 6-A   | 62  | CRQ  | C-CA3-N3-C1     |
| 1   | 26-A  | 62  | CRQ  | C-CA3-N3-C1     |
| 1   | 29-A  | 62  | CRQ  | N2-CA2-CB2-CG2  |
| 1   | 25-A  | 62  | CRQ  | C-CA3-N3-C1     |
| 1   | 45-A  | 62  | CRQ  | C-CA3-N3-C2     |
| 1   | 20-A  | 62  | CRQ  | C1-CA1-CB1-CG1  |
| 1   | 44-A  | 62  | CRQ  | C1-CA1-CB1-CG1  |
| 1   | 47-A  | 62  | CRQ  | CA1-CB1-CG1-CD3 |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | 1-A   | 1                |
| 1   | 5-A   | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 5     | A     | 62:CRQ    | C      | 65:ASN    | N      | 1.20         |
| 1     | A     | 62:CRQ    | C      | 65:ASN    | N      | 1.18         |

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9      |
|-----|-------|---------------|--------|--------------|-----------------------|------------|
| 1   | 1-A   | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 2-A   | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 3-A   | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 4-A   | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 5-A   | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 6-A   | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 7-A   | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 8-A   | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 9-A   | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 10-A  | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 11-A  | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 12-A  | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 13-A  | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 14-A  | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 15-A  | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 16-A  | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 17-A  | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 18-A  | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 19-A  | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 20-A  | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 21-A  | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 22-A  | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 23-A  | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |
| 1   | 24-A  | 213/229 (93%) | 0.91   | 31 (14%) 2 2 | 22, 29, 37, 41        | 213 (100%) |

*Continued on next page...*



Continued from previous page...

| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9        |
|-----|-------|-------------------|--------|----------------|-----------------------|--------------|
| 1   | 25-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 26-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 27-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 28-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 29-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 30-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 31-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 32-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 33-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 34-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 35-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 36-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 37-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 38-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 39-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 40-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 41-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 42-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 43-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 44-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 45-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 46-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| 1   | 47-A  | 213/229 (93%)     | 0.91   | 31 (14%) 2 2   | 22, 29, 37, 41        | 213 (100%)   |
| All | All   | 10011/10763 (93%) | 0.91   | 1457 (14%) 2 2 | 22, 29, 37, 41        | 10011 (100%) |

All (1457) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 1-A   | 217 | TYR  | 11.3 |
| 1   | 2-A   | 217 | TYR  | 11.3 |
| 1   | 3-A   | 217 | TYR  | 11.3 |
| 1   | 4-A   | 217 | TYR  | 11.3 |
| 1   | 5-A   | 217 | TYR  | 11.3 |
| 1   | 6-A   | 217 | TYR  | 11.3 |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 7-A   | 217 | TYR  | 11.3 |
| 1   | 8-A   | 217 | TYR  | 11.3 |
| 1   | 9-A   | 217 | TYR  | 11.3 |
| 1   | 10-A  | 217 | TYR  | 11.3 |
| 1   | 11-A  | 217 | TYR  | 11.3 |
| 1   | 12-A  | 217 | TYR  | 11.3 |
| 1   | 13-A  | 217 | TYR  | 11.3 |
| 1   | 14-A  | 217 | TYR  | 11.3 |
| 1   | 15-A  | 217 | TYR  | 11.3 |
| 1   | 16-A  | 217 | TYR  | 11.3 |
| 1   | 17-A  | 217 | TYR  | 11.3 |
| 1   | 18-A  | 217 | TYR  | 11.3 |
| 1   | 19-A  | 217 | TYR  | 11.3 |
| 1   | 20-A  | 217 | TYR  | 11.3 |
| 1   | 21-A  | 217 | TYR  | 11.3 |
| 1   | 22-A  | 217 | TYR  | 11.3 |
| 1   | 23-A  | 217 | TYR  | 11.3 |
| 1   | 24-A  | 217 | TYR  | 11.3 |
| 1   | 25-A  | 217 | TYR  | 11.3 |
| 1   | 26-A  | 217 | TYR  | 11.3 |
| 1   | 27-A  | 217 | TYR  | 11.3 |
| 1   | 28-A  | 217 | TYR  | 11.3 |
| 1   | 29-A  | 217 | TYR  | 11.3 |
| 1   | 30-A  | 217 | TYR  | 11.3 |
| 1   | 31-A  | 217 | TYR  | 11.3 |
| 1   | 32-A  | 217 | TYR  | 11.3 |
| 1   | 33-A  | 217 | TYR  | 11.3 |
| 1   | 34-A  | 217 | TYR  | 11.3 |
| 1   | 35-A  | 217 | TYR  | 11.3 |
| 1   | 36-A  | 217 | TYR  | 11.3 |
| 1   | 37-A  | 217 | TYR  | 11.3 |
| 1   | 38-A  | 217 | TYR  | 11.3 |
| 1   | 39-A  | 217 | TYR  | 11.3 |
| 1   | 40-A  | 217 | TYR  | 11.3 |
| 1   | 41-A  | 217 | TYR  | 11.3 |
| 1   | 42-A  | 217 | TYR  | 11.3 |
| 1   | 43-A  | 217 | TYR  | 11.3 |
| 1   | 44-A  | 217 | TYR  | 11.3 |
| 1   | 45-A  | 217 | TYR  | 11.3 |
| 1   | 46-A  | 217 | TYR  | 11.3 |
| 1   | 47-A  | 217 | TYR  | 11.3 |
| 1   | 1-A   | 6   | PRO  | 6.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 2-A   | 6   | PRO  | 6.7  |
| 1   | 3-A   | 6   | PRO  | 6.7  |
| 1   | 4-A   | 6   | PRO  | 6.7  |
| 1   | 5-A   | 6   | PRO  | 6.7  |
| 1   | 6-A   | 6   | PRO  | 6.7  |
| 1   | 7-A   | 6   | PRO  | 6.7  |
| 1   | 8-A   | 6   | PRO  | 6.7  |
| 1   | 9-A   | 6   | PRO  | 6.7  |
| 1   | 10-A  | 6   | PRO  | 6.7  |
| 1   | 11-A  | 6   | PRO  | 6.7  |
| 1   | 12-A  | 6   | PRO  | 6.7  |
| 1   | 13-A  | 6   | PRO  | 6.7  |
| 1   | 14-A  | 6   | PRO  | 6.7  |
| 1   | 15-A  | 6   | PRO  | 6.7  |
| 1   | 16-A  | 6   | PRO  | 6.7  |
| 1   | 17-A  | 6   | PRO  | 6.7  |
| 1   | 18-A  | 6   | PRO  | 6.7  |
| 1   | 19-A  | 6   | PRO  | 6.7  |
| 1   | 20-A  | 6   | PRO  | 6.7  |
| 1   | 21-A  | 6   | PRO  | 6.7  |
| 1   | 22-A  | 6   | PRO  | 6.7  |
| 1   | 23-A  | 6   | PRO  | 6.7  |
| 1   | 24-A  | 6   | PRO  | 6.7  |
| 1   | 25-A  | 6   | PRO  | 6.7  |
| 1   | 26-A  | 6   | PRO  | 6.7  |
| 1   | 27-A  | 6   | PRO  | 6.7  |
| 1   | 28-A  | 6   | PRO  | 6.7  |
| 1   | 29-A  | 6   | PRO  | 6.7  |
| 1   | 30-A  | 6   | PRO  | 6.7  |
| 1   | 31-A  | 6   | PRO  | 6.7  |
| 1   | 32-A  | 6   | PRO  | 6.7  |
| 1   | 33-A  | 6   | PRO  | 6.7  |
| 1   | 34-A  | 6   | PRO  | 6.7  |
| 1   | 35-A  | 6   | PRO  | 6.7  |
| 1   | 36-A  | 6   | PRO  | 6.7  |
| 1   | 37-A  | 6   | PRO  | 6.7  |
| 1   | 38-A  | 6   | PRO  | 6.7  |
| 1   | 39-A  | 6   | PRO  | 6.7  |
| 1   | 40-A  | 6   | PRO  | 6.7  |
| 1   | 41-A  | 6   | PRO  | 6.7  |
| 1   | 42-A  | 6   | PRO  | 6.7  |
| 1   | 43-A  | 6   | PRO  | 6.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 44-A  | 6   | PRO  | 6.7  |
| 1   | 45-A  | 6   | PRO  | 6.7  |
| 1   | 46-A  | 6   | PRO  | 6.7  |
| 1   | 47-A  | 6   | PRO  | 6.7  |
| 1   | 1-A   | 152 | VAL  | 6.1  |
| 1   | 2-A   | 152 | VAL  | 6.1  |
| 1   | 3-A   | 152 | VAL  | 6.1  |
| 1   | 4-A   | 152 | VAL  | 6.1  |
| 1   | 5-A   | 152 | VAL  | 6.1  |
| 1   | 6-A   | 152 | VAL  | 6.1  |
| 1   | 7-A   | 152 | VAL  | 6.1  |
| 1   | 8-A   | 152 | VAL  | 6.1  |
| 1   | 9-A   | 152 | VAL  | 6.1  |
| 1   | 10-A  | 152 | VAL  | 6.1  |
| 1   | 11-A  | 152 | VAL  | 6.1  |
| 1   | 12-A  | 152 | VAL  | 6.1  |
| 1   | 13-A  | 152 | VAL  | 6.1  |
| 1   | 14-A  | 152 | VAL  | 6.1  |
| 1   | 15-A  | 152 | VAL  | 6.1  |
| 1   | 16-A  | 152 | VAL  | 6.1  |
| 1   | 17-A  | 152 | VAL  | 6.1  |
| 1   | 18-A  | 152 | VAL  | 6.1  |
| 1   | 19-A  | 152 | VAL  | 6.1  |
| 1   | 20-A  | 152 | VAL  | 6.1  |
| 1   | 21-A  | 152 | VAL  | 6.1  |
| 1   | 22-A  | 152 | VAL  | 6.1  |
| 1   | 23-A  | 152 | VAL  | 6.1  |
| 1   | 24-A  | 152 | VAL  | 6.1  |
| 1   | 25-A  | 152 | VAL  | 6.1  |
| 1   | 26-A  | 152 | VAL  | 6.1  |
| 1   | 27-A  | 152 | VAL  | 6.1  |
| 1   | 28-A  | 152 | VAL  | 6.1  |
| 1   | 29-A  | 152 | VAL  | 6.1  |
| 1   | 30-A  | 152 | VAL  | 6.1  |
| 1   | 31-A  | 152 | VAL  | 6.1  |
| 1   | 32-A  | 152 | VAL  | 6.1  |
| 1   | 33-A  | 152 | VAL  | 6.1  |
| 1   | 34-A  | 152 | VAL  | 6.1  |
| 1   | 35-A  | 152 | VAL  | 6.1  |
| 1   | 36-A  | 152 | VAL  | 6.1  |
| 1   | 37-A  | 152 | VAL  | 6.1  |
| 1   | 38-A  | 152 | VAL  | 6.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 39-A  | 152 | VAL  | 6.1  |
| 1   | 40-A  | 152 | VAL  | 6.1  |
| 1   | 41-A  | 152 | VAL  | 6.1  |
| 1   | 42-A  | 152 | VAL  | 6.1  |
| 1   | 43-A  | 152 | VAL  | 6.1  |
| 1   | 44-A  | 152 | VAL  | 6.1  |
| 1   | 45-A  | 152 | VAL  | 6.1  |
| 1   | 46-A  | 152 | VAL  | 6.1  |
| 1   | 47-A  | 152 | VAL  | 6.1  |
| 1   | 1-A   | 150 | ASP  | 5.1  |
| 1   | 2-A   | 150 | ASP  | 5.1  |
| 1   | 3-A   | 150 | ASP  | 5.1  |
| 1   | 4-A   | 150 | ASP  | 5.1  |
| 1   | 5-A   | 150 | ASP  | 5.1  |
| 1   | 6-A   | 150 | ASP  | 5.1  |
| 1   | 7-A   | 150 | ASP  | 5.1  |
| 1   | 8-A   | 150 | ASP  | 5.1  |
| 1   | 9-A   | 150 | ASP  | 5.1  |
| 1   | 10-A  | 150 | ASP  | 5.1  |
| 1   | 11-A  | 150 | ASP  | 5.1  |
| 1   | 12-A  | 150 | ASP  | 5.1  |
| 1   | 13-A  | 150 | ASP  | 5.1  |
| 1   | 14-A  | 150 | ASP  | 5.1  |
| 1   | 15-A  | 150 | ASP  | 5.1  |
| 1   | 16-A  | 150 | ASP  | 5.1  |
| 1   | 17-A  | 150 | ASP  | 5.1  |
| 1   | 18-A  | 150 | ASP  | 5.1  |
| 1   | 19-A  | 150 | ASP  | 5.1  |
| 1   | 20-A  | 150 | ASP  | 5.1  |
| 1   | 21-A  | 150 | ASP  | 5.1  |
| 1   | 22-A  | 150 | ASP  | 5.1  |
| 1   | 23-A  | 150 | ASP  | 5.1  |
| 1   | 24-A  | 150 | ASP  | 5.1  |
| 1   | 25-A  | 150 | ASP  | 5.1  |
| 1   | 26-A  | 150 | ASP  | 5.1  |
| 1   | 27-A  | 150 | ASP  | 5.1  |
| 1   | 28-A  | 150 | ASP  | 5.1  |
| 1   | 29-A  | 150 | ASP  | 5.1  |
| 1   | 30-A  | 150 | ASP  | 5.1  |
| 1   | 31-A  | 150 | ASP  | 5.1  |
| 1   | 32-A  | 150 | ASP  | 5.1  |
| 1   | 33-A  | 150 | ASP  | 5.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 34-A  | 150 | ASP  | 5.1  |
| 1   | 35-A  | 150 | ASP  | 5.1  |
| 1   | 36-A  | 150 | ASP  | 5.1  |
| 1   | 37-A  | 150 | ASP  | 5.1  |
| 1   | 38-A  | 150 | ASP  | 5.1  |
| 1   | 39-A  | 150 | ASP  | 5.1  |
| 1   | 40-A  | 150 | ASP  | 5.1  |
| 1   | 41-A  | 150 | ASP  | 5.1  |
| 1   | 42-A  | 150 | ASP  | 5.1  |
| 1   | 43-A  | 150 | ASP  | 5.1  |
| 1   | 44-A  | 150 | ASP  | 5.1  |
| 1   | 45-A  | 150 | ASP  | 5.1  |
| 1   | 46-A  | 150 | ASP  | 5.1  |
| 1   | 47-A  | 150 | ASP  | 5.1  |
| 1   | 1-A   | 111 | GLY  | 5.0  |
| 1   | 2-A   | 111 | GLY  | 5.0  |
| 1   | 3-A   | 111 | GLY  | 5.0  |
| 1   | 4-A   | 111 | GLY  | 5.0  |
| 1   | 5-A   | 111 | GLY  | 5.0  |
| 1   | 6-A   | 111 | GLY  | 5.0  |
| 1   | 7-A   | 111 | GLY  | 5.0  |
| 1   | 8-A   | 111 | GLY  | 5.0  |
| 1   | 9-A   | 111 | GLY  | 5.0  |
| 1   | 10-A  | 111 | GLY  | 5.0  |
| 1   | 11-A  | 111 | GLY  | 5.0  |
| 1   | 12-A  | 111 | GLY  | 5.0  |
| 1   | 13-A  | 111 | GLY  | 5.0  |
| 1   | 14-A  | 111 | GLY  | 5.0  |
| 1   | 15-A  | 111 | GLY  | 5.0  |
| 1   | 16-A  | 111 | GLY  | 5.0  |
| 1   | 17-A  | 111 | GLY  | 5.0  |
| 1   | 18-A  | 111 | GLY  | 5.0  |
| 1   | 19-A  | 111 | GLY  | 5.0  |
| 1   | 20-A  | 111 | GLY  | 5.0  |
| 1   | 21-A  | 111 | GLY  | 5.0  |
| 1   | 22-A  | 111 | GLY  | 5.0  |
| 1   | 23-A  | 111 | GLY  | 5.0  |
| 1   | 24-A  | 111 | GLY  | 5.0  |
| 1   | 25-A  | 111 | GLY  | 5.0  |
| 1   | 26-A  | 111 | GLY  | 5.0  |
| 1   | 27-A  | 111 | GLY  | 5.0  |
| 1   | 28-A  | 111 | GLY  | 5.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 29-A  | 111 | GLY  | 5.0  |
| 1   | 30-A  | 111 | GLY  | 5.0  |
| 1   | 31-A  | 111 | GLY  | 5.0  |
| 1   | 32-A  | 111 | GLY  | 5.0  |
| 1   | 33-A  | 111 | GLY  | 5.0  |
| 1   | 34-A  | 111 | GLY  | 5.0  |
| 1   | 35-A  | 111 | GLY  | 5.0  |
| 1   | 36-A  | 111 | GLY  | 5.0  |
| 1   | 37-A  | 111 | GLY  | 5.0  |
| 1   | 38-A  | 111 | GLY  | 5.0  |
| 1   | 39-A  | 111 | GLY  | 5.0  |
| 1   | 40-A  | 111 | GLY  | 5.0  |
| 1   | 41-A  | 111 | GLY  | 5.0  |
| 1   | 42-A  | 111 | GLY  | 5.0  |
| 1   | 43-A  | 111 | GLY  | 5.0  |
| 1   | 44-A  | 111 | GLY  | 5.0  |
| 1   | 45-A  | 111 | GLY  | 5.0  |
| 1   | 46-A  | 111 | GLY  | 5.0  |
| 1   | 47-A  | 111 | GLY  | 5.0  |
| 1   | 1-A   | 49  | PRO  | 4.9  |
| 1   | 2-A   | 49  | PRO  | 4.9  |
| 1   | 3-A   | 49  | PRO  | 4.9  |
| 1   | 4-A   | 49  | PRO  | 4.9  |
| 1   | 5-A   | 49  | PRO  | 4.9  |
| 1   | 6-A   | 49  | PRO  | 4.9  |
| 1   | 7-A   | 49  | PRO  | 4.9  |
| 1   | 8-A   | 49  | PRO  | 4.9  |
| 1   | 9-A   | 49  | PRO  | 4.9  |
| 1   | 10-A  | 49  | PRO  | 4.9  |
| 1   | 11-A  | 49  | PRO  | 4.9  |
| 1   | 12-A  | 49  | PRO  | 4.9  |
| 1   | 13-A  | 49  | PRO  | 4.9  |
| 1   | 14-A  | 49  | PRO  | 4.9  |
| 1   | 15-A  | 49  | PRO  | 4.9  |
| 1   | 16-A  | 49  | PRO  | 4.9  |
| 1   | 17-A  | 49  | PRO  | 4.9  |
| 1   | 18-A  | 49  | PRO  | 4.9  |
| 1   | 19-A  | 49  | PRO  | 4.9  |
| 1   | 20-A  | 49  | PRO  | 4.9  |
| 1   | 21-A  | 49  | PRO  | 4.9  |
| 1   | 22-A  | 49  | PRO  | 4.9  |
| 1   | 23-A  | 49  | PRO  | 4.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 24-A  | 49  | PRO  | 4.9  |
| 1   | 25-A  | 49  | PRO  | 4.9  |
| 1   | 26-A  | 49  | PRO  | 4.9  |
| 1   | 27-A  | 49  | PRO  | 4.9  |
| 1   | 28-A  | 49  | PRO  | 4.9  |
| 1   | 29-A  | 49  | PRO  | 4.9  |
| 1   | 30-A  | 49  | PRO  | 4.9  |
| 1   | 31-A  | 49  | PRO  | 4.9  |
| 1   | 32-A  | 49  | PRO  | 4.9  |
| 1   | 33-A  | 49  | PRO  | 4.9  |
| 1   | 34-A  | 49  | PRO  | 4.9  |
| 1   | 35-A  | 49  | PRO  | 4.9  |
| 1   | 36-A  | 49  | PRO  | 4.9  |
| 1   | 37-A  | 49  | PRO  | 4.9  |
| 1   | 38-A  | 49  | PRO  | 4.9  |
| 1   | 39-A  | 49  | PRO  | 4.9  |
| 1   | 40-A  | 49  | PRO  | 4.9  |
| 1   | 41-A  | 49  | PRO  | 4.9  |
| 1   | 42-A  | 49  | PRO  | 4.9  |
| 1   | 43-A  | 49  | PRO  | 4.9  |
| 1   | 44-A  | 49  | PRO  | 4.9  |
| 1   | 45-A  | 49  | PRO  | 4.9  |
| 1   | 46-A  | 49  | PRO  | 4.9  |
| 1   | 47-A  | 49  | PRO  | 4.9  |
| 1   | 1-A   | 48  | ALA  | 4.5  |
| 1   | 2-A   | 48  | ALA  | 4.5  |
| 1   | 3-A   | 48  | ALA  | 4.5  |
| 1   | 4-A   | 48  | ALA  | 4.5  |
| 1   | 5-A   | 48  | ALA  | 4.5  |
| 1   | 6-A   | 48  | ALA  | 4.5  |
| 1   | 7-A   | 48  | ALA  | 4.5  |
| 1   | 8-A   | 48  | ALA  | 4.5  |
| 1   | 9-A   | 48  | ALA  | 4.5  |
| 1   | 10-A  | 48  | ALA  | 4.5  |
| 1   | 11-A  | 48  | ALA  | 4.5  |
| 1   | 12-A  | 48  | ALA  | 4.5  |
| 1   | 13-A  | 48  | ALA  | 4.5  |
| 1   | 14-A  | 48  | ALA  | 4.5  |
| 1   | 15-A  | 48  | ALA  | 4.5  |
| 1   | 16-A  | 48  | ALA  | 4.5  |
| 1   | 17-A  | 48  | ALA  | 4.5  |
| 1   | 18-A  | 48  | ALA  | 4.5  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 19-A  | 48  | ALA  | 4.5  |
| 1   | 20-A  | 48  | ALA  | 4.5  |
| 1   | 21-A  | 48  | ALA  | 4.5  |
| 1   | 22-A  | 48  | ALA  | 4.5  |
| 1   | 23-A  | 48  | ALA  | 4.5  |
| 1   | 24-A  | 48  | ALA  | 4.5  |
| 1   | 25-A  | 48  | ALA  | 4.5  |
| 1   | 26-A  | 48  | ALA  | 4.5  |
| 1   | 27-A  | 48  | ALA  | 4.5  |
| 1   | 28-A  | 48  | ALA  | 4.5  |
| 1   | 29-A  | 48  | ALA  | 4.5  |
| 1   | 30-A  | 48  | ALA  | 4.5  |
| 1   | 31-A  | 48  | ALA  | 4.5  |
| 1   | 32-A  | 48  | ALA  | 4.5  |
| 1   | 33-A  | 48  | ALA  | 4.5  |
| 1   | 34-A  | 48  | ALA  | 4.5  |
| 1   | 35-A  | 48  | ALA  | 4.5  |
| 1   | 36-A  | 48  | ALA  | 4.5  |
| 1   | 37-A  | 48  | ALA  | 4.5  |
| 1   | 38-A  | 48  | ALA  | 4.5  |
| 1   | 39-A  | 48  | ALA  | 4.5  |
| 1   | 40-A  | 48  | ALA  | 4.5  |
| 1   | 41-A  | 48  | ALA  | 4.5  |
| 1   | 42-A  | 48  | ALA  | 4.5  |
| 1   | 43-A  | 48  | ALA  | 4.5  |
| 1   | 44-A  | 48  | ALA  | 4.5  |
| 1   | 45-A  | 48  | ALA  | 4.5  |
| 1   | 46-A  | 48  | ALA  | 4.5  |
| 1   | 47-A  | 48  | ALA  | 4.5  |
| 1   | 1-A   | 74  | ASP  | 4.3  |
| 1   | 2-A   | 74  | ASP  | 4.3  |
| 1   | 3-A   | 74  | ASP  | 4.3  |
| 1   | 4-A   | 74  | ASP  | 4.3  |
| 1   | 5-A   | 74  | ASP  | 4.3  |
| 1   | 6-A   | 74  | ASP  | 4.3  |
| 1   | 7-A   | 74  | ASP  | 4.3  |
| 1   | 8-A   | 74  | ASP  | 4.3  |
| 1   | 9-A   | 74  | ASP  | 4.3  |
| 1   | 10-A  | 74  | ASP  | 4.3  |
| 1   | 11-A  | 74  | ASP  | 4.3  |
| 1   | 12-A  | 74  | ASP  | 4.3  |
| 1   | 13-A  | 74  | ASP  | 4.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 14-A  | 74  | ASP  | 4.3  |
| 1   | 15-A  | 74  | ASP  | 4.3  |
| 1   | 16-A  | 74  | ASP  | 4.3  |
| 1   | 17-A  | 74  | ASP  | 4.3  |
| 1   | 18-A  | 74  | ASP  | 4.3  |
| 1   | 19-A  | 74  | ASP  | 4.3  |
| 1   | 20-A  | 74  | ASP  | 4.3  |
| 1   | 21-A  | 74  | ASP  | 4.3  |
| 1   | 22-A  | 74  | ASP  | 4.3  |
| 1   | 23-A  | 74  | ASP  | 4.3  |
| 1   | 24-A  | 74  | ASP  | 4.3  |
| 1   | 25-A  | 74  | ASP  | 4.3  |
| 1   | 26-A  | 74  | ASP  | 4.3  |
| 1   | 27-A  | 74  | ASP  | 4.3  |
| 1   | 28-A  | 74  | ASP  | 4.3  |
| 1   | 29-A  | 74  | ASP  | 4.3  |
| 1   | 30-A  | 74  | ASP  | 4.3  |
| 1   | 31-A  | 74  | ASP  | 4.3  |
| 1   | 32-A  | 74  | ASP  | 4.3  |
| 1   | 33-A  | 74  | ASP  | 4.3  |
| 1   | 34-A  | 74  | ASP  | 4.3  |
| 1   | 35-A  | 74  | ASP  | 4.3  |
| 1   | 36-A  | 74  | ASP  | 4.3  |
| 1   | 37-A  | 74  | ASP  | 4.3  |
| 1   | 38-A  | 74  | ASP  | 4.3  |
| 1   | 39-A  | 74  | ASP  | 4.3  |
| 1   | 40-A  | 74  | ASP  | 4.3  |
| 1   | 41-A  | 74  | ASP  | 4.3  |
| 1   | 42-A  | 74  | ASP  | 4.3  |
| 1   | 43-A  | 74  | ASP  | 4.3  |
| 1   | 44-A  | 74  | ASP  | 4.3  |
| 1   | 45-A  | 74  | ASP  | 4.3  |
| 1   | 46-A  | 74  | ASP  | 4.3  |
| 1   | 47-A  | 74  | ASP  | 4.3  |
| 1   | 1-A   | 3   | VAL  | 4.2  |
| 1   | 2-A   | 3   | VAL  | 4.2  |
| 1   | 3-A   | 3   | VAL  | 4.2  |
| 1   | 4-A   | 3   | VAL  | 4.2  |
| 1   | 5-A   | 3   | VAL  | 4.2  |
| 1   | 6-A   | 3   | VAL  | 4.2  |
| 1   | 7-A   | 3   | VAL  | 4.2  |
| 1   | 8-A   | 3   | VAL  | 4.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 9-A   | 3   | VAL  | 4.2  |
| 1   | 10-A  | 3   | VAL  | 4.2  |
| 1   | 11-A  | 3   | VAL  | 4.2  |
| 1   | 12-A  | 3   | VAL  | 4.2  |
| 1   | 13-A  | 3   | VAL  | 4.2  |
| 1   | 14-A  | 3   | VAL  | 4.2  |
| 1   | 15-A  | 3   | VAL  | 4.2  |
| 1   | 16-A  | 3   | VAL  | 4.2  |
| 1   | 17-A  | 3   | VAL  | 4.2  |
| 1   | 18-A  | 3   | VAL  | 4.2  |
| 1   | 19-A  | 3   | VAL  | 4.2  |
| 1   | 20-A  | 3   | VAL  | 4.2  |
| 1   | 21-A  | 3   | VAL  | 4.2  |
| 1   | 22-A  | 3   | VAL  | 4.2  |
| 1   | 23-A  | 3   | VAL  | 4.2  |
| 1   | 24-A  | 3   | VAL  | 4.2  |
| 1   | 25-A  | 3   | VAL  | 4.2  |
| 1   | 26-A  | 3   | VAL  | 4.2  |
| 1   | 27-A  | 3   | VAL  | 4.2  |
| 1   | 28-A  | 3   | VAL  | 4.2  |
| 1   | 29-A  | 3   | VAL  | 4.2  |
| 1   | 30-A  | 3   | VAL  | 4.2  |
| 1   | 31-A  | 3   | VAL  | 4.2  |
| 1   | 32-A  | 3   | VAL  | 4.2  |
| 1   | 33-A  | 3   | VAL  | 4.2  |
| 1   | 34-A  | 3   | VAL  | 4.2  |
| 1   | 35-A  | 3   | VAL  | 4.2  |
| 1   | 36-A  | 3   | VAL  | 4.2  |
| 1   | 37-A  | 3   | VAL  | 4.2  |
| 1   | 38-A  | 3   | VAL  | 4.2  |
| 1   | 39-A  | 3   | VAL  | 4.2  |
| 1   | 40-A  | 3   | VAL  | 4.2  |
| 1   | 41-A  | 3   | VAL  | 4.2  |
| 1   | 42-A  | 3   | VAL  | 4.2  |
| 1   | 43-A  | 3   | VAL  | 4.2  |
| 1   | 44-A  | 3   | VAL  | 4.2  |
| 1   | 45-A  | 3   | VAL  | 4.2  |
| 1   | 46-A  | 3   | VAL  | 4.2  |
| 1   | 47-A  | 3   | VAL  | 4.2  |
| 1   | 1-A   | 151 | GLY  | 4.1  |
| 1   | 2-A   | 151 | GLY  | 4.1  |
| 1   | 3-A   | 151 | GLY  | 4.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 4-A   | 151 | GLY  | 4.1  |
| 1   | 5-A   | 151 | GLY  | 4.1  |
| 1   | 6-A   | 151 | GLY  | 4.1  |
| 1   | 7-A   | 151 | GLY  | 4.1  |
| 1   | 8-A   | 151 | GLY  | 4.1  |
| 1   | 9-A   | 151 | GLY  | 4.1  |
| 1   | 10-A  | 151 | GLY  | 4.1  |
| 1   | 11-A  | 151 | GLY  | 4.1  |
| 1   | 12-A  | 151 | GLY  | 4.1  |
| 1   | 13-A  | 151 | GLY  | 4.1  |
| 1   | 14-A  | 151 | GLY  | 4.1  |
| 1   | 15-A  | 151 | GLY  | 4.1  |
| 1   | 16-A  | 151 | GLY  | 4.1  |
| 1   | 17-A  | 151 | GLY  | 4.1  |
| 1   | 18-A  | 151 | GLY  | 4.1  |
| 1   | 19-A  | 151 | GLY  | 4.1  |
| 1   | 20-A  | 151 | GLY  | 4.1  |
| 1   | 21-A  | 151 | GLY  | 4.1  |
| 1   | 22-A  | 151 | GLY  | 4.1  |
| 1   | 23-A  | 151 | GLY  | 4.1  |
| 1   | 24-A  | 151 | GLY  | 4.1  |
| 1   | 25-A  | 151 | GLY  | 4.1  |
| 1   | 26-A  | 151 | GLY  | 4.1  |
| 1   | 27-A  | 151 | GLY  | 4.1  |
| 1   | 28-A  | 151 | GLY  | 4.1  |
| 1   | 29-A  | 151 | GLY  | 4.1  |
| 1   | 30-A  | 151 | GLY  | 4.1  |
| 1   | 31-A  | 151 | GLY  | 4.1  |
| 1   | 32-A  | 151 | GLY  | 4.1  |
| 1   | 33-A  | 151 | GLY  | 4.1  |
| 1   | 34-A  | 151 | GLY  | 4.1  |
| 1   | 35-A  | 151 | GLY  | 4.1  |
| 1   | 36-A  | 151 | GLY  | 4.1  |
| 1   | 37-A  | 151 | GLY  | 4.1  |
| 1   | 38-A  | 151 | GLY  | 4.1  |
| 1   | 39-A  | 151 | GLY  | 4.1  |
| 1   | 40-A  | 151 | GLY  | 4.1  |
| 1   | 41-A  | 151 | GLY  | 4.1  |
| 1   | 42-A  | 151 | GLY  | 4.1  |
| 1   | 43-A  | 151 | GLY  | 4.1  |
| 1   | 44-A  | 151 | GLY  | 4.1  |
| 1   | 45-A  | 151 | GLY  | 4.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 46-A  | 151 | GLY  | 4.1  |
| 1   | 47-A  | 151 | GLY  | 4.1  |
| 1   | 1-A   | 128 | ASN  | 3.8  |
| 1   | 2-A   | 128 | ASN  | 3.8  |
| 1   | 3-A   | 128 | ASN  | 3.8  |
| 1   | 4-A   | 128 | ASN  | 3.8  |
| 1   | 5-A   | 128 | ASN  | 3.8  |
| 1   | 6-A   | 128 | ASN  | 3.8  |
| 1   | 7-A   | 128 | ASN  | 3.8  |
| 1   | 8-A   | 128 | ASN  | 3.8  |
| 1   | 9-A   | 128 | ASN  | 3.8  |
| 1   | 10-A  | 128 | ASN  | 3.8  |
| 1   | 11-A  | 128 | ASN  | 3.8  |
| 1   | 12-A  | 128 | ASN  | 3.8  |
| 1   | 13-A  | 128 | ASN  | 3.8  |
| 1   | 14-A  | 128 | ASN  | 3.8  |
| 1   | 15-A  | 128 | ASN  | 3.8  |
| 1   | 16-A  | 128 | ASN  | 3.8  |
| 1   | 17-A  | 128 | ASN  | 3.8  |
| 1   | 18-A  | 128 | ASN  | 3.8  |
| 1   | 19-A  | 128 | ASN  | 3.8  |
| 1   | 20-A  | 128 | ASN  | 3.8  |
| 1   | 21-A  | 128 | ASN  | 3.8  |
| 1   | 22-A  | 128 | ASN  | 3.8  |
| 1   | 23-A  | 128 | ASN  | 3.8  |
| 1   | 24-A  | 128 | ASN  | 3.8  |
| 1   | 25-A  | 128 | ASN  | 3.8  |
| 1   | 26-A  | 128 | ASN  | 3.8  |
| 1   | 27-A  | 128 | ASN  | 3.8  |
| 1   | 28-A  | 128 | ASN  | 3.8  |
| 1   | 29-A  | 128 | ASN  | 3.8  |
| 1   | 30-A  | 128 | ASN  | 3.8  |
| 1   | 31-A  | 128 | ASN  | 3.8  |
| 1   | 32-A  | 128 | ASN  | 3.8  |
| 1   | 33-A  | 128 | ASN  | 3.8  |
| 1   | 34-A  | 128 | ASN  | 3.8  |
| 1   | 35-A  | 128 | ASN  | 3.8  |
| 1   | 36-A  | 128 | ASN  | 3.8  |
| 1   | 37-A  | 128 | ASN  | 3.8  |
| 1   | 38-A  | 128 | ASN  | 3.8  |
| 1   | 39-A  | 128 | ASN  | 3.8  |
| 1   | 40-A  | 128 | ASN  | 3.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 41-A  | 128 | ASN  | 3.8  |
| 1   | 42-A  | 128 | ASN  | 3.8  |
| 1   | 43-A  | 128 | ASN  | 3.8  |
| 1   | 44-A  | 128 | ASN  | 3.8  |
| 1   | 45-A  | 128 | ASN  | 3.8  |
| 1   | 46-A  | 128 | ASN  | 3.8  |
| 1   | 47-A  | 128 | ASN  | 3.8  |
| 1   | 1-A   | 202 | LYS  | 3.7  |
| 1   | 2-A   | 202 | LYS  | 3.7  |
| 1   | 3-A   | 202 | LYS  | 3.7  |
| 1   | 4-A   | 202 | LYS  | 3.7  |
| 1   | 5-A   | 202 | LYS  | 3.7  |
| 1   | 6-A   | 202 | LYS  | 3.7  |
| 1   | 7-A   | 202 | LYS  | 3.7  |
| 1   | 8-A   | 202 | LYS  | 3.7  |
| 1   | 9-A   | 202 | LYS  | 3.7  |
| 1   | 10-A  | 202 | LYS  | 3.7  |
| 1   | 11-A  | 202 | LYS  | 3.7  |
| 1   | 12-A  | 202 | LYS  | 3.7  |
| 1   | 13-A  | 202 | LYS  | 3.7  |
| 1   | 14-A  | 202 | LYS  | 3.7  |
| 1   | 15-A  | 202 | LYS  | 3.7  |
| 1   | 16-A  | 202 | LYS  | 3.7  |
| 1   | 17-A  | 202 | LYS  | 3.7  |
| 1   | 18-A  | 202 | LYS  | 3.7  |
| 1   | 19-A  | 202 | LYS  | 3.7  |
| 1   | 20-A  | 202 | LYS  | 3.7  |
| 1   | 21-A  | 202 | LYS  | 3.7  |
| 1   | 22-A  | 202 | LYS  | 3.7  |
| 1   | 23-A  | 202 | LYS  | 3.7  |
| 1   | 24-A  | 202 | LYS  | 3.7  |
| 1   | 25-A  | 202 | LYS  | 3.7  |
| 1   | 26-A  | 202 | LYS  | 3.7  |
| 1   | 27-A  | 202 | LYS  | 3.7  |
| 1   | 28-A  | 202 | LYS  | 3.7  |
| 1   | 29-A  | 202 | LYS  | 3.7  |
| 1   | 30-A  | 202 | LYS  | 3.7  |
| 1   | 31-A  | 202 | LYS  | 3.7  |
| 1   | 32-A  | 202 | LYS  | 3.7  |
| 1   | 33-A  | 202 | LYS  | 3.7  |
| 1   | 34-A  | 202 | LYS  | 3.7  |
| 1   | 35-A  | 202 | LYS  | 3.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 36-A  | 202 | LYS  | 3.7  |
| 1   | 37-A  | 202 | LYS  | 3.7  |
| 1   | 38-A  | 202 | LYS  | 3.7  |
| 1   | 39-A  | 202 | LYS  | 3.7  |
| 1   | 40-A  | 202 | LYS  | 3.7  |
| 1   | 41-A  | 202 | LYS  | 3.7  |
| 1   | 42-A  | 202 | LYS  | 3.7  |
| 1   | 43-A  | 202 | LYS  | 3.7  |
| 1   | 44-A  | 202 | LYS  | 3.7  |
| 1   | 45-A  | 202 | LYS  | 3.7  |
| 1   | 46-A  | 202 | LYS  | 3.7  |
| 1   | 47-A  | 202 | LYS  | 3.7  |
| 1   | 1-A   | 110 | GLU  | 3.5  |
| 1   | 2-A   | 110 | GLU  | 3.5  |
| 1   | 3-A   | 110 | GLU  | 3.5  |
| 1   | 4-A   | 110 | GLU  | 3.5  |
| 1   | 5-A   | 110 | GLU  | 3.5  |
| 1   | 6-A   | 110 | GLU  | 3.5  |
| 1   | 7-A   | 110 | GLU  | 3.5  |
| 1   | 8-A   | 110 | GLU  | 3.5  |
| 1   | 9-A   | 110 | GLU  | 3.5  |
| 1   | 10-A  | 110 | GLU  | 3.5  |
| 1   | 11-A  | 110 | GLU  | 3.5  |
| 1   | 12-A  | 110 | GLU  | 3.5  |
| 1   | 13-A  | 110 | GLU  | 3.5  |
| 1   | 14-A  | 110 | GLU  | 3.5  |
| 1   | 15-A  | 110 | GLU  | 3.5  |
| 1   | 16-A  | 110 | GLU  | 3.5  |
| 1   | 17-A  | 110 | GLU  | 3.5  |
| 1   | 18-A  | 110 | GLU  | 3.5  |
| 1   | 19-A  | 110 | GLU  | 3.5  |
| 1   | 20-A  | 110 | GLU  | 3.5  |
| 1   | 21-A  | 110 | GLU  | 3.5  |
| 1   | 22-A  | 110 | GLU  | 3.5  |
| 1   | 23-A  | 110 | GLU  | 3.5  |
| 1   | 24-A  | 110 | GLU  | 3.5  |
| 1   | 25-A  | 110 | GLU  | 3.5  |
| 1   | 26-A  | 110 | GLU  | 3.5  |
| 1   | 27-A  | 110 | GLU  | 3.5  |
| 1   | 28-A  | 110 | GLU  | 3.5  |
| 1   | 29-A  | 110 | GLU  | 3.5  |
| 1   | 30-A  | 110 | GLU  | 3.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 31-A  | 110 | GLU  | 3.5  |
| 1   | 32-A  | 110 | GLU  | 3.5  |
| 1   | 33-A  | 110 | GLU  | 3.5  |
| 1   | 34-A  | 110 | GLU  | 3.5  |
| 1   | 35-A  | 110 | GLU  | 3.5  |
| 1   | 36-A  | 110 | GLU  | 3.5  |
| 1   | 37-A  | 110 | GLU  | 3.5  |
| 1   | 38-A  | 110 | GLU  | 3.5  |
| 1   | 39-A  | 110 | GLU  | 3.5  |
| 1   | 40-A  | 110 | GLU  | 3.5  |
| 1   | 41-A  | 110 | GLU  | 3.5  |
| 1   | 42-A  | 110 | GLU  | 3.5  |
| 1   | 43-A  | 110 | GLU  | 3.5  |
| 1   | 44-A  | 110 | GLU  | 3.5  |
| 1   | 45-A  | 110 | GLU  | 3.5  |
| 1   | 46-A  | 110 | GLU  | 3.5  |
| 1   | 47-A  | 110 | GLU  | 3.5  |
| 1   | 1-A   | 127 | PRO  | 3.4  |
| 1   | 2-A   | 127 | PRO  | 3.4  |
| 1   | 3-A   | 127 | PRO  | 3.4  |
| 1   | 4-A   | 127 | PRO  | 3.4  |
| 1   | 5-A   | 127 | PRO  | 3.4  |
| 1   | 6-A   | 127 | PRO  | 3.4  |
| 1   | 7-A   | 127 | PRO  | 3.4  |
| 1   | 8-A   | 127 | PRO  | 3.4  |
| 1   | 9-A   | 127 | PRO  | 3.4  |
| 1   | 10-A  | 127 | PRO  | 3.4  |
| 1   | 11-A  | 127 | PRO  | 3.4  |
| 1   | 12-A  | 127 | PRO  | 3.4  |
| 1   | 13-A  | 127 | PRO  | 3.4  |
| 1   | 14-A  | 127 | PRO  | 3.4  |
| 1   | 15-A  | 127 | PRO  | 3.4  |
| 1   | 16-A  | 127 | PRO  | 3.4  |
| 1   | 17-A  | 127 | PRO  | 3.4  |
| 1   | 18-A  | 127 | PRO  | 3.4  |
| 1   | 19-A  | 127 | PRO  | 3.4  |
| 1   | 20-A  | 127 | PRO  | 3.4  |
| 1   | 21-A  | 127 | PRO  | 3.4  |
| 1   | 22-A  | 127 | PRO  | 3.4  |
| 1   | 23-A  | 127 | PRO  | 3.4  |
| 1   | 24-A  | 127 | PRO  | 3.4  |
| 1   | 25-A  | 127 | PRO  | 3.4  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 26-A  | 127 | PRO  | 3.4  |
| 1   | 27-A  | 127 | PRO  | 3.4  |
| 1   | 28-A  | 127 | PRO  | 3.4  |
| 1   | 29-A  | 127 | PRO  | 3.4  |
| 1   | 30-A  | 127 | PRO  | 3.4  |
| 1   | 31-A  | 127 | PRO  | 3.4  |
| 1   | 32-A  | 127 | PRO  | 3.4  |
| 1   | 33-A  | 127 | PRO  | 3.4  |
| 1   | 34-A  | 127 | PRO  | 3.4  |
| 1   | 35-A  | 127 | PRO  | 3.4  |
| 1   | 36-A  | 127 | PRO  | 3.4  |
| 1   | 37-A  | 127 | PRO  | 3.4  |
| 1   | 38-A  | 127 | PRO  | 3.4  |
| 1   | 39-A  | 127 | PRO  | 3.4  |
| 1   | 40-A  | 127 | PRO  | 3.4  |
| 1   | 41-A  | 127 | PRO  | 3.4  |
| 1   | 42-A  | 127 | PRO  | 3.4  |
| 1   | 43-A  | 127 | PRO  | 3.4  |
| 1   | 44-A  | 127 | PRO  | 3.4  |
| 1   | 45-A  | 127 | PRO  | 3.4  |
| 1   | 46-A  | 127 | PRO  | 3.4  |
| 1   | 47-A  | 127 | PRO  | 3.4  |
| 1   | 1-A   | 198 | LEU  | 3.4  |
| 1   | 2-A   | 198 | LEU  | 3.4  |
| 1   | 3-A   | 198 | LEU  | 3.4  |
| 1   | 4-A   | 198 | LEU  | 3.4  |
| 1   | 5-A   | 198 | LEU  | 3.4  |
| 1   | 6-A   | 198 | LEU  | 3.4  |
| 1   | 7-A   | 198 | LEU  | 3.4  |
| 1   | 8-A   | 198 | LEU  | 3.4  |
| 1   | 9-A   | 198 | LEU  | 3.4  |
| 1   | 10-A  | 198 | LEU  | 3.4  |
| 1   | 11-A  | 198 | LEU  | 3.4  |
| 1   | 12-A  | 198 | LEU  | 3.4  |
| 1   | 13-A  | 198 | LEU  | 3.4  |
| 1   | 14-A  | 198 | LEU  | 3.4  |
| 1   | 15-A  | 198 | LEU  | 3.4  |
| 1   | 16-A  | 198 | LEU  | 3.4  |
| 1   | 17-A  | 198 | LEU  | 3.4  |
| 1   | 18-A  | 198 | LEU  | 3.4  |
| 1   | 19-A  | 198 | LEU  | 3.4  |
| 1   | 20-A  | 198 | LEU  | 3.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 21-A  | 198 | LEU  | 3.4  |
| 1   | 22-A  | 198 | LEU  | 3.4  |
| 1   | 23-A  | 198 | LEU  | 3.4  |
| 1   | 24-A  | 198 | LEU  | 3.4  |
| 1   | 25-A  | 198 | LEU  | 3.4  |
| 1   | 26-A  | 198 | LEU  | 3.4  |
| 1   | 27-A  | 198 | LEU  | 3.4  |
| 1   | 28-A  | 198 | LEU  | 3.4  |
| 1   | 29-A  | 198 | LEU  | 3.4  |
| 1   | 30-A  | 198 | LEU  | 3.4  |
| 1   | 31-A  | 198 | LEU  | 3.4  |
| 1   | 32-A  | 198 | LEU  | 3.4  |
| 1   | 33-A  | 198 | LEU  | 3.4  |
| 1   | 34-A  | 198 | LEU  | 3.4  |
| 1   | 35-A  | 198 | LEU  | 3.4  |
| 1   | 36-A  | 198 | LEU  | 3.4  |
| 1   | 37-A  | 198 | LEU  | 3.4  |
| 1   | 38-A  | 198 | LEU  | 3.4  |
| 1   | 39-A  | 198 | LEU  | 3.4  |
| 1   | 40-A  | 198 | LEU  | 3.4  |
| 1   | 41-A  | 198 | LEU  | 3.4  |
| 1   | 42-A  | 198 | LEU  | 3.4  |
| 1   | 43-A  | 198 | LEU  | 3.4  |
| 1   | 44-A  | 198 | LEU  | 3.4  |
| 1   | 45-A  | 198 | LEU  | 3.4  |
| 1   | 46-A  | 198 | LEU  | 3.4  |
| 1   | 47-A  | 198 | LEU  | 3.4  |
| 1   | 1-A   | 216 | ARG  | 3.4  |
| 1   | 2-A   | 216 | ARG  | 3.4  |
| 1   | 3-A   | 216 | ARG  | 3.4  |
| 1   | 4-A   | 216 | ARG  | 3.4  |
| 1   | 5-A   | 216 | ARG  | 3.4  |
| 1   | 6-A   | 216 | ARG  | 3.4  |
| 1   | 7-A   | 216 | ARG  | 3.4  |
| 1   | 8-A   | 216 | ARG  | 3.4  |
| 1   | 9-A   | 216 | ARG  | 3.4  |
| 1   | 10-A  | 216 | ARG  | 3.4  |
| 1   | 11-A  | 216 | ARG  | 3.4  |
| 1   | 12-A  | 216 | ARG  | 3.4  |
| 1   | 13-A  | 216 | ARG  | 3.4  |
| 1   | 14-A  | 216 | ARG  | 3.4  |
| 1   | 15-A  | 216 | ARG  | 3.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 16-A  | 216 | ARG  | 3.4  |
| 1   | 17-A  | 216 | ARG  | 3.4  |
| 1   | 18-A  | 216 | ARG  | 3.4  |
| 1   | 19-A  | 216 | ARG  | 3.4  |
| 1   | 20-A  | 216 | ARG  | 3.4  |
| 1   | 21-A  | 216 | ARG  | 3.4  |
| 1   | 22-A  | 216 | ARG  | 3.4  |
| 1   | 23-A  | 216 | ARG  | 3.4  |
| 1   | 24-A  | 216 | ARG  | 3.4  |
| 1   | 25-A  | 216 | ARG  | 3.4  |
| 1   | 26-A  | 216 | ARG  | 3.4  |
| 1   | 27-A  | 216 | ARG  | 3.4  |
| 1   | 28-A  | 216 | ARG  | 3.4  |
| 1   | 29-A  | 216 | ARG  | 3.4  |
| 1   | 30-A  | 216 | ARG  | 3.4  |
| 1   | 31-A  | 216 | ARG  | 3.4  |
| 1   | 32-A  | 216 | ARG  | 3.4  |
| 1   | 33-A  | 216 | ARG  | 3.4  |
| 1   | 34-A  | 216 | ARG  | 3.4  |
| 1   | 35-A  | 216 | ARG  | 3.4  |
| 1   | 36-A  | 216 | ARG  | 3.4  |
| 1   | 37-A  | 216 | ARG  | 3.4  |
| 1   | 38-A  | 216 | ARG  | 3.4  |
| 1   | 39-A  | 216 | ARG  | 3.4  |
| 1   | 40-A  | 216 | ARG  | 3.4  |
| 1   | 41-A  | 216 | ARG  | 3.4  |
| 1   | 42-A  | 216 | ARG  | 3.4  |
| 1   | 43-A  | 216 | ARG  | 3.4  |
| 1   | 44-A  | 216 | ARG  | 3.4  |
| 1   | 45-A  | 216 | ARG  | 3.4  |
| 1   | 46-A  | 216 | ARG  | 3.4  |
| 1   | 47-A  | 216 | ARG  | 3.4  |
| 1   | 1-A   | 153 | LEU  | 3.1  |
| 1   | 2-A   | 153 | LEU  | 3.1  |
| 1   | 3-A   | 153 | LEU  | 3.1  |
| 1   | 4-A   | 153 | LEU  | 3.1  |
| 1   | 5-A   | 153 | LEU  | 3.1  |
| 1   | 6-A   | 153 | LEU  | 3.1  |
| 1   | 7-A   | 153 | LEU  | 3.1  |
| 1   | 8-A   | 153 | LEU  | 3.1  |
| 1   | 9-A   | 153 | LEU  | 3.1  |
| 1   | 10-A  | 153 | LEU  | 3.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 11-A  | 153 | LEU  | 3.1  |
| 1   | 12-A  | 153 | LEU  | 3.1  |
| 1   | 13-A  | 153 | LEU  | 3.1  |
| 1   | 14-A  | 153 | LEU  | 3.1  |
| 1   | 15-A  | 153 | LEU  | 3.1  |
| 1   | 16-A  | 153 | LEU  | 3.1  |
| 1   | 17-A  | 153 | LEU  | 3.1  |
| 1   | 18-A  | 153 | LEU  | 3.1  |
| 1   | 19-A  | 153 | LEU  | 3.1  |
| 1   | 20-A  | 153 | LEU  | 3.1  |
| 1   | 21-A  | 153 | LEU  | 3.1  |
| 1   | 22-A  | 153 | LEU  | 3.1  |
| 1   | 23-A  | 153 | LEU  | 3.1  |
| 1   | 24-A  | 153 | LEU  | 3.1  |
| 1   | 25-A  | 153 | LEU  | 3.1  |
| 1   | 26-A  | 153 | LEU  | 3.1  |
| 1   | 27-A  | 153 | LEU  | 3.1  |
| 1   | 28-A  | 153 | LEU  | 3.1  |
| 1   | 29-A  | 153 | LEU  | 3.1  |
| 1   | 30-A  | 153 | LEU  | 3.1  |
| 1   | 31-A  | 153 | LEU  | 3.1  |
| 1   | 32-A  | 153 | LEU  | 3.1  |
| 1   | 33-A  | 153 | LEU  | 3.1  |
| 1   | 34-A  | 153 | LEU  | 3.1  |
| 1   | 35-A  | 153 | LEU  | 3.1  |
| 1   | 36-A  | 153 | LEU  | 3.1  |
| 1   | 37-A  | 153 | LEU  | 3.1  |
| 1   | 38-A  | 153 | LEU  | 3.1  |
| 1   | 39-A  | 153 | LEU  | 3.1  |
| 1   | 40-A  | 153 | LEU  | 3.1  |
| 1   | 41-A  | 153 | LEU  | 3.1  |
| 1   | 42-A  | 153 | LEU  | 3.1  |
| 1   | 43-A  | 153 | LEU  | 3.1  |
| 1   | 44-A  | 153 | LEU  | 3.1  |
| 1   | 45-A  | 153 | LEU  | 3.1  |
| 1   | 46-A  | 153 | LEU  | 3.1  |
| 1   | 47-A  | 153 | LEU  | 3.1  |
| 1   | 1-A   | 2   | SER  | 3.0  |
| 1   | 2-A   | 2   | SER  | 3.0  |
| 1   | 3-A   | 2   | SER  | 3.0  |
| 1   | 4-A   | 2   | SER  | 3.0  |
| 1   | 5-A   | 2   | SER  | 3.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 6-A   | 2   | SER  | 3.0  |
| 1   | 7-A   | 2   | SER  | 3.0  |
| 1   | 8-A   | 2   | SER  | 3.0  |
| 1   | 9-A   | 2   | SER  | 3.0  |
| 1   | 10-A  | 2   | SER  | 3.0  |
| 1   | 11-A  | 2   | SER  | 3.0  |
| 1   | 12-A  | 2   | SER  | 3.0  |
| 1   | 13-A  | 2   | SER  | 3.0  |
| 1   | 14-A  | 2   | SER  | 3.0  |
| 1   | 15-A  | 2   | SER  | 3.0  |
| 1   | 16-A  | 2   | SER  | 3.0  |
| 1   | 17-A  | 2   | SER  | 3.0  |
| 1   | 18-A  | 2   | SER  | 3.0  |
| 1   | 19-A  | 2   | SER  | 3.0  |
| 1   | 20-A  | 2   | SER  | 3.0  |
| 1   | 21-A  | 2   | SER  | 3.0  |
| 1   | 22-A  | 2   | SER  | 3.0  |
| 1   | 23-A  | 2   | SER  | 3.0  |
| 1   | 24-A  | 2   | SER  | 3.0  |
| 1   | 25-A  | 2   | SER  | 3.0  |
| 1   | 26-A  | 2   | SER  | 3.0  |
| 1   | 27-A  | 2   | SER  | 3.0  |
| 1   | 28-A  | 2   | SER  | 3.0  |
| 1   | 29-A  | 2   | SER  | 3.0  |
| 1   | 30-A  | 2   | SER  | 3.0  |
| 1   | 31-A  | 2   | SER  | 3.0  |
| 1   | 32-A  | 2   | SER  | 3.0  |
| 1   | 33-A  | 2   | SER  | 3.0  |
| 1   | 34-A  | 2   | SER  | 3.0  |
| 1   | 35-A  | 2   | SER  | 3.0  |
| 1   | 36-A  | 2   | SER  | 3.0  |
| 1   | 37-A  | 2   | SER  | 3.0  |
| 1   | 38-A  | 2   | SER  | 3.0  |
| 1   | 39-A  | 2   | SER  | 3.0  |
| 1   | 40-A  | 2   | SER  | 3.0  |
| 1   | 41-A  | 2   | SER  | 3.0  |
| 1   | 42-A  | 2   | SER  | 3.0  |
| 1   | 43-A  | 2   | SER  | 3.0  |
| 1   | 44-A  | 2   | SER  | 3.0  |
| 1   | 45-A  | 2   | SER  | 3.0  |
| 1   | 46-A  | 2   | SER  | 3.0  |
| 1   | 47-A  | 2   | SER  | 3.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 1-A   | 51  | PRO  | 3.0  |
| 1   | 2-A   | 51  | PRO  | 3.0  |
| 1   | 3-A   | 51  | PRO  | 3.0  |
| 1   | 4-A   | 51  | PRO  | 3.0  |
| 1   | 5-A   | 51  | PRO  | 3.0  |
| 1   | 6-A   | 51  | PRO  | 3.0  |
| 1   | 7-A   | 51  | PRO  | 3.0  |
| 1   | 8-A   | 51  | PRO  | 3.0  |
| 1   | 9-A   | 51  | PRO  | 3.0  |
| 1   | 10-A  | 51  | PRO  | 3.0  |
| 1   | 11-A  | 51  | PRO  | 3.0  |
| 1   | 12-A  | 51  | PRO  | 3.0  |
| 1   | 13-A  | 51  | PRO  | 3.0  |
| 1   | 14-A  | 51  | PRO  | 3.0  |
| 1   | 15-A  | 51  | PRO  | 3.0  |
| 1   | 16-A  | 51  | PRO  | 3.0  |
| 1   | 17-A  | 51  | PRO  | 3.0  |
| 1   | 18-A  | 51  | PRO  | 3.0  |
| 1   | 19-A  | 51  | PRO  | 3.0  |
| 1   | 20-A  | 51  | PRO  | 3.0  |
| 1   | 21-A  | 51  | PRO  | 3.0  |
| 1   | 22-A  | 51  | PRO  | 3.0  |
| 1   | 23-A  | 51  | PRO  | 3.0  |
| 1   | 24-A  | 51  | PRO  | 3.0  |
| 1   | 25-A  | 51  | PRO  | 3.0  |
| 1   | 26-A  | 51  | PRO  | 3.0  |
| 1   | 27-A  | 51  | PRO  | 3.0  |
| 1   | 28-A  | 51  | PRO  | 3.0  |
| 1   | 29-A  | 51  | PRO  | 3.0  |
| 1   | 30-A  | 51  | PRO  | 3.0  |
| 1   | 31-A  | 51  | PRO  | 3.0  |
| 1   | 32-A  | 51  | PRO  | 3.0  |
| 1   | 33-A  | 51  | PRO  | 3.0  |
| 1   | 34-A  | 51  | PRO  | 3.0  |
| 1   | 35-A  | 51  | PRO  | 3.0  |
| 1   | 36-A  | 51  | PRO  | 3.0  |
| 1   | 37-A  | 51  | PRO  | 3.0  |
| 1   | 38-A  | 51  | PRO  | 3.0  |
| 1   | 39-A  | 51  | PRO  | 3.0  |
| 1   | 40-A  | 51  | PRO  | 3.0  |
| 1   | 41-A  | 51  | PRO  | 3.0  |
| 1   | 42-A  | 51  | PRO  | 3.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 43-A  | 51  | PRO  | 3.0  |
| 1   | 44-A  | 51  | PRO  | 3.0  |
| 1   | 45-A  | 51  | PRO  | 3.0  |
| 1   | 46-A  | 51  | PRO  | 3.0  |
| 1   | 47-A  | 51  | PRO  | 3.0  |
| 1   | 1-A   | 34  | TYR  | 2.9  |
| 1   | 2-A   | 34  | TYR  | 2.9  |
| 1   | 3-A   | 34  | TYR  | 2.9  |
| 1   | 4-A   | 34  | TYR  | 2.9  |
| 1   | 5-A   | 34  | TYR  | 2.9  |
| 1   | 6-A   | 34  | TYR  | 2.9  |
| 1   | 7-A   | 34  | TYR  | 2.9  |
| 1   | 8-A   | 34  | TYR  | 2.9  |
| 1   | 9-A   | 34  | TYR  | 2.9  |
| 1   | 10-A  | 34  | TYR  | 2.9  |
| 1   | 11-A  | 34  | TYR  | 2.9  |
| 1   | 12-A  | 34  | TYR  | 2.9  |
| 1   | 13-A  | 34  | TYR  | 2.9  |
| 1   | 14-A  | 34  | TYR  | 2.9  |
| 1   | 15-A  | 34  | TYR  | 2.9  |
| 1   | 16-A  | 34  | TYR  | 2.9  |
| 1   | 17-A  | 34  | TYR  | 2.9  |
| 1   | 18-A  | 34  | TYR  | 2.9  |
| 1   | 19-A  | 34  | TYR  | 2.9  |
| 1   | 20-A  | 34  | TYR  | 2.9  |
| 1   | 21-A  | 34  | TYR  | 2.9  |
| 1   | 22-A  | 34  | TYR  | 2.9  |
| 1   | 23-A  | 34  | TYR  | 2.9  |
| 1   | 24-A  | 34  | TYR  | 2.9  |
| 1   | 25-A  | 34  | TYR  | 2.9  |
| 1   | 26-A  | 34  | TYR  | 2.9  |
| 1   | 27-A  | 34  | TYR  | 2.9  |
| 1   | 28-A  | 34  | TYR  | 2.9  |
| 1   | 29-A  | 34  | TYR  | 2.9  |
| 1   | 30-A  | 34  | TYR  | 2.9  |
| 1   | 31-A  | 34  | TYR  | 2.9  |
| 1   | 32-A  | 34  | TYR  | 2.9  |
| 1   | 33-A  | 34  | TYR  | 2.9  |
| 1   | 34-A  | 34  | TYR  | 2.9  |
| 1   | 35-A  | 34  | TYR  | 2.9  |
| 1   | 36-A  | 34  | TYR  | 2.9  |
| 1   | 37-A  | 34  | TYR  | 2.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 38-A  | 34  | TYR  | 2.9  |
| 1   | 39-A  | 34  | TYR  | 2.9  |
| 1   | 40-A  | 34  | TYR  | 2.9  |
| 1   | 41-A  | 34  | TYR  | 2.9  |
| 1   | 42-A  | 34  | TYR  | 2.9  |
| 1   | 43-A  | 34  | TYR  | 2.9  |
| 1   | 44-A  | 34  | TYR  | 2.9  |
| 1   | 45-A  | 34  | TYR  | 2.9  |
| 1   | 46-A  | 34  | TYR  | 2.9  |
| 1   | 47-A  | 34  | TYR  | 2.9  |
| 1   | 1-A   | 113 | CYS  | 2.9  |
| 1   | 2-A   | 113 | CYS  | 2.9  |
| 1   | 3-A   | 113 | CYS  | 2.9  |
| 1   | 4-A   | 113 | CYS  | 2.9  |
| 1   | 5-A   | 113 | CYS  | 2.9  |
| 1   | 6-A   | 113 | CYS  | 2.9  |
| 1   | 7-A   | 113 | CYS  | 2.9  |
| 1   | 8-A   | 113 | CYS  | 2.9  |
| 1   | 9-A   | 113 | CYS  | 2.9  |
| 1   | 10-A  | 113 | CYS  | 2.9  |
| 1   | 11-A  | 113 | CYS  | 2.9  |
| 1   | 12-A  | 113 | CYS  | 2.9  |
| 1   | 13-A  | 113 | CYS  | 2.9  |
| 1   | 14-A  | 113 | CYS  | 2.9  |
| 1   | 15-A  | 113 | CYS  | 2.9  |
| 1   | 16-A  | 113 | CYS  | 2.9  |
| 1   | 17-A  | 113 | CYS  | 2.9  |
| 1   | 18-A  | 113 | CYS  | 2.9  |
| 1   | 19-A  | 113 | CYS  | 2.9  |
| 1   | 20-A  | 113 | CYS  | 2.9  |
| 1   | 21-A  | 113 | CYS  | 2.9  |
| 1   | 22-A  | 113 | CYS  | 2.9  |
| 1   | 23-A  | 113 | CYS  | 2.9  |
| 1   | 24-A  | 113 | CYS  | 2.9  |
| 1   | 25-A  | 113 | CYS  | 2.9  |
| 1   | 26-A  | 113 | CYS  | 2.9  |
| 1   | 27-A  | 113 | CYS  | 2.9  |
| 1   | 28-A  | 113 | CYS  | 2.9  |
| 1   | 29-A  | 113 | CYS  | 2.9  |
| 1   | 30-A  | 113 | CYS  | 2.9  |
| 1   | 31-A  | 113 | CYS  | 2.9  |
| 1   | 32-A  | 113 | CYS  | 2.9  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 33-A  | 113 | CYS  | 2.9  |
| 1   | 34-A  | 113 | CYS  | 2.9  |
| 1   | 35-A  | 113 | CYS  | 2.9  |
| 1   | 36-A  | 113 | CYS  | 2.9  |
| 1   | 37-A  | 113 | CYS  | 2.9  |
| 1   | 38-A  | 113 | CYS  | 2.9  |
| 1   | 39-A  | 113 | CYS  | 2.9  |
| 1   | 40-A  | 113 | CYS  | 2.9  |
| 1   | 41-A  | 113 | CYS  | 2.9  |
| 1   | 42-A  | 113 | CYS  | 2.9  |
| 1   | 43-A  | 113 | CYS  | 2.9  |
| 1   | 44-A  | 113 | CYS  | 2.9  |
| 1   | 45-A  | 113 | CYS  | 2.9  |
| 1   | 46-A  | 113 | CYS  | 2.9  |
| 1   | 47-A  | 113 | CYS  | 2.9  |
| 1   | 1-A   | 166 | GLY  | 2.8  |
| 1   | 2-A   | 166 | GLY  | 2.8  |
| 1   | 3-A   | 166 | GLY  | 2.8  |
| 1   | 4-A   | 166 | GLY  | 2.8  |
| 1   | 5-A   | 166 | GLY  | 2.8  |
| 1   | 6-A   | 166 | GLY  | 2.8  |
| 1   | 7-A   | 166 | GLY  | 2.8  |
| 1   | 8-A   | 166 | GLY  | 2.8  |
| 1   | 9-A   | 166 | GLY  | 2.8  |
| 1   | 10-A  | 166 | GLY  | 2.8  |
| 1   | 11-A  | 166 | GLY  | 2.8  |
| 1   | 12-A  | 166 | GLY  | 2.8  |
| 1   | 13-A  | 166 | GLY  | 2.8  |
| 1   | 14-A  | 166 | GLY  | 2.8  |
| 1   | 15-A  | 166 | GLY  | 2.8  |
| 1   | 16-A  | 166 | GLY  | 2.8  |
| 1   | 17-A  | 166 | GLY  | 2.8  |
| 1   | 18-A  | 166 | GLY  | 2.8  |
| 1   | 19-A  | 166 | GLY  | 2.8  |
| 1   | 20-A  | 166 | GLY  | 2.8  |
| 1   | 21-A  | 166 | GLY  | 2.8  |
| 1   | 22-A  | 166 | GLY  | 2.8  |
| 1   | 23-A  | 166 | GLY  | 2.8  |
| 1   | 24-A  | 166 | GLY  | 2.8  |
| 1   | 25-A  | 166 | GLY  | 2.8  |
| 1   | 26-A  | 166 | GLY  | 2.8  |
| 1   | 27-A  | 166 | GLY  | 2.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 28-A  | 166 | GLY  | 2.8  |
| 1   | 29-A  | 166 | GLY  | 2.8  |
| 1   | 30-A  | 166 | GLY  | 2.8  |
| 1   | 31-A  | 166 | GLY  | 2.8  |
| 1   | 32-A  | 166 | GLY  | 2.8  |
| 1   | 33-A  | 166 | GLY  | 2.8  |
| 1   | 34-A  | 166 | GLY  | 2.8  |
| 1   | 35-A  | 166 | GLY  | 2.8  |
| 1   | 36-A  | 166 | GLY  | 2.8  |
| 1   | 37-A  | 166 | GLY  | 2.8  |
| 1   | 38-A  | 166 | GLY  | 2.8  |
| 1   | 39-A  | 166 | GLY  | 2.8  |
| 1   | 40-A  | 166 | GLY  | 2.8  |
| 1   | 41-A  | 166 | GLY  | 2.8  |
| 1   | 42-A  | 166 | GLY  | 2.8  |
| 1   | 43-A  | 166 | GLY  | 2.8  |
| 1   | 44-A  | 166 | GLY  | 2.8  |
| 1   | 45-A  | 166 | GLY  | 2.8  |
| 1   | 46-A  | 166 | GLY  | 2.8  |
| 1   | 47-A  | 166 | GLY  | 2.8  |
| 1   | 1-A   | 112 | ASP  | 2.7  |
| 1   | 2-A   | 112 | ASP  | 2.7  |
| 1   | 3-A   | 112 | ASP  | 2.7  |
| 1   | 4-A   | 112 | ASP  | 2.7  |
| 1   | 5-A   | 112 | ASP  | 2.7  |
| 1   | 6-A   | 112 | ASP  | 2.7  |
| 1   | 7-A   | 112 | ASP  | 2.7  |
| 1   | 8-A   | 112 | ASP  | 2.7  |
| 1   | 9-A   | 112 | ASP  | 2.7  |
| 1   | 10-A  | 112 | ASP  | 2.7  |
| 1   | 11-A  | 112 | ASP  | 2.7  |
| 1   | 12-A  | 112 | ASP  | 2.7  |
| 1   | 13-A  | 112 | ASP  | 2.7  |
| 1   | 14-A  | 112 | ASP  | 2.7  |
| 1   | 15-A  | 112 | ASP  | 2.7  |
| 1   | 16-A  | 112 | ASP  | 2.7  |
| 1   | 17-A  | 112 | ASP  | 2.7  |
| 1   | 18-A  | 112 | ASP  | 2.7  |
| 1   | 19-A  | 112 | ASP  | 2.7  |
| 1   | 20-A  | 112 | ASP  | 2.7  |
| 1   | 21-A  | 112 | ASP  | 2.7  |
| 1   | 22-A  | 112 | ASP  | 2.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 23-A  | 112 | ASP  | 2.7  |
| 1   | 24-A  | 112 | ASP  | 2.7  |
| 1   | 25-A  | 112 | ASP  | 2.7  |
| 1   | 26-A  | 112 | ASP  | 2.7  |
| 1   | 27-A  | 112 | ASP  | 2.7  |
| 1   | 28-A  | 112 | ASP  | 2.7  |
| 1   | 29-A  | 112 | ASP  | 2.7  |
| 1   | 30-A  | 112 | ASP  | 2.7  |
| 1   | 31-A  | 112 | ASP  | 2.7  |
| 1   | 32-A  | 112 | ASP  | 2.7  |
| 1   | 33-A  | 112 | ASP  | 2.7  |
| 1   | 34-A  | 112 | ASP  | 2.7  |
| 1   | 35-A  | 112 | ASP  | 2.7  |
| 1   | 36-A  | 112 | ASP  | 2.7  |
| 1   | 37-A  | 112 | ASP  | 2.7  |
| 1   | 38-A  | 112 | ASP  | 2.7  |
| 1   | 39-A  | 112 | ASP  | 2.7  |
| 1   | 40-A  | 112 | ASP  | 2.7  |
| 1   | 41-A  | 112 | ASP  | 2.7  |
| 1   | 42-A  | 112 | ASP  | 2.7  |
| 1   | 43-A  | 112 | ASP  | 2.7  |
| 1   | 44-A  | 112 | ASP  | 2.7  |
| 1   | 45-A  | 112 | ASP  | 2.7  |
| 1   | 46-A  | 112 | ASP  | 2.7  |
| 1   | 47-A  | 112 | ASP  | 2.7  |
| 1   | 1-A   | 98  | GLN  | 2.7  |
| 1   | 2-A   | 98  | GLN  | 2.7  |
| 1   | 3-A   | 98  | GLN  | 2.7  |
| 1   | 4-A   | 98  | GLN  | 2.7  |
| 1   | 5-A   | 98  | GLN  | 2.7  |
| 1   | 6-A   | 98  | GLN  | 2.7  |
| 1   | 7-A   | 98  | GLN  | 2.7  |
| 1   | 8-A   | 98  | GLN  | 2.7  |
| 1   | 9-A   | 98  | GLN  | 2.7  |
| 1   | 10-A  | 98  | GLN  | 2.7  |
| 1   | 11-A  | 98  | GLN  | 2.7  |
| 1   | 12-A  | 98  | GLN  | 2.7  |
| 1   | 13-A  | 98  | GLN  | 2.7  |
| 1   | 14-A  | 98  | GLN  | 2.7  |
| 1   | 15-A  | 98  | GLN  | 2.7  |
| 1   | 16-A  | 98  | GLN  | 2.7  |
| 1   | 17-A  | 98  | GLN  | 2.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 18-A  | 98  | GLN  | 2.7  |
| 1   | 19-A  | 98  | GLN  | 2.7  |
| 1   | 20-A  | 98  | GLN  | 2.7  |
| 1   | 21-A  | 98  | GLN  | 2.7  |
| 1   | 22-A  | 98  | GLN  | 2.7  |
| 1   | 23-A  | 98  | GLN  | 2.7  |
| 1   | 24-A  | 98  | GLN  | 2.7  |
| 1   | 25-A  | 98  | GLN  | 2.7  |
| 1   | 26-A  | 98  | GLN  | 2.7  |
| 1   | 27-A  | 98  | GLN  | 2.7  |
| 1   | 28-A  | 98  | GLN  | 2.7  |
| 1   | 29-A  | 98  | GLN  | 2.7  |
| 1   | 30-A  | 98  | GLN  | 2.7  |
| 1   | 31-A  | 98  | GLN  | 2.7  |
| 1   | 32-A  | 98  | GLN  | 2.7  |
| 1   | 33-A  | 98  | GLN  | 2.7  |
| 1   | 34-A  | 98  | GLN  | 2.7  |
| 1   | 35-A  | 98  | GLN  | 2.7  |
| 1   | 36-A  | 98  | GLN  | 2.7  |
| 1   | 37-A  | 98  | GLN  | 2.7  |
| 1   | 38-A  | 98  | GLN  | 2.7  |
| 1   | 39-A  | 98  | GLN  | 2.7  |
| 1   | 40-A  | 98  | GLN  | 2.7  |
| 1   | 41-A  | 98  | GLN  | 2.7  |
| 1   | 42-A  | 98  | GLN  | 2.7  |
| 1   | 43-A  | 98  | GLN  | 2.7  |
| 1   | 44-A  | 98  | GLN  | 2.7  |
| 1   | 45-A  | 98  | GLN  | 2.7  |
| 1   | 46-A  | 98  | GLN  | 2.7  |
| 1   | 47-A  | 98  | GLN  | 2.7  |
| 1   | 1-A   | 199 | SER  | 2.6  |
| 1   | 2-A   | 199 | SER  | 2.6  |
| 1   | 3-A   | 199 | SER  | 2.6  |
| 1   | 4-A   | 199 | SER  | 2.6  |
| 1   | 5-A   | 199 | SER  | 2.6  |
| 1   | 6-A   | 199 | SER  | 2.6  |
| 1   | 7-A   | 199 | SER  | 2.6  |
| 1   | 8-A   | 199 | SER  | 2.6  |
| 1   | 9-A   | 199 | SER  | 2.6  |
| 1   | 10-A  | 199 | SER  | 2.6  |
| 1   | 11-A  | 199 | SER  | 2.6  |
| 1   | 12-A  | 199 | SER  | 2.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 13-A  | 199 | SER  | 2.6  |
| 1   | 14-A  | 199 | SER  | 2.6  |
| 1   | 15-A  | 199 | SER  | 2.6  |
| 1   | 16-A  | 199 | SER  | 2.6  |
| 1   | 17-A  | 199 | SER  | 2.6  |
| 1   | 18-A  | 199 | SER  | 2.6  |
| 1   | 19-A  | 199 | SER  | 2.6  |
| 1   | 20-A  | 199 | SER  | 2.6  |
| 1   | 21-A  | 199 | SER  | 2.6  |
| 1   | 22-A  | 199 | SER  | 2.6  |
| 1   | 23-A  | 199 | SER  | 2.6  |
| 1   | 24-A  | 199 | SER  | 2.6  |
| 1   | 25-A  | 199 | SER  | 2.6  |
| 1   | 26-A  | 199 | SER  | 2.6  |
| 1   | 27-A  | 199 | SER  | 2.6  |
| 1   | 28-A  | 199 | SER  | 2.6  |
| 1   | 29-A  | 199 | SER  | 2.6  |
| 1   | 30-A  | 199 | SER  | 2.6  |
| 1   | 31-A  | 199 | SER  | 2.6  |
| 1   | 32-A  | 199 | SER  | 2.6  |
| 1   | 33-A  | 199 | SER  | 2.6  |
| 1   | 34-A  | 199 | SER  | 2.6  |
| 1   | 35-A  | 199 | SER  | 2.6  |
| 1   | 36-A  | 199 | SER  | 2.6  |
| 1   | 37-A  | 199 | SER  | 2.6  |
| 1   | 38-A  | 199 | SER  | 2.6  |
| 1   | 39-A  | 199 | SER  | 2.6  |
| 1   | 40-A  | 199 | SER  | 2.6  |
| 1   | 41-A  | 199 | SER  | 2.6  |
| 1   | 42-A  | 199 | SER  | 2.6  |
| 1   | 43-A  | 199 | SER  | 2.6  |
| 1   | 44-A  | 199 | SER  | 2.6  |
| 1   | 45-A  | 199 | SER  | 2.6  |
| 1   | 46-A  | 199 | SER  | 2.6  |
| 1   | 47-A  | 199 | SER  | 2.6  |
| 1   | 1-A   | 7   | GLU  | 2.5  |
| 1   | 2-A   | 7   | GLU  | 2.5  |
| 1   | 3-A   | 7   | GLU  | 2.5  |
| 1   | 4-A   | 7   | GLU  | 2.5  |
| 1   | 5-A   | 7   | GLU  | 2.5  |
| 1   | 6-A   | 7   | GLU  | 2.5  |
| 1   | 7-A   | 7   | GLU  | 2.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 8-A   | 7   | GLU  | 2.5  |
| 1   | 9-A   | 7   | GLU  | 2.5  |
| 1   | 10-A  | 7   | GLU  | 2.5  |
| 1   | 11-A  | 7   | GLU  | 2.5  |
| 1   | 12-A  | 7   | GLU  | 2.5  |
| 1   | 13-A  | 7   | GLU  | 2.5  |
| 1   | 14-A  | 7   | GLU  | 2.5  |
| 1   | 15-A  | 7   | GLU  | 2.5  |
| 1   | 16-A  | 7   | GLU  | 2.5  |
| 1   | 17-A  | 7   | GLU  | 2.5  |
| 1   | 18-A  | 7   | GLU  | 2.5  |
| 1   | 19-A  | 7   | GLU  | 2.5  |
| 1   | 20-A  | 7   | GLU  | 2.5  |
| 1   | 21-A  | 7   | GLU  | 2.5  |
| 1   | 22-A  | 7   | GLU  | 2.5  |
| 1   | 23-A  | 7   | GLU  | 2.5  |
| 1   | 24-A  | 7   | GLU  | 2.5  |
| 1   | 25-A  | 7   | GLU  | 2.5  |
| 1   | 26-A  | 7   | GLU  | 2.5  |
| 1   | 27-A  | 7   | GLU  | 2.5  |
| 1   | 28-A  | 7   | GLU  | 2.5  |
| 1   | 29-A  | 7   | GLU  | 2.5  |
| 1   | 30-A  | 7   | GLU  | 2.5  |
| 1   | 31-A  | 7   | GLU  | 2.5  |
| 1   | 32-A  | 7   | GLU  | 2.5  |
| 1   | 33-A  | 7   | GLU  | 2.5  |
| 1   | 34-A  | 7   | GLU  | 2.5  |
| 1   | 35-A  | 7   | GLU  | 2.5  |
| 1   | 36-A  | 7   | GLU  | 2.5  |
| 1   | 37-A  | 7   | GLU  | 2.5  |
| 1   | 38-A  | 7   | GLU  | 2.5  |
| 1   | 39-A  | 7   | GLU  | 2.5  |
| 1   | 40-A  | 7   | GLU  | 2.5  |
| 1   | 41-A  | 7   | GLU  | 2.5  |
| 1   | 42-A  | 7   | GLU  | 2.5  |
| 1   | 43-A  | 7   | GLU  | 2.5  |
| 1   | 44-A  | 7   | GLU  | 2.5  |
| 1   | 45-A  | 7   | GLU  | 2.5  |
| 1   | 46-A  | 7   | GLU  | 2.5  |
| 1   | 47-A  | 7   | GLU  | 2.5  |
| 1   | 1-A   | 143 | THR  | 2.4  |
| 1   | 2-A   | 143 | THR  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 3-A   | 143 | THR  | 2.4  |
| 1   | 4-A   | 143 | THR  | 2.4  |
| 1   | 5-A   | 143 | THR  | 2.4  |
| 1   | 6-A   | 143 | THR  | 2.4  |
| 1   | 7-A   | 143 | THR  | 2.4  |
| 1   | 8-A   | 143 | THR  | 2.4  |
| 1   | 9-A   | 143 | THR  | 2.4  |
| 1   | 10-A  | 143 | THR  | 2.4  |
| 1   | 11-A  | 143 | THR  | 2.4  |
| 1   | 12-A  | 143 | THR  | 2.4  |
| 1   | 13-A  | 143 | THR  | 2.4  |
| 1   | 14-A  | 143 | THR  | 2.4  |
| 1   | 15-A  | 143 | THR  | 2.4  |
| 1   | 16-A  | 143 | THR  | 2.4  |
| 1   | 17-A  | 143 | THR  | 2.4  |
| 1   | 18-A  | 143 | THR  | 2.4  |
| 1   | 19-A  | 143 | THR  | 2.4  |
| 1   | 20-A  | 143 | THR  | 2.4  |
| 1   | 21-A  | 143 | THR  | 2.4  |
| 1   | 22-A  | 143 | THR  | 2.4  |
| 1   | 23-A  | 143 | THR  | 2.4  |
| 1   | 24-A  | 143 | THR  | 2.4  |
| 1   | 25-A  | 143 | THR  | 2.4  |
| 1   | 26-A  | 143 | THR  | 2.4  |
| 1   | 27-A  | 143 | THR  | 2.4  |
| 1   | 28-A  | 143 | THR  | 2.4  |
| 1   | 29-A  | 143 | THR  | 2.4  |
| 1   | 30-A  | 143 | THR  | 2.4  |
| 1   | 31-A  | 143 | THR  | 2.4  |
| 1   | 32-A  | 143 | THR  | 2.4  |
| 1   | 33-A  | 143 | THR  | 2.4  |
| 1   | 34-A  | 143 | THR  | 2.4  |
| 1   | 35-A  | 143 | THR  | 2.4  |
| 1   | 36-A  | 143 | THR  | 2.4  |
| 1   | 37-A  | 143 | THR  | 2.4  |
| 1   | 38-A  | 143 | THR  | 2.4  |
| 1   | 39-A  | 143 | THR  | 2.4  |
| 1   | 40-A  | 143 | THR  | 2.4  |
| 1   | 41-A  | 143 | THR  | 2.4  |
| 1   | 42-A  | 143 | THR  | 2.4  |
| 1   | 43-A  | 143 | THR  | 2.4  |
| 1   | 44-A  | 143 | THR  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 45-A  | 143 | THR  | 2.4  |
| 1   | 46-A  | 143 | THR  | 2.4  |
| 1   | 47-A  | 143 | THR  | 2.4  |
| 1   | 1-A   | 132 | MET  | 2.2  |
| 1   | 2-A   | 132 | MET  | 2.2  |
| 1   | 3-A   | 132 | MET  | 2.2  |
| 1   | 4-A   | 132 | MET  | 2.2  |
| 1   | 5-A   | 132 | MET  | 2.2  |
| 1   | 6-A   | 132 | MET  | 2.2  |
| 1   | 7-A   | 132 | MET  | 2.2  |
| 1   | 8-A   | 132 | MET  | 2.2  |
| 1   | 9-A   | 132 | MET  | 2.2  |
| 1   | 10-A  | 132 | MET  | 2.2  |
| 1   | 11-A  | 132 | MET  | 2.2  |
| 1   | 12-A  | 132 | MET  | 2.2  |
| 1   | 13-A  | 132 | MET  | 2.2  |
| 1   | 14-A  | 132 | MET  | 2.2  |
| 1   | 15-A  | 132 | MET  | 2.2  |
| 1   | 16-A  | 132 | MET  | 2.2  |
| 1   | 17-A  | 132 | MET  | 2.2  |
| 1   | 18-A  | 132 | MET  | 2.2  |
| 1   | 19-A  | 132 | MET  | 2.2  |
| 1   | 20-A  | 132 | MET  | 2.2  |
| 1   | 21-A  | 132 | MET  | 2.2  |
| 1   | 22-A  | 132 | MET  | 2.2  |
| 1   | 23-A  | 132 | MET  | 2.2  |
| 1   | 24-A  | 132 | MET  | 2.2  |
| 1   | 25-A  | 132 | MET  | 2.2  |
| 1   | 26-A  | 132 | MET  | 2.2  |
| 1   | 27-A  | 132 | MET  | 2.2  |
| 1   | 28-A  | 132 | MET  | 2.2  |
| 1   | 29-A  | 132 | MET  | 2.2  |
| 1   | 30-A  | 132 | MET  | 2.2  |
| 1   | 31-A  | 132 | MET  | 2.2  |
| 1   | 32-A  | 132 | MET  | 2.2  |
| 1   | 33-A  | 132 | MET  | 2.2  |
| 1   | 34-A  | 132 | MET  | 2.2  |
| 1   | 35-A  | 132 | MET  | 2.2  |
| 1   | 36-A  | 132 | MET  | 2.2  |
| 1   | 37-A  | 132 | MET  | 2.2  |
| 1   | 38-A  | 132 | MET  | 2.2  |
| 1   | 39-A  | 132 | MET  | 2.2  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 40-A  | 132 | MET  | 2.2  |
| 1   | 41-A  | 132 | MET  | 2.2  |
| 1   | 42-A  | 132 | MET  | 2.2  |
| 1   | 43-A  | 132 | MET  | 2.2  |
| 1   | 44-A  | 132 | MET  | 2.2  |
| 1   | 45-A  | 132 | MET  | 2.2  |
| 1   | 46-A  | 132 | MET  | 2.2  |
| 1   | 47-A  | 132 | MET  | 2.2  |
| 1   | 1-A   | 147 | TYR  | 2.2  |
| 1   | 2-A   | 147 | TYR  | 2.2  |
| 1   | 3-A   | 147 | TYR  | 2.2  |
| 1   | 4-A   | 147 | TYR  | 2.2  |
| 1   | 5-A   | 147 | TYR  | 2.2  |
| 1   | 6-A   | 147 | TYR  | 2.2  |
| 1   | 7-A   | 147 | TYR  | 2.2  |
| 1   | 8-A   | 147 | TYR  | 2.2  |
| 1   | 9-A   | 147 | TYR  | 2.2  |
| 1   | 10-A  | 147 | TYR  | 2.2  |
| 1   | 11-A  | 147 | TYR  | 2.2  |
| 1   | 12-A  | 147 | TYR  | 2.2  |
| 1   | 13-A  | 147 | TYR  | 2.2  |
| 1   | 14-A  | 147 | TYR  | 2.2  |
| 1   | 15-A  | 147 | TYR  | 2.2  |
| 1   | 16-A  | 147 | TYR  | 2.2  |
| 1   | 17-A  | 147 | TYR  | 2.2  |
| 1   | 18-A  | 147 | TYR  | 2.2  |
| 1   | 19-A  | 147 | TYR  | 2.2  |
| 1   | 20-A  | 147 | TYR  | 2.2  |
| 1   | 21-A  | 147 | TYR  | 2.2  |
| 1   | 22-A  | 147 | TYR  | 2.2  |
| 1   | 23-A  | 147 | TYR  | 2.2  |
| 1   | 24-A  | 147 | TYR  | 2.2  |
| 1   | 25-A  | 147 | TYR  | 2.2  |
| 1   | 26-A  | 147 | TYR  | 2.2  |
| 1   | 27-A  | 147 | TYR  | 2.2  |
| 1   | 28-A  | 147 | TYR  | 2.2  |
| 1   | 29-A  | 147 | TYR  | 2.2  |
| 1   | 30-A  | 147 | TYR  | 2.2  |
| 1   | 31-A  | 147 | TYR  | 2.2  |
| 1   | 32-A  | 147 | TYR  | 2.2  |
| 1   | 33-A  | 147 | TYR  | 2.2  |
| 1   | 34-A  | 147 | TYR  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 35-A  | 147 | TYR  | 2.2  |
| 1   | 36-A  | 147 | TYR  | 2.2  |
| 1   | 37-A  | 147 | TYR  | 2.2  |
| 1   | 38-A  | 147 | TYR  | 2.2  |
| 1   | 39-A  | 147 | TYR  | 2.2  |
| 1   | 40-A  | 147 | TYR  | 2.2  |
| 1   | 41-A  | 147 | TYR  | 2.2  |
| 1   | 42-A  | 147 | TYR  | 2.2  |
| 1   | 43-A  | 147 | TYR  | 2.2  |
| 1   | 44-A  | 147 | TYR  | 2.2  |
| 1   | 45-A  | 147 | TYR  | 2.2  |
| 1   | 46-A  | 147 | TYR  | 2.2  |
| 1   | 47-A  | 147 | TYR  | 2.2  |
| 1   | 1-A   | 148 | VAL  | 2.1  |
| 1   | 2-A   | 148 | VAL  | 2.1  |
| 1   | 3-A   | 148 | VAL  | 2.1  |
| 1   | 4-A   | 148 | VAL  | 2.1  |
| 1   | 5-A   | 148 | VAL  | 2.1  |
| 1   | 6-A   | 148 | VAL  | 2.1  |
| 1   | 7-A   | 148 | VAL  | 2.1  |
| 1   | 8-A   | 148 | VAL  | 2.1  |
| 1   | 9-A   | 148 | VAL  | 2.1  |
| 1   | 10-A  | 148 | VAL  | 2.1  |
| 1   | 11-A  | 148 | VAL  | 2.1  |
| 1   | 12-A  | 148 | VAL  | 2.1  |
| 1   | 13-A  | 148 | VAL  | 2.1  |
| 1   | 14-A  | 148 | VAL  | 2.1  |
| 1   | 15-A  | 148 | VAL  | 2.1  |
| 1   | 16-A  | 148 | VAL  | 2.1  |
| 1   | 17-A  | 148 | VAL  | 2.1  |
| 1   | 18-A  | 148 | VAL  | 2.1  |
| 1   | 19-A  | 148 | VAL  | 2.1  |
| 1   | 20-A  | 148 | VAL  | 2.1  |
| 1   | 21-A  | 148 | VAL  | 2.1  |
| 1   | 22-A  | 148 | VAL  | 2.1  |
| 1   | 23-A  | 148 | VAL  | 2.1  |
| 1   | 24-A  | 148 | VAL  | 2.1  |
| 1   | 25-A  | 148 | VAL  | 2.1  |
| 1   | 26-A  | 148 | VAL  | 2.1  |
| 1   | 27-A  | 148 | VAL  | 2.1  |
| 1   | 28-A  | 148 | VAL  | 2.1  |
| 1   | 29-A  | 148 | VAL  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 30-A  | 148 | VAL  | 2.1  |
| 1   | 31-A  | 148 | VAL  | 2.1  |
| 1   | 32-A  | 148 | VAL  | 2.1  |
| 1   | 33-A  | 148 | VAL  | 2.1  |
| 1   | 34-A  | 148 | VAL  | 2.1  |
| 1   | 35-A  | 148 | VAL  | 2.1  |
| 1   | 36-A  | 148 | VAL  | 2.1  |
| 1   | 37-A  | 148 | VAL  | 2.1  |
| 1   | 38-A  | 148 | VAL  | 2.1  |
| 1   | 39-A  | 148 | VAL  | 2.1  |
| 1   | 40-A  | 148 | VAL  | 2.1  |
| 1   | 41-A  | 148 | VAL  | 2.1  |
| 1   | 42-A  | 148 | VAL  | 2.1  |
| 1   | 43-A  | 148 | VAL  | 2.1  |
| 1   | 44-A  | 148 | VAL  | 2.1  |
| 1   | 45-A  | 148 | VAL  | 2.1  |
| 1   | 46-A  | 148 | VAL  | 2.1  |
| 1   | 47-A  | 148 | VAL  | 2.1  |
| 1   | 1-A   | 57  | LEU  | 2.1  |
| 1   | 2-A   | 57  | LEU  | 2.1  |
| 1   | 3-A   | 57  | LEU  | 2.1  |
| 1   | 4-A   | 57  | LEU  | 2.1  |
| 1   | 5-A   | 57  | LEU  | 2.1  |
| 1   | 6-A   | 57  | LEU  | 2.1  |
| 1   | 7-A   | 57  | LEU  | 2.1  |
| 1   | 8-A   | 57  | LEU  | 2.1  |
| 1   | 9-A   | 57  | LEU  | 2.1  |
| 1   | 10-A  | 57  | LEU  | 2.1  |
| 1   | 11-A  | 57  | LEU  | 2.1  |
| 1   | 12-A  | 57  | LEU  | 2.1  |
| 1   | 13-A  | 57  | LEU  | 2.1  |
| 1   | 14-A  | 57  | LEU  | 2.1  |
| 1   | 15-A  | 57  | LEU  | 2.1  |
| 1   | 16-A  | 57  | LEU  | 2.1  |
| 1   | 17-A  | 57  | LEU  | 2.1  |
| 1   | 18-A  | 57  | LEU  | 2.1  |
| 1   | 19-A  | 57  | LEU  | 2.1  |
| 1   | 20-A  | 57  | LEU  | 2.1  |
| 1   | 21-A  | 57  | LEU  | 2.1  |
| 1   | 22-A  | 57  | LEU  | 2.1  |
| 1   | 23-A  | 57  | LEU  | 2.1  |
| 1   | 24-A  | 57  | LEU  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 25-A  | 57  | LEU  | 2.1  |
| 1   | 26-A  | 57  | LEU  | 2.1  |
| 1   | 27-A  | 57  | LEU  | 2.1  |
| 1   | 28-A  | 57  | LEU  | 2.1  |
| 1   | 29-A  | 57  | LEU  | 2.1  |
| 1   | 30-A  | 57  | LEU  | 2.1  |
| 1   | 31-A  | 57  | LEU  | 2.1  |
| 1   | 32-A  | 57  | LEU  | 2.1  |
| 1   | 33-A  | 57  | LEU  | 2.1  |
| 1   | 34-A  | 57  | LEU  | 2.1  |
| 1   | 35-A  | 57  | LEU  | 2.1  |
| 1   | 36-A  | 57  | LEU  | 2.1  |
| 1   | 37-A  | 57  | LEU  | 2.1  |
| 1   | 38-A  | 57  | LEU  | 2.1  |
| 1   | 39-A  | 57  | LEU  | 2.1  |
| 1   | 40-A  | 57  | LEU  | 2.1  |
| 1   | 41-A  | 57  | LEU  | 2.1  |
| 1   | 42-A  | 57  | LEU  | 2.1  |
| 1   | 43-A  | 57  | LEU  | 2.1  |
| 1   | 44-A  | 57  | LEU  | 2.1  |
| 1   | 45-A  | 57  | LEU  | 2.1  |
| 1   | 46-A  | 57  | LEU  | 2.1  |
| 1   | 47-A  | 57  | LEU  | 2.1  |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 1   | CRQ  | 29-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                | 24    |
| 1   | CRQ  | 16-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                | 24    |
| 1   | CRQ  | 25-A  | 62  | 24/25 | 0.94 | 0.16 | 22,23,24,25                | 24    |
| 1   | CRQ  | 31-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                | 24    |
| 1   | CRQ  | 30-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                | 24    |
| 1   | CRQ  | 35-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                | 24    |
| 1   | CRQ  | 24-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                | 24    |
| 1   | CRQ  | 3-A   | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                | 24    |
| 1   | CRQ  | 2-A   | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                | 24    |
| 1   | CRQ  | 7-A   | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                | 24    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 1   | CRQ  | 18-A  | 62  | 24/25 | 0.94 | 0.16 | 22,23,24,25                 | 24    |
| 1   | CRQ  | 4-A   | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 23-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 13-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 27-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 22-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 21-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 41-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 47-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 20-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 36-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 6-A   | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 33-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 37-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 1-A   | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 39-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 19-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 10-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 44-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 45-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 40-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 11-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 28-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 8-A   | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 26-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 38-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 5-A   | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 17-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 12-A  | 62  | 24/25 | 0.94 | 0.16 | 22,23,24,25                 | 24    |
| 1   | CRQ  | 9-A   | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 14-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 34-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 32-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 15-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 43-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 46-A  | 62  | 24/25 | 0.94 | 0.16 | 22,22,24,25                 | 24    |
| 1   | CRQ  | 42-A  | 62  | 24/25 | 0.94 | 0.16 | 22,23,24,25                 | 24    |

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.